Supplemental Material for: "Destructive Error Interference in Product-Formula Lattice Simulation"

Minh C. Tran,[1,2,3] Su-Kuan Chu,[1,2] Yuan Su,[1,4,5] Andrew M. Childs,[1,4,5] and Alexey V. Gorshkov[1,2,3]

[1] *Joint Center for Quantum Information and Computer Science, NIST/University of Maryland, College Park, Maryland 20742, USA*
[2] *Joint Quantum Institute, NIST/University of Maryland, College Park, Maryland 20742, USA*
[3] *Kavli Institute for Theoretical Physics, University of California, Santa Barbara, California 93106, USA*
[4] *Department of Computer Science, University of Maryland, College Park, Maryland 20742, USA*
[5] *Institute for Advanced Computer Studies, University of Maryland, College Park, Maryland 20742, USA*

(Dated: January 22, 2020)

The Supplemental Material provides more mathematical details for the derivations of the error bound in the paper. Specifically, Sec. S1 explains how we write the k-th order error δ_k into a commutator. Section S2 provides an upper bound for a sum of different evolutions of δ. Finally, in Sec. S3, we show how we bound the norm of Δ_k in Eq. (16).

S1. STRUCTURE OF δ_k

In this section, we present the proof of Lemma 1, which says that we can write δ_k into a sum of a commutator and an operator of higher order. First, we need the following recursive relation between the δ_k operators.

Lemma S1. *For $k \geq 2$, we have the following recursive relation:*

$$\delta_{k+1} = H_1\delta_k + \delta_k H_2 - [H^k, H_2]. \tag{S1}$$

Proof. We prove the lemma by expanding both $U_{t/r}$ and $U^{(1)}_{t/r}U^{(2)}_{t/r}$ in orders of t/r:

$$U^{(1)}_{t/r}U^{(2)}_{t/r} = e^{-iH_1 t/r}e^{-iH_2 t/r} = \sum_{k=0}^{\infty}\frac{1}{k!}A_k\left(\frac{-it}{r}\right)^k, \tag{S2}$$

$$U_{t/r} = e^{-iHt/r} = \sum_{k=0}^{\infty}\frac{1}{k!}B_k\left(\frac{-it}{r}\right)^k, \tag{S3}$$

where

$$A_k \coloneqq \sum_{j=0}^{k}\binom{k}{j}H_1^j H_2^{k-j}, \quad B_k \coloneqq H^k = (H_1+H_2)^k. \tag{S4}$$

With these notations, we have the relation $\delta_k = B_k - A_k$. It is also straightforward to verify the recursive relations for A_k and B_k:

$$A_{k+1} = H_1A_k + A_kH_2, \tag{S5}$$

$$\begin{aligned}B_{k+1} &= H^{k+1} = HB_k = (H_1+H_2)(A_k+\delta_k)\\ &= H_1A_k + H_1\delta_k + B_kH_2 - [B_k, H_2]\\ &= H_1A_k + H_1\delta_k + (A_k+\delta_k)H_2 - [B_k,H_2]\\ &= (H_1A_k + A_kH_2) + H_1\delta_k + \delta_kH_2 - \left[H^k, H_2\right]\\ &= A_{k+1} + H_1\delta_k + \delta_kH_2 - \left[H^k, H_2\right].\end{aligned} \tag{S6}$$

By definition, we have

$$\delta_{k+1} = B_{k+1} - A_{k+1} = H_1\delta_k + \delta_kH_2 - \left[H^k, H_2\right]. \tag{S7}$$

Therefore, the lemma follows. ☐

We now construct the operators S_k, V_k in Lemma 1 inductively on k. For $k = 2$, we have $\delta_2 = [H, H_2]$. Thus Lemma 1 is true for $k = 2$ with $S_2 = H_2$ and $V_2 = 0$. Assume that Lemma 1 is true up to k, i.e. there exist S_k, V_k such that $\delta_k = [H, S_k] + V_k$, we shall prove that it is also true for $k + 1$. Using Lemma S1, we have

$$\begin{aligned}\delta_{k+1} &= H_1\delta_k + \delta_k H_2 - [H^k, H_2]\\ &= [H_1, \delta_k] + \delta_k H - [H^k, H_2]\\ &= [H_1, [H, S_k] + V_k] + V_k H + [H, S_k]H - [H^k, H_2]. \end{aligned}\tag{S8}$$

We use the following commutator identities:

$$[H, S_k]H = [H, S_k H], \tag{S9}$$

$$[H^k, H_2] = [H, \sum_{j=0}^{k-1} H^{k-1-j} H_2 H^j]. \tag{S10}$$

With some trivial manipulations, we can write $\delta_{k+1} = [H, S_{k+1}] + V_{k+1}$, where

$$S_{k+1} = S_k H - \sum_{j=0}^{k-1} H^{k-1-j} H_2 H^j, \tag{S11}$$

$$V_{k+1} = [H_1, [H, S_k]] + H_1 V_k + V_k H_2. \tag{S12}$$

Finally, we show that the operators S_k, V_k constructed using the above recursive relations satisfy the norm bounds in Eqs. (10) to (12). We need the following lemma about the structure of S_k, V_k.

Lemma S2. *For integer $k \geq 2$, the operators S_k, V_k constructed from Eqs. (S11) and (S12) can be written as*

$$V_k = \sum_{i=1}^{n_k} v_{k,i}, \quad n_k \leq \xi e^{k-2} n^{k-2}, \tag{S13}$$

$$S_k = \sum_{i=1}^{m_k} s_{k,i}, \quad m_k \leq \frac{k(k-1)}{2} n^{k-1}, \tag{S14}$$

where ξ is a constant, $v_{k,i}, s_{k,i}$ are operators supported on at most $2(k-1)$ sites and

$$\|s_{k,i}\| \leq 1, \quad \|v_{k,i}\| \leq 1, \tag{S15}$$

for all i.

Proof. Denote by $\mathrm{supp}\,(X)$ the support size of an operator X, i.e. the number of sites X acts nontrivially on. We say that the number of terms in V_k is x if there exists a decomposition $V_k = \sum_{j=1}^{x} v_j$ such that $\|v_j\| \leq 1$ for all j. For $k = 2$, the lemma is true by definition. Assume that the lemma is true up to some $k \geq 2$, we shall prove that it holds for $k + 1$.

First, we argue for the bounds on the number of terms m_{k+1}, n_{k+1} in S_{k+1}, V_{k+1} respectively. Since there are m_k terms in S_k, using Eq. (S11), it is straightforward to bound m_{k+1}—the number of terms in S_{k+1}:

$$m_{k+1} \leq m_k n + k n^k \leq \frac{k(k-1)}{2} n^k + k n^k = \frac{k(k+1)}{2} n^k. \tag{S16}$$

To bound n_{k+1}, the number of terms in V_{k+1}, we use Eq. (S12) and note that $s_{k,i}$ can non-commute with at most $2\mathrm{supp}\,(s_{k,i}) = 4(k-1)$ terms from H. Therefore, the number of terms in $[H, S_k]$ is at most $4(k-1)m_k$. Each of these terms has its support size increased by at most one (to $2k - 1$) compared to the terms of S_k. Repeating the argument for $[H_1, [H, S_k]]$, the number of terms in V_{k+1} can be bounded as follow:

$$n_{k+1} \leq 2(2k-1)4(k-1)m_k + n n_k \tag{S17}$$

$$\leq 8k^4 n^{k-1} + \xi e^{k-2} n^{k-1} \tag{S18}$$

$$< 2\xi e^{k-2} n^{k-1} < \xi e^{k-1} n^{k-1}, \tag{S19}$$

where $\xi = \frac{2048}{e^2(e-1)}$ and we have used the fact that $8k^4 + \xi e^{k-2} < \xi e^{k-1}$ for all $k \geq 2$. Therefore, the number of terms n_{k+1}, m_{k+1} are bounded according to Eqs. (S13) and (S14).

It is also apparent from this construction that each iteration in Eqs. (S11) and (S12) increases the support size of the constituent terms in S_k, V_k by at most 2. Therefore, Lemma S2 follows. □

With Lemma S2, it is straightforward to show that the norms of $V_k, S_k, [H, S_k]$ are upper bounded by the their number of terms:

$$\|V_k\| \leq n_k = O\left(e^{k-2}n^{k-2}\right) \tag{S20}$$

$$\|S_k\| \leq m_k = O\left(k^2 n^{k-1}\right), \tag{S21}$$

$$\|[H, S_k]\| \leq 4(k-1)m_k = O\left(k^3 n^{k-1}\right). \tag{S22}$$

These bounds complete the proof of Lemma 1.

S2. SUM OF EVOLUTIONS OF δ

In this section, we present the proof of Lemma 2, which provides an upper bound for the sum of evolution of an operator with different times.

Proof. We denote by $\tau := t/r$ and

$$\Sigma_a(X) := \sum_{j=0}^{a-1} U_{j\tau}\left[H, X\right] U_{j\tau}^\dagger \tau, \tag{S23}$$

where X is an arbitrary time-independent operator, a is a positive integer, and $U_t = \exp(-iHt)$ as before.

First, we need to turn the sum $\Sigma_a(X)$ into a sum of several integrals using the following lemma.

Lemma S3. *Define*

$$F[X] := -\frac{1}{\tau}\int_0^\tau ds \int_0^s dv U_v\left[H, X\right] U_v^\dagger, \tag{S24}$$

$$I_t(X) := \int_0^t U_s\left[H, X\right] U_s^\dagger ds. \tag{S25}$$

For all τ such that $n\tau < 1$, where n is the number of sites in the system, we have

$$\Sigma_a(X) = \sum_{k=0}^{\infty} I_{a\tau}(F^{\circ k}[X])), \tag{S26}$$

where $F^{\circ k}$ the k-th iterate of a function F, i.e. the composition $F^{\circ k}[X] = F[F[\ldots F[X]\ldots]]$, with $F^{\circ 0}$ being the identity function.

Proof. To prove the claim, we note that

$$I_{a\tau}(X) = \int_0^{a\tau} U_s\left[H, X\right] U_s^\dagger ds = \sum_{j=0}^{a-1}\int_{j\tau}^{(j+1)\tau} U_s\left[H, X\right] U_s^\dagger ds = \sum_{j=0}^{a-1} U_{j\tau}\left(\int_0^\tau U_s\left[H, X\right] U_s^\dagger ds\right) U_{j\tau}^\dagger. \tag{S27}$$

Therefore, we have

$$\begin{aligned}
\Sigma_a(X) - I_{a\tau}(X) &= \sum_{j=0}^{a-1} U_{j\tau}\left(\left[H, X\right]\tau - \int_0^\tau U_s\left[H, X\right] U_s^\dagger ds\right) U_{j\tau}^\dagger \\
&= \sum_{j=0}^{a-1} U_{j\tau}\int_0^\tau ds\left(\left[H, X\right] - U_s\left[H, X\right] U_s^\dagger\right) U_{j\tau}^\dagger \\
&= \sum_{j=0}^{a-1} U_{j\tau}\int_0^\tau ds\int_s^0 dv U_v\left[H, \left[H, X\right]\right] U_v^\dagger U_{j\tau}^\dagger \\
&= \sum_{j=0}^{a-1} U_{j\tau}\left[H, \frac{1}{\tau}\int_0^\tau ds\int_s^0 dv U_v\left[H, X\right] U_v^\dagger\right] U_{j\tau}^\dagger \tau \\
&= \Sigma_a(F[X])).
\end{aligned} \tag{S28}$$

To get the second last line, we use the fact that H and U_t commute in order to move the integral inside the commutator. Repeated applications of this recursive relation yields Eq. (S26). The condition $n\tau < 1$ ensures that the sum in Eq. (S26) converges (See Lemma S4). □

Lemma S4 below is a consequence of Lemma S3.

Lemma S4. *If X is time-independent and $\mu := \frac{nt}{r} < 1$, $\|\Sigma_a(X)\| \leq \frac{2}{1-\mu}\|X\|$.*

Proof. To prove Lemma S4, we note that

$$\|F[X]\| \leq \tau \|H\| \|X\| \leq \mu \|X\| . \tag{S29}$$

Therefore, $\left\|F^{\circ k}[X]\right\| \leq \mu^k \|X\|$. Note also that for the time-independent X,

$$I_{a\tau}(X) = \int_0^{a\tau} U_s [H, X] U_s^\dagger ds = U_{a\tau} X U_{a\tau}^\dagger - X, \tag{S30}$$

and therefore $\|I_{a\tau}(X)\| \leq 2\|X\|$. Using Lemma S3, we have

$$\begin{aligned}
\|\Sigma_a(X)\| &\leq \sum_{k=0}^{\infty} \left\|I_{a\tau}(F^{\circ k}[X])\right\| \leq 2 \sum_{k=0}^{\infty} \left\|F^{\circ k}[X]\right\| \\
&\leq 2\|X\| \sum_{k=0}^{\infty} \mu^k = \frac{2}{1-\mu}\|X\| \\
&= O(\|X\|) ,
\end{aligned} \tag{S31}$$

where we have assumed $\mu = \frac{nt}{r} < 1$ so that the sum converges. Therefore, the lemma follows. □

To prove the Lemma 2, we write $\delta = [H, S] + V$ with S, V bounded by Eq. (14). We then use Lemma S4 with $X = S$ and the triangle inequality to get

$$\left\| \sum_{j=0}^{a-1} U_{j\tau} \delta\, U_{j\tau}^\dagger \right\| \leq \left\| \frac{1}{\tau} \Sigma_a(S) \right\| + \left\| \sum_{j=0}^{a-1} U_{j\tau} V\, U_{j\tau}^\dagger \right\| \tag{S32}$$

$$= O\left(\frac{1}{\tau}\|S\|\right) + O(a\|V\|) \tag{S33}$$

$$= O\left(\frac{nt}{r}\right) + O\left(a\frac{nt^3}{r^3}\right). \tag{S34}$$

Thus, the lemma follows. □

S3. UPPER BOUND ON Δ_k

In this section, we show how we bound the norms of Δ_k in Eq. (16). For that, we use Lemma 2 together with the bound on $\|\delta\|$ [Eq. (13)]:

$$\begin{aligned}
\|\Delta_k\| &= \left\| \sum_{i_1=0}^{r-k} \sum_{i_2=0}^{r-k-i_1} \sum_{i_3=0}^{r-k-i_1-i_2} \cdots \sum_{i_k=0}^{r-k-i_1-i_2-\cdots-i_k} \underbrace{U_{t/r}^{i_1} \delta U_{t/r}^{i_2} \delta U_{t/r}^{i_3} \delta \cdots}_{\delta \text{ appears } k \text{ times}} U_{t/r}^{r-k-i_1-i_2-\cdots-i_k} \right\| \\
&\leq \sum_{i_1=0}^{r-k} \sum_{i_2=0}^{r-k-i_1} \sum_{i_3=0}^{r-k-i_1-i_2} \cdots \|\delta\|^{k-1} \left\| \sum_{i_k=0}^{r-k-i_1-i_2-\cdots-i_k} U_{t/r}^{i_k} \delta U_{t/r}^{-i_k} \right\| \\
&\leq r^{k-1} \|\delta\|^{k-1} O\left(\frac{nt}{r} + \frac{nt^3}{r^2}\right).
\end{aligned} \tag{S35}$$

Thus, Eq. (16) follows.