EchoKey Unified Reversible Coin Framework

From First Principles to TSP and Chemistry

Warning — brain–melting math, not for the weak.

0. Contract of the Reader

We will not comfort you. We will define everything we use, move fast, and prove the essential claims. No literature review. No apologetics. If you don't like a symbol, rename it. *Everything is explicit and reproducible in the provided code.*

Roadmap **New framework → Reversible core → Application: TSP → Application: Chemistry**.

1 The Unified Reversible Coin Framework

1.1 Abstract problem

Let Ω be a finite set of *configurations*. A configuration $x \in \Omega$ has a real-valued objective $\Phi(x) \in \mathbb{R}$ (length, energy, cost, etc.). Fix an anchored indexing $\iota : \Omega \to \{0, \dots, M-1\}$ with inverse τ.

Let $\mathcal{K} = \{0, 1, \dots, d\}$ denote *moves*: $k = 0$ means *stay*; for $k \geq 1$, a local, invertible update $s_k : \Omega \to \Omega$. Define local deltas

$$\Delta\Phi_k(x) \coloneqq \Phi(s_k(x)) - \Phi(x). \tag{1}$$

1.2 Registers and padding

The position register uses $q_{\text{pos}} = \lceil \log_2 M \rceil$ qubits; the coin uses $q_{\text{coin}} = \lceil \log_2(d+1) \rceil$ qubits. Embed real states into computational basis and define projectors $P_{\text{real}}, P_{\text{pad}}$ as before.

1.3 EchoKey–7 feature map and coin

For each (x, k) we compute a 7–feature vector $\boldsymbol{F}(x,k) \in \mathbb{R}^7$ (CYC, REC, FRA, OUT, INT, NON, ADA). The domain–specific part is **INT**:

$$\mathrm{INT}(x,k) \coloneqq -\Delta\Phi_k(x). \tag{2}$$

With weights $\boldsymbol{W} \in \mathbb{R}^7$ we get scores $s_k(x) = \boldsymbol{W}^\top \boldsymbol{F}(x,k)$, a marginized stay score s_0, and a softmax coin distribution $r_k(x)$ at inverse temperature β. Define

$$|c_i\rangle \coloneqq \sum_{k=0}^{d} \sqrt{r_k(\tau(i))}\, |k\rangle\,. \tag{3}$$

1.4 Exact inhomogeneous coin and shift

Block-diagonal coin with per-index state preparation

$$U_{\text{coin}} = \left(\sum_{i=0}^{M-1} |i\rangle\langle i| \otimes S_i \right) + P_{\text{pad}} \otimes I, \qquad S_i |0\rangle = |c_i\rangle . \tag{4}$$

Coin-controlled shift via permutation matrices Π_k for each move as in the previous writeup:

$$U_{\text{shift}} := |0\rangle\langle 0| \otimes I + \sum_{k=1}^{d} |k\rangle\langle k| \otimes (\Pi_k \oplus I_{\text{pad}}). \tag{5}$$

One step: $U = U_{\text{shift}} U_{\text{coin}}$.

2 Reversible Core (Bennett Sandwich)

2.1 Goal and tables

We compute the two's-complement word of $\Delta\Phi_k(\tau(i))$ into a work register Δ using a ROM-style, idempotent XOR, copy its sign bit, apply a controlled marker rotation, and *uncompute*.

Let $T \in \mathbb{Z}^{M \times (d+1)}$ with $T_{i,0} = 0$ and $T_{i,k} = \Delta\Phi_k(\tau(i))$. Choose width b for two's-complement.

2.2 ROM load: idempotent

Selection predicates $\sigma_{i,k}$ gate multi-controlled NOTs which XOR the constant pattern of $T_{i,k}$ into Δ. Call this U_{ROM}. By construction $U_{\text{ROM}}^2 = I$ (bitwise toggles cancel under the same control).

2.3 Use and uncompute

Let s be the sign bit of Δ. Apply CNOT($s \to f$) and CRY(λ) from f to a marker m: U_{use}. The full sandwich

$$\mathcal{U} = U_{\text{ROM}} U_{\text{use}} U_{\text{ROM}} \tag{6}$$

returns all work/chain ancillas to $|0\rangle$; only (f, m) record the sign-dependent effect.

Claim (unitarity and cleanliness). For any clean input, $\mathcal{U}$ leaves $|p\rangle\,|c\rangle\,\left|0^b\right\rangle\,|0\rangle\,|m\rangle\,\left|0^A\right\rangle$ as $|p\rangle\,|c\rangle\,\left|0^b\right\rangle\,|f(p,c)\rangle\,\left(\mathrm{RY}(\lambda)^{f(p,c)}\,|m\rangle\right)\left|0^A\right\rangle$ with $f(p,c) = \mathbf{1}_{\{T_{p,c}<0\}}$. Proof is identical to the previous TSP core and follows directly from idempotence and locality of uncomputation.

3 Application I: TSP (anchored tours, adjacent swaps)

3.1 Model

Cities $\{0, \ldots, N-1\}$, symmetric metric $D \in \mathbb{R}^{N \times N}$ with $D_{ii} = 0$ and $D_{ij} = D_{ji}$. Configurations Ω are closed tours anchored at 0; $M = (N-1)!$. Objective $\Phi = L$: tour length. Moves $k \in \{1, \ldots, N-2\}$ swap positions $k, k+1$ (interior). Stay is $k = 0$.

The exact three-edge delta is

$$\Delta L_k(t; D) = \underbrace{\left(D_{t_{k-1},t_{k+1}} + D_{t_{k+1},t_k} + D_{t_k,t_{k+2}}\right)}_{\text{after}} - \underbrace{\left(D_{t_{k-1},t_k} + D_{t_k,t_{k+1}} + D_{t_{k+1},t_{k+2}}\right)}_{\text{before}}, \tag{7}$$

indices modulo N. Use Eq. (2) with $\Delta\Phi = \Delta L$.

3.2 Symmetry note

For symmetric D, t and its reversal t^{rev} have equal length. In classical summaries we count a hit if the measured tour equals the optimum or its reversal.

3.3 Minimal reproduction

1. Build D from seeded random coordinates; enumerate anchored tours and indices.
2. Construct U_{coin} with EchoKey–7 scores; construct U_{shift} from adjacent swaps.
3. Build T with ΔL and verify the Bennett sandwich: after first ROM load, $\Pr[\Delta = 0^b]$ drops; after the full sandwich it returns to 1; ancillas are 0; fidelity of $\mathcal{U}^\dagger\mathcal{U}$ is 1 up to FP.

4 Application II: Chemistry (configurations, local moves, energy deltas)

4.1 Model

Let configurations $x \in \Omega$ denote molecular or lattice states drawn from a finite design set (e.g., discretized conformers, reaction graph nodes, or small basis expansions). Objective is *energy* $\Phi = E(x)$ from a chosen backend (classical oracle, surrogate, table, or exact for tiny systems). Local moves s_k are reversible updates (e.g., bond reorder, angle flip, site swap, basis toggle) defined so that s_k and s_k^{-1} both lie in $\mathcal{K}$.

The domain-specific delta is

$$\Delta E_k(x) = E(s_k x) - E(x), \qquad \text{and} \quad \mathrm{INT}(x,k) = -\Delta E_k(x). \tag{8}$$

All remaining features (CYC, REC, FRA, OUT, NON, ADA) are instantiated analogously: e.g., CYC via KNN in a geometry graph; OUT via z-scores of local bond/angle deviations; NON via signed-square penalties.

4.2 Reversible energy predicate

Construct $T_{i,k} = \Delta E_k(\tau(i))$ and use the same ROM sandwich. Only the *sign* of ΔE is consumed to mark favorable directions without erasing ΔE; then we uncompute.

4.3 Minimal reproduction

1. Define a finite chemistry sandbox Ω (e.g., small molecule with enumerated conformers or a reaction micrograph) and reversible moves $\{s_k\}$.
2. Tabulate energies $E(x)$ (or a validated surrogate) and build T of ΔE.
3. Run the same $U_{\mathrm{coin}}/U_{\mathrm{shift}}$ pipeline and the Bennett sandwich; verify console identities as in TSP.

5 Complexity and Resources

Coin blocks. M controlled state preparations on q_{coin} targets with q_{pos} controls. Exact, factorial-in-N; intended for small truth-machine instances.

Shift. One coin-controlled permutation per move; naive embedding yields depth $\Theta(2^{q_{\mathrm{pos}}})$; acceptable for tiny M.

ROM. Per nonzero bit of $T_{i,k}$, one multi-controlled NOT with a v-chain; selection ancillas are locally uncomputed.

Use. One CNOT (sign to flag) + one CRY(λ) (flag to marker).

6 CLI and Repo Layout

The reference Python scripts mirror the unified pipeline:

- `tsp_reversible_coin.py` — TSP instance: anchored tours, EchoKey–7 coin, ROM delta for ΔL.
- `chem_reversible_coin.py` — Chemistry instance: finite configuration sandbox, EchoKey–7 coin, ROM delta for ΔE.

Both expose analogous flags (seed, steps, β schedule, stay gap, repeats). Outputs print the reversible proof counters (work register zeroes, ancilla zeros, fidelity checks) and the classical summaries (hits including symmetry-equivalents).

7 What is and is not being claimed

- We do not claim polynomial scaling. The inhomogeneous coin is intentionally exact and factorial in M.
- We *do* claim full unitarity of every step, exactness of local deltas (ΔL or ΔE), and a textbook Bennett sandwich.
- We *do not* hide classical DP/VCI oracles inside U; any heavy baseline is evaluation-only and optionally skipped.

Last Words

One framework, two domains: standard coined-walk search plus a clean, fully reversible arithmetic core. No mysticism. No erasure. No mercy.