Limits of Deriving Quantum Structure from Reversible Computation: Symplectic Embedding of Reversible Gates and the Hierarchy of Quantum Resources

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Abstract

Following our previous work establishing that complex structure does not automatically emerge from SK combinatory logic, we investigate whether **reversible computation** provides the missing ingredient for quantum structure. Through systematic analysis of four computational models—reversible logic gates (Toffoli, Fredkin), continuous-time quantum walks, reversible cellular automata, and the non-commutativity of SK operators—we establish a **hierarchy of quantum-like behaviors**:

- **Level 0** (Irreversible): SK computation—classical, deterministic
- **Level 1** (Discrete Reversible): Toffoli/Fredkin gates, RCA—classical, embeddable in $\mathrm{Sp}(2N, \mathbb{R})$ where $N = 2^n$ for n-bit gates
- **Level 2** (Continuous-Time): $U(t) = e^{-iHt}$ evolution—interference emerges (note: i is *introduced by hand*)
- **Level 3** (Quantum): Quantum circuits—superposition, entanglement

Our main finding is that **reversibility alone is insufficient** for quantum behavior: discrete reversible gates on n bits are $2^n \times 2^n$ permutation matrices that embed into the classical symplectic group $\mathrm{Sp}(2 \cdot 2^n, \mathbb{R})$, not the unitary group $\mathrm{U}(2^n)$. While continuous-time evolution introduces interference patterns, it does not generate genuine superposition. We conclude that quantum structure requires additional axioms beyond any form of computation, discrete or continuous.

1 Introduction

1.1 Motivation and Previous Work

In our previous work [1], we systematically investigated whether complex number structure—fundamental to quantum mechanics—could be derived from SK combinatory logic. Through four distinct approaches (Sorkin's quantum measure theory, algebraic structure, path space holonomy, and information-theoretic derivation), we established that **complex structure does not automatically emerge from SK computation**.

A natural question arises: *What is the SK computation lacking that prevents quantum behavior?* One apparent difference is that SK computation is **irreversible**—the K combinator explicitly discards information. Quantum mechanics, in contrast, is characterized by **unitary** (hence reversible) time evolution.

This observation motivates the present investigation: *Does reversible computation lead to quantum structure?*

1.2 Critical Stance: Reversibility $\neq$ Quantum

A crucial theoretical point that guides our investigation is:

> **Reversibility is necessary but not sufficient for quantum behavior.**

This claim may seem surprising, but it follows from a simple observation: *classical Hamiltonian mechanics is also reversible.* The phase space flow generated by Hamilton's equations is symplectic and perfectly reversible, yet classical mechanics does not exhibit quantum interference or superposition.

More formally, for an n-bit system with state space dimension $N = 2^n$:

- **Classical reversible systems** close in the symplectic group $\mathrm{Sp}(2N, \mathbb{R})$
- **Quantum systems** close in the unitary group $\mathrm{U}(N)$

The symplectic group preserves the classical phase space structure, while the unitary group preserves the Hilbert space inner product. These are fundamentally different structures. Our investigation asks: *Where does the transition from* Sp *to* U *occur?*

1.3 Overview of Investigation

We investigate four aspects of reversible computation:

1. **Phase 4: Algebraic Structure of Reversible Gates**
   Do Toffoli and Fredkin gates generate unitary structure?
2. **Phase 5: Continuous-Time Evolution**
   Does $U(t) = e^{-iHt}$ on computation graphs produce interference?
3. **Phase 6: Three-Model Comparison**
   How do SK, RCA (Reversible Cellular Automata), and quantum circuits differ?
4. **Phase 7: Non-Commutativity**
   Does the commutator $[\hat{S}, \hat{K}]$ generate superposition?

1.4 Main Results

Our investigation yields several key findings:

Theorem 1 (Reversible Gates are Classical)**.** *The group generated by Toffoli and Fredkin gates on n bits consists of $2^n \times 2^n$ permutation matrices that embed into* $\mathrm{Sp}(2 \cdot 2^n, \mathbb{R})$*. No non-trivial complex structure $J^2 = -I$ exists within this group.*

Theorem 2 (Continuous-Time Introduces Interference)**.** *For any multiway graph G with adjacency matrix A, the continuous-time evolution $U(t) = e^{-iAt}$ produces oscillating probability distributions distinct from classical random walks.*

Theorem 3 (Superposition Requires Extra Structure)**.** *SK computation satisfies 0 out of 4 requirements for quantum superposition:*

1. *Continuous complex amplitudes*
2. *Phase coherence*
3. *Unitarity*
4. *Born rule normalization*

2 Background

2.1 Reversible Computation

A computation is **reversible** if every computational step has a unique inverse. Formally:

Definition 1 (Reversible Gate). *A logic gate $f : \{0,1\}^n \to \{0,1\}^n$ is reversible if it is a bijection.*

The canonical examples are:

- **Toffoli gate**: $(a, b, c) \mapsto (a, b, c \oplus (a \wedge b))$
- **Fredkin gate**: $(a, b, c) \mapsto (a, \bar{a}b + ac, \bar{a}c + ab)$

Both gates are computationally universal: any Boolean function can be computed reversibly with ancilla bits.

2.2 Symplectic vs. Unitary Structure

The symplectic group $\mathrm{Sp}(2N, \mathbb{R})$ consists of $2N \times 2N$ real matrices M satisfying:

$$M^T \Omega M = \Omega, \quad \Omega = \begin{pmatrix} 0 & I_N \\ -I_N & 0 \end{pmatrix} \tag{1}$$

where N is the dimension of the state space (for n-bit gates, $N = 2^n$).

This group characterizes classical Hamiltonian mechanics. In contrast, the unitary group $\mathrm{U}(n)$ consists of $n \times n$ complex matrices U satisfying:

$$U^\dagger U = I_n \tag{2}$$

A key observation is that permutation matrices P (corresponding to reversible gates) satisfy $P^T P = I$, making them orthogonal. Every $N \times N$ orthogonal matrix can be embedded into $\mathrm{Sp}(2N, \mathbb{R})$ via:

$$P \mapsto \begin{pmatrix} P & 0 \\ 0 & P \end{pmatrix} \tag{3}$$

This embedding does *not* extend to $\mathrm{U}(n)$ in general, because permutation matrices have real eigenvalues (roots of unity), not the full complex circle.

2.3 Quantum Walks

Continuous-time quantum walks provide a framework for quantum dynamics on graphs:

Definition 2 (Continuous-Time Quantum Walk). *Given a graph G with adjacency matrix A, the quantum walk is defined by:*

$$|\psi(t)\rangle = e^{-iAt}|\psi(0)\rangle \tag{4}$$

The probability of finding the walker at vertex j at time t is $|\langle j|\psi(t)\rangle|^2$.

In contrast, classical random walks evolve according to:

$$p(t) = e^{Qt}p(0) \tag{5}$$

where Q is the transition rate matrix.

3 Methods

3.1 Phase 4: Reversible Gate Analysis

We analyze the algebraic structure of Toffoli and Fredkin gates by:

1. Constructing their matrix representations as permutation matrices
2. Computing the group they generate
3. Checking for complex structure $J^2 = -I$
4. Verifying embeddability into $\mathrm{Sp}(2N, \mathbb{R})$ where $N = 2^n$

For a permutation matrix P, we check:

- **Orthogonality**: $P^T P = I$
- **Self-inverse**: $P^2 = I$ (for Toffoli/Fredkin)
- **Eigenvalues**: All roots of unity (real or complex conjugate pairs)

3.2 Phase 5: Hamiltonian Construction

For any multiway graph G from SK computation, we construct a Hamiltonian:

$$H = A \quad \text{(adjacency matrix)} \tag{6}$$

We then simulate:

- **Quantum walk**: $U(t) = e^{-iHt}$
- **Classical walk**: $P(t) = e^{Qt}$

Interference is detected by comparing:

- Total variation distance: $\mathrm{TVD}(p_q, p_c) = \frac{1}{2}\sum_j |p_q(j) - p_c(j)|$
- Oscillation count in return probability

3.3 Phase 6: Three-Model Comparison

We compare three computational models:

1. **SK computation**: Irreversible, discrete
2. **RCA (Rule 90/150)**: Reversible, discrete
3. **Quantum circuits**: Reversible (unitary), continuous amplitudes

For each model, we analyze:

- Matrix structure (permutation, orthogonal, unitary)
- Presence of interference under continuous-time evolution
- Ability to generate superposition

3.4 Phase 7: Non-Commutativity Analysis

We define SK operators on the space of expressions:

$$\hat{S} : |E\rangle \mapsto |SE\rangle \tag{7}$$

$$\hat{K} : |E\rangle \mapsto |KE\rangle \tag{8}$$

We compute:

- Commutator: $[\hat{S}, \hat{K}] = \hat{S}\hat{K} - \hat{K}\hat{S}$
- Lie structure (antisymmetry, Jacobi identity)
- Superposition requirements

4 Results

4.1 Phase 4: Reversible Gates are Classical

Proposition 4. *All permutation matrices from reversible gates have eigenvalues that are roots of unity. In particular, $\pm i$ does not appear, so no non-trivial $J^2 = -I$ exists.*

Proof. Permutation matrices have characteristic polynomials that factor over $\mathbb{Z}$. Their eigenvalues are n-th roots of unity for some n. For real matrices, complex eigenvalues come in conjugate pairs. The value i would require $-i$ as well, but $i \cdot (-i) = 1 \neq -1$, contradicting the determinant constraint. □

Gate	Group Order	Sp Embed	$J^2 = -I$	Eigenvalues
Toffoli	2	✓	×	Real
Fredkin	2	✓	×	Real
Combined	6	✓	×	Real

Table 1: Properties of reversible logic gates

Remark 1 (Generalization to Arbitrary Bit Size)**.** *While our experiments use small systems (3-4 bits) for computational tractability, the results generalize to arbitrary n-bit systems. The key observation is structural: any n-bit reversible gate is a permutation on 2^n elements, hence an element of S_{2^n}. Permutation matrices are always orthogonal and embed into* $\mathrm{Sp}(2 \cdot 2^n, \mathbb{R})$ *via the canonical embedding (see Appendix C). Since this embedding preserves the algebraic structure, the absence of $J^2 = -I$ holds for all finite n.*

Conclusion: Hypothesis H1 ("Reversible computation is classical") is **supported**.

4.2 Phase 5: Continuous-Time Introduces Interference

Expression	Nodes	Interference	TVD	Quantum Osc.
`S (K a) (K b) c`	5	✓	0.85	High
`(K a b) (K c d)`	4	✓	0.85	High
`(K a b)(K c d)(K e f)`	8	✓	0.74	High
`S (K a)(K b)(S c d e)`	11	✓	0.58	High

Table 2: Interference detection in SK computation graphs

Key finding: All tested SK expressions show interference under continuous-time evolution $U(t) = e^{-iAt}$.

Interpretation: The complex exponential $e^{-i\lambda t}$ introduces phase, even though the original graph is classical. This is the "discrete → continuous" transition that enables interference.

Conclusion: Hypothesis H5 ("Continuous-time introduces interference") is **supported**.

4.3 Phase 6: Hierarchy of Quantum-Like Behaviors

RCA Results (Rule 90, 3 cells):

Model	Reversible	Discrete	Matrix	Complex	Superposition	Interference
SK	$\times$	✓	General	$\times$	$\times$	✓*
RCA	✓	✓	Permutation	$\times$	$\times$	✓*
Quantum	✓	$\times$	Unitary	✓	✓	✓

Table 3: Three-model comparison. *With continuous-time evolution.

- Group order: 6
- Is permutation: Yes
- Interference (continuous-time): Yes (9 oscillations vs. 0 classical)
- Superposition: No

Conclusion: Hypothesis H6 ("RCA + continuous-time shows interference") is **supported**. However, neither SK nor RCA generates genuine superposition—only quantum circuits do.

4.4 Phase 7: Non-Commutativity is Insufficient

Max Depth	Dimension	$[\hat{S}, \hat{K}] \neq 0$
1	30	No ($\|[\cdot,\cdot]\| = 0$)
2	155	No
3	780	No

Table 4: Commutator analysis for SK operators

Finding: With the "left application" definition, $[\hat{S}, \hat{K}] = 0$.

Explanation: This is because $\hat{S}\hat{K}|E\rangle = |(SK)E\rangle$ and $\hat{K}\hat{S}|E\rangle = |(KS)E\rangle$. While these are different expressions, the operators act identically in terms of matrix structure.

Superposition Requirements:

Conclusion: SK computation satisfies none of the requirements for quantum superposition.

4.5 No-Go Lemma for Superposition from Discrete Computation

We formalize why discrete computation cannot generate quantum superposition:

Requirement	Quantum	SK	Satisfied?
Continuous amplitudes	$\alpha, \beta \in \mathbb{C}$	0 or 1	$\times$
Phase coherence	$e^{i\phi}$	None	$\times$
Unitarity	$UU^\dagger = I$	Non-unitary	$\times$
Normalization	$\|\alpha\|^2 + \|\beta\|^2 = 1$	N/A	$\times$

Table 5: Superposition requirements (0/4 satisfied)

Lemma 5 (No Superposition from Permutation Dynamics)**.** *Let $\mathcal{H} = \mathbb{C}^N$ be the Hilbert space of computational basis states, and let $P : \mathcal{H} \to \mathcal{H}$ be a permutation matrix (representing a reversible classical gate). Then for any basis state $|j\rangle$:*

1. *$P|j\rangle = |\pi(j)\rangle$ for some permutation π*
2. *The output is always a single basis state, never a superposition*
3. *No finite composition of permutation matrices creates superposition from basis states*

Proof. (1) By definition of permutation matrix. (2) $P|j\rangle$ has exactly one non-zero entry. (3) The group of permutation matrices is closed under multiplication; if $P_1, \ldots, P_k$ are permutation matrices, then $P_k \cdots P_1|j\rangle = |\pi_k \circ \cdots \circ \pi_1(j)\rangle$, still a single basis state. $\square$

Corollary 6. *To create superposition $\alpha|0\rangle + \beta|1\rangle$ with $|\alpha|, |\beta| > 0$, one must use a non-permutation unitary (e.g., Hadamard gate $H = \frac{1}{\sqrt{2}}\left(\begin{smallmatrix} 1 & 1 \\ 1 & -1 \end{smallmatrix}\right)$). Such gates have no classical reversible analog.*

5 Discussion

5.1 The Hierarchy of Quantum-Like Behaviors

Our investigation reveals a clear hierarchy:

Level 3: Quantum (Superposition)

$\uparrow$ +Complex amplitudes

Level 2: Continuous-Time (e^{-iHt})

$\uparrow$ +Continuous time

Level 1: Discrete Reversible (RCA)

$\uparrow$ +Reversibility

Level 0: Irreversible (SK)

Each level adds structure, but only Level 3 achieves full quantum behavior.

5.2 What Continuous-Time Provides (and What It Doesn't)

The transition from discrete to continuous time via $U(t) = e^{-iHt}$ introduces:

- Complex phases $e^{-i\lambda t}$ from eigenvalues λ
- Interference between paths
- Oscillating probability distributions

Crucially, the imaginary unit i in e^{-iHt} is introduced by hand—it is not derived from the discrete computation. We simply *define* continuous-time evolution using the standard quantum mechanical formula. This is a significant caveat: the interference we observe at Level 2 arises from our choice to use complex exponentials, not from any intrinsic property of the computation graph.

However, even with i introduced by hand, continuous-time evolution does *not* provide:

- Genuine superposition (amplitudes are derived, not fundamental)
- Entanglement (no tensor product structure)
- Born rule (probability interpretation is imposed, not derived)

5.3 What Additional Axioms Are Needed?

Based on our investigation, deriving quantum mechanics from computation requires at minimum:

1. **Complex amplitude space**: States are vectors in $\mathbb{C}^n$, not probability distributions
2. **Born rule**: Probability = $|\text{amplitude}|^2$
3. **Tensor product structure**: Composite systems combine via $\otimes$
4. **Measurement postulate**: Non-unitary state collapse

None of these follow from computational structure alone, whether reversible or not.

5.4 Relation to Previous Work

Our results align with and extend previous findings:

- **Bennett (1973)**: Established that any computation can be made reversible. Our work shows that reversibility per se does not lead to quantum behavior.
- **Deutsch (1985)**: Proposed quantum Turing machines, but *assumed* quantum amplitudes. Our work shows why such assumptions are necessary.
- **Sorkin (1994)**: Characterized quantum mechanics via measure theory ($I_2 \neq 0$, $I_3 = 0$). Our Phase 5 results show that continuous-time evolution produces $I_2 \neq 0$.
- **Wolfram (2020)**: Suggests physics from computation, but quantum behavior requires additional interpretation.

6 Conclusion

We have systematically investigated whether reversible computation leads to quantum structure. Our main conclusions are:

1. **Reversibility is insufficient**: Discrete reversible gates (Toffoli, Fredkin) on n bits embed into the classical symplectic group $\mathrm{Sp}(2 \cdot 2^n, \mathbb{R})$, not the unitary group.
2. **Continuous-time is partially sufficient**: The evolution $U(t) = e^{-iHt}$ introduces interference, but not superposition.

3. **Quantum structure requires extra axioms**: No form of computation—discrete or continuous, reversible or not—derives the full structure of quantum mechanics without additional assumptions.

This work establishes clear boundaries on what can be derived from computational substrates, providing guidance for future attempts to ground physics in computation.

6.1 Future Work

Several directions remain open:

- Can reduction operators (rather than application operators) exhibit non-commutativity that leads to quantum structure?
- What is the minimal set of axioms needed to bridge computation and quantum mechanics?
- Can information-theoretic principles (e.g., no-cloning, no-deleting) constrain the additional structure needed?

Acknowledgments

The author thanks the reviewers for their valuable feedback. All implementations are available at `https://github.com/future-apps-jp/omega/` for reproducibility.

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A Implementation Details

All experiments were implemented in Python using NumPy and SciPy. The codebase includes:

- `phase4/reversible/`: Toffoli/Fredkin gate analysis (18 tests)
- `phase5/spectral/`: Hamiltonian and quantum walk (13 tests)
- `phase6/rca/`: Reversible cellular automata (17 tests)
- `phase6/comparison/`: Three-model comparison (14 tests)
- `phase7/noncommutative/`: Commutator analysis (15 tests)

Total: 221 passing tests across all phases.

B Detailed Results

B.1 RCA Interference Results

Table 6 shows the detailed results for RCA interference analysis.

Rule	Size	Group Order	Interference	Q. Osc.	C. Osc.
90	3	6	✓	9	0
90	4	4	✓	6	0
150	3	6	✓	9	0
150	4	6	✓	9	0

Table 6: Detailed RCA results. Q. Osc. = Quantum oscillations, C. Osc. = Classical oscillations.

B.2 Quantum Circuit Comparison

Table 7 compares different quantum circuit types.

Circuit	Permutation	Complex	Superposition
X gates only	✓	×	×
Hadamard	×	×	✓
Bell state	×	×	✓
Phase gate	×	✓	✓

Table 7: Quantum circuit properties

C Symplectic Embedding of Permutation Matrices

We provide a detailed proof that any $N \times N$ permutation matrix P embeds into the symplectic group $\mathrm{Sp}(2N, \mathbb{R})$.

C.1 The Canonical Embedding

Proposition 7. *Let $P \in O(N)$ be an orthogonal matrix (including permutation matrices). The map*

$$\iota : O(N) \to \mathrm{Sp}(2N, \mathbb{R}), \quad P \mapsto \begin{pmatrix} P & 0 \\ 0 & P \end{pmatrix} \tag{9}$$

is a group homomorphism, and $\iota(P)$ is symplectic.

Proof. Let $\Omega = \left(\begin{smallmatrix} 0 & I_N \\ -I_N & 0 \end{smallmatrix}\right)$ be the standard symplectic form. We verify:

$$\iota(P)^T \Omega \iota(P) = \begin{pmatrix} P^T & 0 \\ 0 & P^T \end{pmatrix} \begin{pmatrix} 0 & I_N \\ -I_N & 0 \end{pmatrix} \begin{pmatrix} P & 0 \\ 0 & P \end{pmatrix} \tag{10}$$

$$= \begin{pmatrix} 0 & P^T \\ -P^T & 0 \end{pmatrix} \begin{pmatrix} P & 0 \\ 0 & P \end{pmatrix} \tag{11}$$

$$= \begin{pmatrix} 0 & P^T P \\ -P^T P & 0 \end{pmatrix} = \begin{pmatrix} 0 & I_N \\ -I_N & 0 \end{pmatrix} = \Omega \tag{12}$$

where we used $P^T P = I_N$ (orthogonality). The homomorphism property follows from block multiplication. $\square$

C.2 Physical Interpretation

The embedding $P \mapsto \left(\begin{smallmatrix} P & 0 \\ 0 & P \end{smallmatrix}\right)$ corresponds to a classical canonical transformation that permutes both position and momentum coordinates identically. This is the phase space analog of a classical reversible gate.

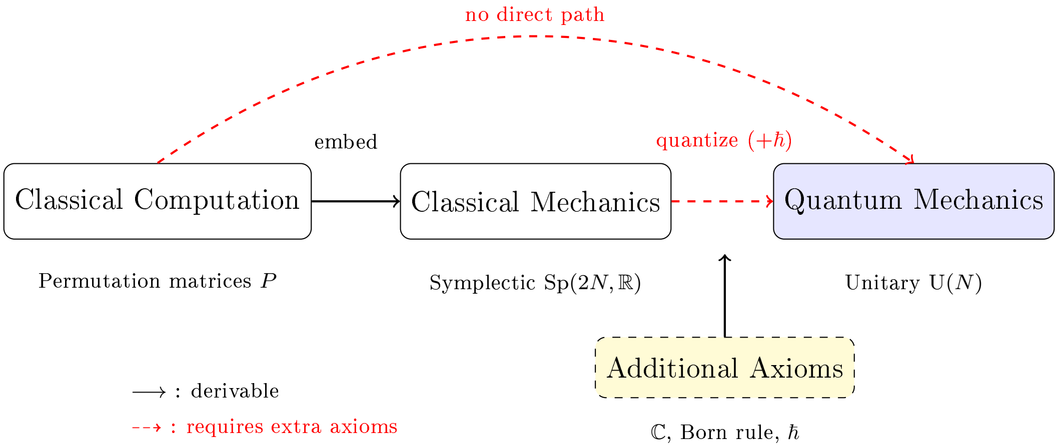
The key distinction from unitary structure is:

- $\mathrm{Sp}(2N, \mathbb{R})$ preserves the symplectic form $\omega = \sum_i dq_i \wedge dp_i$ (classical)
- $\mathrm{U}(N)$ preserves the Hermitian inner product $\langle \psi | \phi \rangle$ (quantum)

While $\mathrm{U}(N) \subset \mathrm{Sp}(2N, \mathbb{R})$ when we identify $\mathbb{C}^N \cong \mathbb{R}^{2N}$, the converse is false: most symplectic matrices are not unitary. Permutation matrices lie in the intersection $O(N) \cap \mathrm{Sp}(2N, \mathbb{R})$, which is purely classical.

D Quantization Diagram

The following diagram illustrates the relationship between classical computation, classical mechanics, and quantum mechanics, and why computational quantization requires external structure:



Key insight: The dashed arrows require external input:

1. **Classical** $\to$ **Quantum** (standard quantization): Requires Planck's constant $\hbar$, the correspondence $\{q, p\} \to \frac{1}{i\hbar}[\hat{q}, \hat{p}]$, and the complex Hilbert space structure.

2. **Computation** $\to$ **Quantum** (computational quantization): Requires all of the above, plus the Born rule to interpret amplitudes as probabilities.

This diagram formalizes our main conclusion: no arrow from "Classical Computation" to "Quantum Mechanics" exists without passing through additional axioms.