

Supplemental Material for Certifying When Temporal Order Can Be Ignored in Continuous-Time Quantum Walks

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1 Purpose and relation to the main text

The main manuscript contains the complete proofs of all stated theorems, lemmas, propositions, and corollaries. This supplement provides calculations that would interrupt the main argument: the exact exponential of one edge event, the full three-vertex matrices, the connection with the Magnus expansion, and the numerical protocol used to produce the reported table. No experimental data are used.

2 Exact edge event and computational cost

For an edge $e = \{u, v\}$, put

$$X_e = |u\rangle\langle v| + |v\rangle\langle u|, \quad P_e = |u\rangle\langle u| + |v\rangle\langle v|.$$

Direct multiplication gives

$$X_e^2 = P_e, \quad X_e^3 = X_e.$$

Separating the even and odd terms in the exponential series therefore yields

$$e^{-i\alpha X_e} = I + (\cos \alpha - 1)P_e - i \sin \alpha X_e. \quad (1)$$

Thus an event unitary is the identity except for the block indexed by (u, v) :

$$\begin{pmatrix} \cos \alpha & -i \sin \alpha \\ -i \sin \alpha & \cos \alpha \end{pmatrix}.$$

This identity was used in the numerical calculations. It avoids computing a dense matrix exponential for every event.

If the full propagator is stored, multiplying it on the left by one event unitary rotates only two rows and costs $O(n)$ arithmetic operations. Constructing the sequential propagator therefore costs $O(mn)$ after the event list is known. The dense exponential of the aggregate action costs $O(n^3)$ with a standard scaling-and-squaring implementation [1]. The total dense-work estimate for the protocol used here is therefore $O(mn + n^3)$, not $O(n^3)$ independently of the number of events. Sparse or Krylov methods can be preferable when only the action on a few states is needed.

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3 Complete three-vertex calculation

Use the ordered basis $(|a\rangle, |b\rangle, |c\rangle)$ and abbreviate $c_\theta = \cos \theta$, $s_\theta = \sin \theta$. The two event unitaries are

$$E_{ab} = \begin{pmatrix} c_\theta & -is_\theta & 0 \\ -is_\theta & c_\theta & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad E_{bc} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & c_\theta & -is_\theta \\ 0 & -is_\theta & c_\theta \end{pmatrix}.$$

When ab acts first and bc acts second,

$$U_{ab \rightarrow bc} = E_{bc} E_{ab} = \begin{pmatrix} c_\theta & -is_\theta & 0 \\ -ic_\theta s_\theta & c_\theta^2 & -is_\theta \\ -s_\theta^2 & -ic_\theta s_\theta & c_\theta \end{pmatrix}. \quad (2)$$

Hence

$$\langle c | U_{ab \rightarrow bc} | a \rangle = -s_\theta^2.$$

For the reversed order,

$$U_{bc \rightarrow ab} = E_{ab} E_{bc} = \begin{pmatrix} c_\theta & -ic_\theta s_\theta & -s_\theta^2 \\ -is_\theta & c_\theta^2 & -ic_\theta s_\theta \\ 0 & -is_\theta & c_\theta \end{pmatrix}, \quad (3)$$

and therefore $\langle c | U_{bc \rightarrow ab} | a \rangle = 0$.

The aggregate action is

$$S = \theta \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} = \theta K.$$

The matrix K satisfies $K^3 = 2K$. Its exponential can consequently be written without diagonalization:

$$e^{-i\theta K} = I - \frac{i \sin(\sqrt{2}\theta)}{\sqrt{2}} K + \frac{\cos(\sqrt{2}\theta) - 1}{2} K^2. \quad (4)$$

Because $(K^2)_{ca} = 1$,

$$\langle c | e^{-i\theta K} | a \rangle = \frac{\cos(\sqrt{2}\theta) - 1}{2} = -\frac{1}{2} [1 - \cos(\sqrt{2}\theta)].$$

This confirms the negative sign used in the main manuscript. Multiplying all hopping terms by minus one does not change this two-step sign, so a positive sign would be inconsistent with either uniform hopping convention.

The commutator is

$$[\theta X_{\{a,b\}}, \theta X_{\{b,c\}}] = \theta^2 (|a\rangle \langle c| - |c\rangle \langle a|),$$

whose norm is θ^2 . The temporal-wedge certificate is therefore $\mathcal{W} = \theta^2/2$.

4 Signed commutators, cancellation, and the Magnus expansion

For a piecewise-constant Hamiltonian with integrated actions A_r , the first two Magnus terms are [2, 3]

$$\Omega_1 = -i \sum_r A_r, \quad \Omega_2 = -\frac{1}{2} \sum_{r>q} [A_r, A_q]. \quad (5)$$

The weak-pulse expansion in the main text is consistent with [equation \(5\)](#), but the nonperturbative theorem does not require the Magnus series to converge.

The difference between the signed quantity

$$C = \sum_{r>q} [A_r, A_q]$$

and the unsigned temporal-wedge budget is essential. For example, consider a scaled three-event sequence A, B, A . Its second-order commutator sum is

$$[B, A] + [A, A] + [A, B] = 0$$

even when $[A, B] \neq 0$. The leading quadratic error cancels, although the individual temporal wedges remain present and the unsigned certificate is positive. This example explains why a large certificate is inconclusive: the theorem is designed to avoid false assurances, not to predict the exact error in every sequence.

The same distinction appears in product-formula analysis. Commutator-scaling bounds are robust and computable, whereas sharper estimates can exploit algebraic cancellation or locality [4, 5]. The present wedge formula is the specialization appropriate to sequential single-edge hopping.

5 Numerical protocol and checks

All calculations used Python 3.12.13, NumPy 2.3.5, and SciPy 1.17.0 with IEEE 754 double-precision complex arithmetic. NumPy’s PCG64 random-number generator was initialized once with seed 20260821. Parameter pairs were visited in the order $n = 8, 16, 32$, and within each value of n , $a = 0.02, 0.05, 0.08$. The following steps were carried out for each pair (n, a) , with $n \in \{8, 16, 32\}$, $a \in \{0.02, 0.05, 0.08\}$, and $m = 2n$:

1. Form the lexicographically ordered list of all $\binom{n}{2}$ unordered loop-free edges.
2. Draw m edge indices independently and uniformly with replacement.
3. Draw m pulse areas independently from the uniform distribution on $[a/2, a]$.
4. Start from $U = I_n$. For events $r = 1, \dots, m$, form the two-row update in [equation \(1\)](#) and replace $U \leftarrow e^{-iA_r} U$.
5. Form $S = \sum_r A_r$ and compute $U_{\text{av}} = e^{-iS}$ by a dense scaling-and-squaring matrix exponential.
6. Repeat step 4 with the event list reversed to obtain U_{rev} .
7. Compute

$$\begin{aligned} \varepsilon_{\text{op}} &= \|U - U_{\text{av}}\|_2, & \varepsilon_{\text{rev}} &= \|U - U_{\text{rev}}\|_2, \\ \Delta_{\text{pro}} &= 1 - \frac{|\text{Tr}(U^\dagger U_{\text{av}})|^2}{n^2}, \end{aligned}$$

and the temporal-wedge budget from the event list.

8. Repeat the preceding steps 200 times and report the median.

The spectral norm was evaluated as the largest singular value. Event unitarity and aggregate unitarity were checked through $\|U^\dagger U - I\|_2$; the largest residual across the reported runs was below 1.2×10^{-15} . Recomputing every aggregate exponential through Hermitian eigendecomposition changed the propagator by less than 4.7×10^{-15} in spectral norm. The largest observed ratios were

$$\max \frac{\varepsilon_{\text{op}}}{\mathcal{W}} = 0.256, \quad \max \frac{\varepsilon_{\text{rev}}}{2\mathcal{W}} = 0.256.$$

For $n = 16$, least-squares fits of the logarithm of the medians against $\log a$ gave

$$\varepsilon_{\text{op}} \propto a^{1.9925}, \quad \varepsilon_{\text{rev}} \propto a^{1.9877}, \quad \Delta_{\text{pro}} \propto a^{3.9893}.$$

These fits are descriptive checks over three pulse ranges, not asymptotic parameter estimates. Their purpose is to verify the orders predicted by the analytic expansion.

6 Scope of the model

Idle intervals and drift. With no background Hamiltonian, an idle interval generates the identity and can be omitted from the event product. If a drift H_0 is present, an interval with controlled edge Hamiltonian H_r instead has action $\Delta_r(H_0 + H_r)$. The general commutator bound in the main text still applies to these layer actions, but the edge-only wedge formula no longer captures all commutators.

Simultaneous and overlapping controls. Controls that act over the same interval should be combined as

$$H^{(\ell)} = \sum_{e \in E_\ell} J_e^{(\ell)} X_e$$

before the layer exponential is formed. Assigning an arbitrary sequential order to genuinely simultaneous noncommuting controls would define a different physical protocol. For smooth overlaps, the time-ordered exponential or a controlled discretization is required; time-dependent simulation methods provide the appropriate broader setting [6].

Directionality and open dynamics. The hopping operator $X_{\{u,v\}}$ is Hermitian and invariant under interchanging u and v . The model is therefore not a directed quantum channel. Dissipative directionality, measurements, and decoherence require a Lindblad or other open-system description and are outside the claims of the main text.

Many excitations. The Hilbert space here contains a single excitation. Interacting many-excitation models can have commutators and locality structures that are not determined only by edge intersections. The general matrix bound remains valid for finite-dimensional Hermitian layer actions, but the graph specialization would have to be derived again for the chosen many-body Hamiltonian.

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