Supplemental Material for
"Bounding the finite-size error of quantum many-body dynamics simulations"

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The supplemental material fills in technical details of the basic results in the main text. We first prove the ground state FSE bound in Eq. (7) under the gap assumption we mentioned there. Then we give the full derivation of the dynamics FSE bound for correlated initial state, Eq. (9). We then compare our dynamics error bounds to perturbation theory at early times and show that they are qualitatively tight for a large class of product initial states, i.e. they grow with time as t^a with the correct exponent a. The remaining task is to give a detailed derivation of the improved error bound in PBC given in Eq. (6). An important intermediate step is to prove Eq. (S18), which is an analog of Eq. (4), expressing the FSE in terms of a LR commutator. We give three different methods to numerically upper bound the LR commutator that appears in the rhs of Eq. (S18). The first one is to evaluate the series in Eq. (S20), which combines the methods in Refs. [1, 2]. This leads to the tightest bound, but is only efficiently computable in special cases. The second one is to numerically solve the differential equation (S30) and then calculate Eq. (S39). This method (which is based on Ref. [2]) is only slightly looser than the first one but is computationally efficient in general. The third method makes further simplifications which result in the simple analytic expression in Eq. (6), whose constants are given in Eqs. (S52,S53,S55). We emphasize that for any desired system, one may compute the LR bound and use it in the error formulas Eqs. (4) and (S18). In this way, as LR bounds are refined in the future or extended to more general systems (e.g. long-range interacting [3–5], bosonic [6], or continuum ones), these refinements can immediately be used in the FSE bounds.

FSEs in gapped non-degenerate ground states

In this section we prove the exponential decay of FSE in gapped non-degenerate ground states under the assumption stated in the main text. Recall that $\hat{H}$ is the Hamiltonian in the thermodynamic limit, and $\hat{H}' = \hat{H} - \Delta\hat{H}$ is obtained from $\hat{H}$ by removing the boundary links. The interpolated Hamiltonian $\hat{H}(\lambda) = (1-\lambda)\hat{H} + \lambda\hat{H}' = \hat{H} - \lambda\Delta\hat{H}$ is assumed to have a non-degenerate ground state $|G(\lambda)\rangle$ and is uniformly gapped $\Delta(\lambda) \geq \Delta > 0$, for all $\lambda \in [0,1]$. The basic idea is that, as the parameter λ is varied from 0 to 1, we keep track of how fast $|G(\lambda)\rangle$ changes, as well as $\langle\hat{S}_l\rangle_\lambda \equiv \langle G(\lambda)|\hat{S}_l|G(\lambda)\rangle$. Suppose $|G(\lambda)\rangle$ is properly normalized such that $\langle G(\lambda)|G(\lambda)\rangle = 1$ and phase chosen such that $\langle G(\lambda)|\frac{d}{d\lambda}|G(\lambda)\rangle = 0$ for any $\lambda \in [0,1]$. Then first order non-degenerate perturbation theory gives

$$\frac{d}{d\lambda}|G(\lambda)\rangle = -\frac{\bar{P}_G(\lambda)}{E_0(\lambda) - \hat{H}(\lambda)}\Delta\hat{H}|G(\lambda)\rangle, \tag{S1}$$

where $E_0(\lambda)$ is the ground state energy of $\hat{H}(\lambda)$ and $\bar{P}_G(\lambda) \equiv \hat{\mathbb{1}} - |G(\lambda)\rangle\langle G(\lambda)|$ is the projection operator to the space of excited states. Therefore, we have the integral formula for the FSE δS_l:

$$\delta S_l \equiv \langle\hat{S}_l\rangle_1 - \langle\hat{S}_l\rangle_0 = -\int_0^1 d\lambda[\langle G(\lambda)|\hat{S}_l\frac{\bar{P}_G(\lambda)}{E_0(\lambda) - \hat{H}(\lambda)}\Delta\hat{H}|G(\lambda)\rangle + \text{H.c.}]. \tag{S2}$$

The integrand looks similar to the ground state correlator between $\hat{S}_l$ and $\Delta\hat{H}$, so it's natural to guess that it should decay exponentially in a gapped system. This is verified by the following theorem (which is similar to the exponential clustering theorem in non-degenerate gapped ground states [7]):

Theorem 1. *Let $\hat{A}_X, \hat{B}_Y$ be arbitrary local observables with unit norm, supported on non-overlapping regions X, Y, respectively. Let $|G\rangle$ be the unique ground state of locally-interacting Hamiltonian $\hat{H}$ with spectral gap Δ. Then the quantity $f_{XY} \equiv \langle G|\hat{A}_X\frac{\bar{P}_G}{E_0-\hat{H}}\hat{B}_Y|G\rangle + \text{c.c.}$ is upper bounded by*

$$|f_{XY}| \leq C\sqrt{d_{XY}}e^{-d_{XY}/\xi}, \quad \text{where} \quad \xi^{-1} = \begin{cases} \frac{\Delta}{2v} & \text{if } \Delta \leq v \\ \frac{1}{2}W(\frac{\Delta^2 e}{v^2}) & \text{if } \Delta > v, \end{cases} \tag{S3}$$

where v is the LR velocity, $W(x)$ is the Lambert-W function, C is a constant depending on $\hat{A}_X$ and $\hat{B}_Y$, and d_{XY} is the distance between X and Y.

Proof. Using the identity

$$\begin{aligned}
&\int_{-\infty}^{\infty} e^{-\alpha T^2} dT \int_0^T dt \langle G|[\hat{A}_X(t), \hat{B}_Y]|G\rangle \\
&= i\int_{-\infty}^{\infty} dT e^{-\alpha T^2} \{\langle G|\hat{A}_X \frac{1-e^{i(E_0-\hat{H})T}}{E_0-\hat{H}} \hat{B}_Y|G\rangle + \text{H.c.}\} \\
&= i\sqrt{\frac{\pi}{\alpha}} \{\langle G|\hat{A}_X \frac{\bar{P}_G}{E_0-\hat{H}} [1-e^{-\frac{(E_0-\hat{H})^2}{4\alpha}}] \hat{B}_Y|G\rangle + \text{H.c.}\},
\end{aligned} \tag{S4}$$

where $\alpha > 0$ is a parameter to be specified later, we have

$$\begin{aligned}
f_{XY} &= \{\langle G|\hat{A}_X \frac{\bar{P}_G}{E_0-\hat{H}} e^{-\frac{(E_0-\hat{H})^2}{4\alpha}} \hat{B}_Y|G\rangle + \text{H.c.}\} \\
&\quad -i\sqrt{\frac{\alpha}{\pi}} \int_{-\infty}^{\infty} e^{-\alpha T^2} dT \int_0^T dt \langle G|[\hat{A}_X(t), \hat{B}_Y]|G\rangle.
\end{aligned} \tag{S5}$$

Therefore

$$\begin{aligned}
|f_{XY}| &\le 2\frac{e^{-\frac{\Delta^2}{4\alpha}}}{\Delta} + \sqrt{\frac{\alpha}{\pi}} \int_{-\infty}^{\infty} e^{-\alpha T^2} dT \int_0^T dt \|[\hat{A}_X(t), \hat{B}_Y]\| \\
&\le 2\frac{e^{-\frac{\Delta^2}{4\alpha}}}{\Delta} + 2\sqrt{\frac{\alpha}{\pi}} \int_0^{\infty} e^{-\alpha T^2} [C\left(\frac{vT}{r}\right)^{r+1}_{\le 1} + 2(T - r/v)_{\ge 0}] dT \\
&\le 2\frac{e^{-\frac{\Delta^2}{4\alpha}}}{\Delta} + 2\sqrt{\frac{\alpha}{\pi}} \int_0^{r/v} e^{-\alpha T^2} C\left(\frac{vT}{r}\right)^{r+1} dT + 2\sqrt{\frac{\alpha}{\pi}} \int_{r/v}^{\infty} e^{-\alpha T^2} [C + 2(T - r/v)] dT \\
&\le \frac{2}{\Delta} e^{-\frac{\Delta^2}{4\alpha}} + 2C\sqrt{\frac{\alpha}{\pi}} \frac{r}{v} \max_{0\le T\le r/v} e^{-\alpha T^2} \left(\frac{vT}{r}\right)^{r+1} + C_3 e^{-\alpha r^2/v^2} \\
&= \frac{2}{\Delta} e^{-\frac{\lambda\Delta^2 r}{4}} + C_2 \max_{0\le\tau\le 1/v} e^{-\tau^2 r/\lambda} (v\tau)^{r+1} + C_3 e^{-\frac{r}{\lambda v^2}},
\end{aligned} \tag{S6}$$

where we use the notation $(x)_{\le 1} = \min\{x, 1\}, (x)_{\ge 0} = \max\{x, 0\}$, C is a constant coming from the LR bound that does not depend on r, α, C_2, C_3 are coefficients that only weakly depend on r, α, and in the last line we substituted $T = \tau r$ and $\alpha = 1/(\lambda r)$.

Notice that Eq. (S6) holds for arbitrary positive λ, since the parameter $\alpha > 0$ introduced in Eq. (S4) can be chosen arbitrarily. If we choose λ to be any positive value, we can immediately prove the exponential decay of $|f_{XY}|$ in d_{XY} which leads to Eq. (7) in the main text, since all the three terms in the rhs of Eq. (S6) decay exponentially in r. If we want a better bound, we can choose λ to maximize the smallest decay coefficient $\min\{\lambda\Delta^2/4, \min_{1\le\tau\le 1/v}[\tau^2/\lambda - \ln(v\tau)], 1/(\lambda v^2)\}$, to make the rhs of Eq. (S6) decay in r as fast as possible. For $\Delta \le v$ we choose $\lambda = 2/(\Delta v)$ and the maximum is at $\tau = 1/v$, while for $\Delta > v$, we choose λ to be the solution to the equation $\lambda\Delta^2/2 + \ln(\lambda v^2/2) = 1$, and the maximum occurs at $\tau = \sqrt{\lambda/2}$. In the end we arrive at Eq. (S3). This finishes the proof of our theorem. □

Inserting Eq. (S3) into Eq. (S2), we get

$$|\delta S_l| = |\text{Tr}[\hat{\rho}\hat{S}_l - \hat{\rho}_L\hat{S}_l]| \le C e^{-(L-l)/2\xi'}, \tag{S7}$$

where ξ' is chosen to be slightly larger than the ξ in Eq. (S3) to compensate the $\sqrt{d_{XY}}$ prefactor, and the constant C is adjusted accordingly. This proves Eq. (7) in the main text.

Proof of Eq. (9): bound for dynamics initiated from a correlated initial state

We assume $2vt < L$, since these are the only times we will apply the FSE bounds; at longer times the error bounds become too large to be useful. We have

$$\begin{aligned}
|\mathrm{Tr}[(\hat{\rho}_L - \hat{\rho}_{[L]})\hat{S}_L(t)]| &= |\mathrm{Tr}\{(\hat{\rho}_L - \hat{\rho}_{[L]})\sum_{l=0}^{L}[\hat{S}_l(t) - \hat{S}_{l-1}(t)]\}| \\
&\leq \sum_{l=0}^{L} \|\hat{S}_l(t) - \hat{S}_{l-1}(t)\| |\mathrm{Tr}[(\hat{\rho}_L - \hat{\rho}_{[L]})\hat{O}_l]| \\
&\leq C_1 \sum_{l=0}^{\lfloor 2vt \rfloor} e^{-(L-l)/2\xi} + C_2 \sum_{l=\lceil 2vt \rceil}^{L} (2vt/l)^{\eta l/2} e^{-(L-l)/2\xi} \\
&\leq C_1' e^{(vt-L/2)/\xi} + C_2 \sum_{l=\lceil 2vt \rceil}^{L} e^{\eta(vt-l/2)} e^{-(L-l)/2\xi} \\
&= C_1' e^{(vt-L/2)/\xi} + C_2' e^{\eta(vt-L/2)},
\end{aligned} \tag{S8}$$

where $\hat{O}_l$ is a unit norm operator that only acts nontrivially in X_l, and $\lfloor x \rfloor, \lceil x \rceil$ are the floor and ceiling of x, respectively. The first term in the third line comes from the trivial bound $\|\hat{S}_l(t) - \hat{S}_{l-1}(t)\| \leq 2\|\hat{S}\|$, while the second term comes from the LR bound $\|\hat{S}_l(t) - \hat{S}_{l-1}(t)\| \leq C(2vt/l)^{\eta l/2}$. In the fourth line we use the inequality $(2vt/l)^{\eta l/2} \leq e^{\eta(vt-l/2)}$ to facilitate the calculation, and we sum the geometric series in the last two lines, with constants C_1', C_2' depending at most weakly on t, L. Combined with the second term of Eq. (8), we obtain Eq. (9). One can explicitly compute as needed the constants appearing in this bound for a given model and initial state $\hat{\rho}$.

Comparison of FSE bounds to perturbation theory at early times

We can gain insights into the accuracy of our error bounds by comparing them to the true FSE at lowest order in time. We can do this analytically using the Taylor series expansion of the true FSE. Recall from Eq. (2) that FSE is defined as

$$\delta\langle\hat{S}(t)\rangle_\psi \equiv |\langle e^{i\hat{H}_L t}\hat{S}e^{-i\hat{H}_L t}\rangle_{\psi_L} - \langle e^{i\hat{H}t}\hat{S}e^{-i\hat{H}t}\rangle_\psi|, \tag{S9}$$

where $\hat{H}_L$ is the L-site finite Hamiltonian and ψ_L is the initial product state restricted to this finite chain. The Taylor series expansion of the time evolved operators can be expressed as sums of Lie clusters (nested commutators) involving $\hat{S}$ and terms in the Hamiltonian [see, e.g. Eq. (S11)]. Many small clusters appear in both $\langle e^{i\hat{H}_L t}\hat{S}e^{-i\hat{H}_L t}\rangle_{\psi_L}$ and $\langle e^{i\hat{H}t}\hat{S}e^{-i\hat{H}t}\rangle_\psi$ and therefore cancel each other. Only those clusters whose spatial length is at least half of the system size may contribute to FSE. In the following we treat OBC and PBC separately, starting with OBC.

In OBC, FSE is due to those nested commutators in $\langle e^{-i\hat{H}t}\hat{S}e^{-i\hat{H}t}\rangle$ in which boundary terms appear at least once, since only such clusters are not canceled by any cluster in $\langle e^{-i\hat{H}_L t}\hat{S}e^{-i\hat{H}_L t}\rangle$. The lowest order cluster containing at least a boundary term is proportional to $\langle\hat{C}(\hat{S},\hat{V}_j)\rangle_\psi t^{D(\hat{S},\hat{V}_j)}/D(\hat{S},\hat{V}_j)!$, where $\hat{V}_j$ the boundary term closest to $\hat{S}$, and $\hat{C}(\hat{S},\hat{V}_j)$ is the shortest nested commutator joining $\hat{S}$ and $\hat{V}_j$. Assuming that the expectation value $\langle\hat{C}(\hat{S},\hat{V}_j)\rangle_\psi$ does not vanish (which is true for most initial product states $|\psi\rangle$), the true FSE has the same t dependence as the bound Eq. (5).

In PBC there is a qualitative difference. Any term in the Taylor expansion of $\langle e^{i\hat{H}t}\hat{S}e^{-i\hat{H}t}\rangle_\psi$ in Eq. (S9) whose spatial span is smaller than L do not contribute to FSE, because they cancel the corresponding terms in $\langle e^{i\hat{H}_L t}\hat{S}e^{-i\hat{H}_L t}\rangle_{\psi_L}$ due to translation invariance and the product nature of the initial state, as shown in Fig. S1. Only those terms in $\langle e^{i\hat{H}t}\hat{S}e^{-i\hat{H}t}\rangle_\psi$ which are too long to be embeddable into an L-site periodic system can contribute. More precisely, in PBC, the rhs of Eq. (S9) is contributed by the following two classes of terms:
(1) terms in $\langle e^{i\hat{H}t}\hat{S}e^{-i\hat{H}t}\rangle_\psi$ whose spatial span is larger than L, i.e. terms that are too long to be embeddable in the L-site PBC chain;
(2) terms in $\langle e^{i\hat{H}_L t}\hat{S}e^{-i\hat{H}_L t}\rangle_{\psi_L}$ which wrap around the whole periodic system (wraps around the torus, or the circle in $d = 1$). Such terms do not generally cancel any terms in $\langle e^{i\hat{H}t}\hat{S}e^{-i\hat{H}t}\rangle_\psi$.

The leading order term in both classes are proportional to $t^{\mathcal{L}}$, where $\mathcal{L}$ is the number of Hamiltonian terms in the smallest L-site-unembeddable cluster starting from $\hat{S}$. This $t^{\mathcal{L}}$ behavior is the same as the improved PBC bound in Eq. (6), and the exponent $\mathcal{L}$ is roughly twice as large as the OBC exponent $D(\hat{S}, \hat{V}_j)$. In the next section, we give a rigorous bound for the sum of all terms in each class.

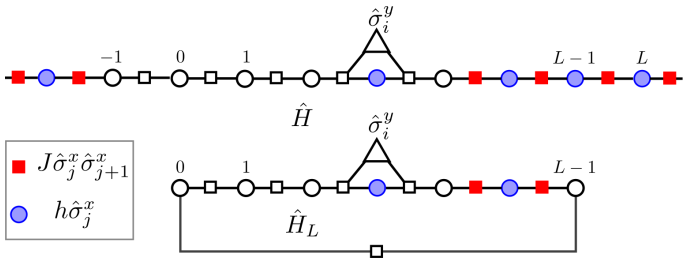

FIG. S1: An example of canceling terms in the Taylor expansions of $e^{i\hat{H}t}\hat{\sigma}_i^y e^{-i\hat{H}t}$ and $e^{i\hat{H}_L t}\hat{\sigma}_i^y e^{-i\hat{H}_L t}$, in the case of 1D TFIM. Vertices represent terms $\hat{h}_j$ of the Hamiltonian $\hat{H} = \sum_j \hat{h}_j$, as well as the observable $\hat{S} = \hat{\sigma}_i^y$, and edges are drawn between terms that do not commute. The spatial span of the two Lie clusters shown in this figure (cluster of open circles, squares, and triangles) are equal and shorter than the system size. The expectation values of these two terms exactly cancel due to translation invariance and the initial state being a product state.

IMPROVED BOUND FOR PBC

For simplicity, we first focus on the 1D case, and later we show that a bound in higher dimension can be obtained by repeatedly using the 1D bound. Consider a translation invariant quantum system on a 1D periodic lattice with L unit cells, described by the Hamiltonian $\hat{H}_L$, and let $\hat{H} = \hat{H}_{L\to\infty}$ be the Hamiltonian in the thermodynamic limit. We will derive an upper bound for the sum of all terms in $e^{-i\hat{H}t}\hat{S}e^{-i\hat{H}t}$ that may contribute to the FSE (i.e. whose spatial span is larger than L), using ideas motivated by Ref. [1], and then do the same for $e^{-i\hat{H}_L t}\hat{S}e^{-i\hat{H}_L t}$.

Let us focus on the first class of terms, i.e. terms in $e^{i\hat{H}t}\hat{S}e^{-i\hat{H}t}$ whose spatial span is larger than L, since the second class can be treated in an identical way. We write the Hamiltonian in the thermodynamic limit as

$$\hat{H} = \sum_{j\in G} \hat{h}_j, \tag{S10}$$

where $\hat{h}_j$ denotes a local term in $\hat{H}$. It is convenient to introduce the notion of the commutativity graph G, defined in Ref. [2]. This is a graph whose vertices j are associated with $\hat{h}_j$ and which has edges from j to j' if and only if $\hat{h}_j$ and $\hat{h}_{j'}$ do not commute. The observable $\hat{S}$ is represented as an external vertex s on G, linked to all the vertices j whose $\hat{h}_j$ do not commute with $\hat{S}$, as shown in Fig. S1. Now we write down the Taylor expansion of $e^{i\hat{H}t}\hat{S}e^{-i\hat{H}t}$. We use bold letters $\mathbf{h}_j = \mathrm{ad}_{\hat{h}_j}$ to denote the adjoint of the corresponding operator $\hat{h}_j$, e.g. $\mathbf{h}_j(\hat{S}) \equiv [\hat{h}_j, \hat{S}]$. We have

$$\begin{aligned} e^{i\hat{H}t}\hat{S}e^{-i\hat{H}t} &= e^{i\mathbf{H}t}(\hat{S}) \\ &= \sum_{n=0}^{\infty} \frac{(it)^n}{n!} \sum_{\substack{j_1,\ldots,j_n\in G \\ T(s,j_1,j_2,\ldots,j_n)\in\mathcal{T}_s}} \mathbf{h}_{j_n}\ldots\mathbf{h}_{j_2}\mathbf{h}_{j_1}\hat{S}, \end{aligned} \tag{S11}$$

where $T(s, j_1, j_2, \ldots, j_n)$ denotes the causal forest of the sequence $(s, j_1, j_2, \ldots, j_n)$, as defined in Ref. [1], and $\mathcal{T}_s$ denotes the set of causal trees starting from the vertex s. In simple terms, we are summing over all the non-vanishing connected Lie clusters on G starting from the vertex s.

Our goal is to upper bound the sum over all the terms in Eq. (S11) whose spatial span is larger than L. For such a Lie cluster, let j_i be the first term in the sequence $j_1, \ldots, j_n$ such that the spatial span of the subsequence $\mathbf{h}_{j_i}\ldots\mathbf{h}_{j_1}\hat{S}$ is larger than L. This means that the spatial span of $\mathbf{h}_{j_{i-1}}\ldots\mathbf{h}_{j_1}\hat{S}$ is less than or equal to L. We call j_i the *earliest unembeddable vertex* (EUV) of the sequence $(s, j_1, j_2, \ldots, j_n)$. Notice that $\hat{h}_{j_i}$ must act nontrivially on at least two unit cells, because otherwise j_i can never be the EUV of any sequence.

The basic idea is to classify the Lie clusters in Eq. (S11) into different families, with each family having the same EUV, and derive an upper bound for the sum over all terms within each family. To this end, let us denote by $[e^{i\mathbf{H}t}(\hat{S})]_k$ the sum of all the L-site unembeddable terms in the rhs of Eq. (S11) whose EUV is k, i.e.

$$[e^{i\mathbf{H}t}(\hat{S})]_k \equiv \sum_{\substack{n\geq 0,\\ T(s,j_1,j_2,\ldots,j_n)\in\mathcal{T}_s,\\ \mathrm{EUV}(s,j_1,j_2,\ldots,j_n)=k}} \frac{(it)^n}{n!}\mathbf{h}_{j_n}\ldots\mathbf{h}_{j_2}\mathbf{h}_{j_1}\hat{S}. \tag{S12}$$

We limit our explicit proof to the nearest neighbor interacting case in which every term $\hat{h}_j$ in the Hamiltonian acts non-trivially on at most two neighboring unit cells. The proof for the general case is the same as for the nearest-neighbor interacting case, but involves keeping track of more complicated notation. Therefore for the general case we omit the proof and present only the final result. Returning to the nearest-neighbor interacting case, for an arbitrary operator $\hat{A}$, let $x_A^{\mathrm{L}}, x_A^{\mathrm{R}}$ denote the x-coordinates of the leftmost and rightmost unit cells on which the operator $\hat{A}$ acts, and let $n_A \equiv x_A^{\mathrm{R}} - x_A^{\mathrm{L}} + 1$ denote the spatial span of $\hat{A}$ (we write $x_k^{\mathrm{L,R}}, n_k$ for the operator $\hat{h}_k$ for simplicity). In the nearest neighboring interacting case, $n_k = 2$ if k is an EUV. Without loss of generality, let us suppose that $x_k^{\mathrm{L}} < x_S^{\mathrm{L}}$ (the other case $x_k^{\mathrm{R}} > x_S^{\mathrm{R}}$ can be treated similarly). In this case we need to have $x_S^{\mathrm{R}} \leq x_k^{\mathrm{R}} + L - 1$, because otherwise the cluster is already unembeddable before $\hat{h}_k$ is attached, contradicting the assumption that k is the EUV. Then we have the following theorem:

Theorem 2.

$$[e^{i\mathbf{H}t}(\hat{S})]_k = i\int_0^t dt'\, e^{i\mathbf{H}(t-t')}\mathbf{h}_k(e^{i\mathbf{H}'_k t'}\hat{S} - e^{i\mathbf{H}_k t'}\hat{S}), \tag{S13}$$

where

$$\hat{H}'_k = \hat{H}_{[x_k^L+1,\ldots,x_k^L+L]}, \qquad \hat{H}_k = \hat{H}_{[x_k^L+1,\ldots,x_k^L+L-1]}, \tag{S14}$$

where $\hat{H}_{[x_k^L+1,\ldots,x_k^L+L]}$ denotes the truncation of $\hat{H}$ to sites $[x_k^L+1,\ldots,x_k^L+L]$, and similarly for $\hat{H}_{[x_k^L+1,\ldots,x_k^L+L-1]}$.

Thm. (2) can be proved by Taylor expanding both sides and explicitly comparing terms, using the same spirit as the proof of Lemma 5 and Lemma 6 in Ref. [1]. Intuitively, $e^{i\mathbf{H}'_k t'}\hat{S}$ gives the sum of all terms in the Taylor expansion of $e^{i\mathbf{H}t'}\hat{S}$ that act inside the region $[x_k^{\mathrm{L}}+1,\ldots,x_k^{\mathrm{L}}+L]$, so $(e^{i\mathbf{H}'_k t'}\hat{S} - e^{i\mathbf{H}_k t'}\hat{S})$ gives the sum of all terms in $e^{i\mathbf{H}t'}\hat{S}$ that act inside the region $[x_k^{\mathrm{L}}+1,\ldots,x_k^{\mathrm{L}}+L]$ and act non-trivially on $x_k^{\mathrm{L}}+L$, since those terms which do not act on $x_k^{\mathrm{L}}+L$ are canceled by $-e^{i\mathbf{H}_k t'}\hat{S}$. Further, only those terms in $(e^{i\mathbf{H}'_k t'}\hat{S} - e^{i\mathbf{H}_k t'}\hat{S})$ that act non-trivially on $x_k^{\mathrm{R}} = x_k^{\mathrm{L}}+1$ can survive the commutation with $\hat{h}_k$ in the rhs of Eq. (S13). In short, the surviving terms in $(e^{i\mathbf{H}'_k t'}\hat{S} - e^{i\mathbf{H}_k t'}\hat{S})$ are those terms that span exactly L unit cells $[x_k^{\mathrm{R}},\ldots,x_k^{\mathrm{L}}+L]$, which are the terms in $e^{i\mathbf{H}t'}\hat{S}$ that are L-site embeddable but become unembeddable immediately after attaching $\mathbf{h}_k$. Therefore the rhs of Eq. (S13) gives the sum of all Lie clusters in $e^{i\mathbf{H}t}(\hat{S})$ with k being the EUV, since the action of $e^{i\mathbf{H}(t-t')}$ happens at a time later than t' and can not change the earliestness of $\hat{h}_k$. [The last sentence can be better understood by noticing that $i\int_0^t dt'\, e^{i\mathbf{H}(t-t')}\mathbf{h}_k e^{i(\mathbf{H}-\mathbf{h}_k)t'}\hat{S}$ simply gives the sum of all terms in $e^{i\mathbf{H}t}\hat{S}$ in which $\hat{h}_k$ appears at least once, with the $\hat{h}_k$ at time t' being the earliest appearance. Therefore it is natural to expect that $i\int_0^t dt'\, e^{i\mathbf{H}(t-t')}\mathbf{h}_k(e^{i\mathbf{H}'_k t'}\hat{S} - e^{i\mathbf{H}_k t'}\hat{S})$ gives a subset of the terms in $i\int_0^t dt'\, e^{i\mathbf{H}(t-t')}\mathbf{h}_k e^{i(\mathbf{H}-\mathbf{h}_k)t'}\hat{S}$, whose EUV is k.]

For more general locally interacting Hamiltonians which involve terms that act non-trivially on more than 2 neighboring unit cells, Thm. (2) is generalized to

$$[e^{i\mathbf{H}t}(\hat{S})]_k = i\sum_{\alpha=1}^{n_k-1}\int_0^t dt'\, e^{i\mathbf{H}(t-t')}\mathbf{h}_k(e^{i\mathbf{H}'_{k,\alpha}t'}\hat{S} - e^{i\mathbf{H}_{k,\alpha}t'}\hat{S}), \tag{S15}$$

where

$$\hat{H}'_{k,\alpha} = \hat{H}_{[x_k^{\mathrm{L}}+\alpha,\ldots,x_k^{\mathrm{L}}+\alpha+L-1]}, \qquad \hat{H}_{k,\alpha} = \hat{H}_{[x_k^{\mathrm{L}}+\alpha,\ldots,x_k^{\mathrm{L}}+\alpha+L-2]}. \tag{S16}$$

We can get an upper bound for the operator norm of the rhs of Eq. (S15) using the triangle inequality and unitary invariance of operator norm. The result is

$$\|e^{i\mathbf{H}t}\hat{S}|_{\mathrm{span}>L}\| \leq \sum_{k,\alpha}\int_0^t dt'\, \|[\hat{h}_k, e^{i\mathbf{H}'_{k,\alpha}t'}(\hat{S}) - e^{i\mathbf{H}_{k,\alpha}t'}(\hat{S})]\|. \tag{S17}$$

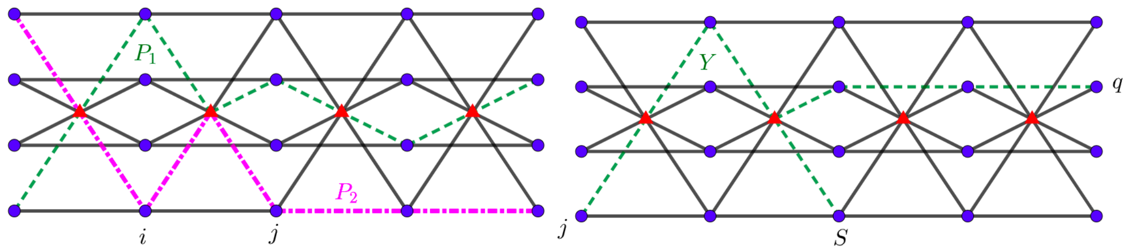

FIG. S2: Examples of irreducible path and Y-shape on the commutativity graph of the FHM. (Left) The dark green, dashed path P_1 is irreducible, while the pink, dot-dashed path P_2 is reducible since the pair (i,j) is not consecutive in P_2 but $(i,j) \in G$. (Right) Example of an irreducible Y-shape.

The second class of terms [those arising from $e^{i\mathbf{H}_L t}(\hat{S})$] can be bounded in a similar way, and it turns out that the resulting upper bound for the second class is identical to the first class, Eq. (S17). Adding up the two classes and taking $n_k = 2$, we get

$$|\delta\langle\hat{S}(t)\rangle| \le 2\sum_{k,\alpha}\int_0^t dt'\, \|[\hat{h}_k, e^{i\mathbf{H}'_{k,\alpha}t'}(\hat{S}) - e^{i\mathbf{H}_{k,\alpha}t'}(\hat{S})]\|. \tag{S18}$$

In the following we give two different approaches to upper bound the commutator in the rhs of Eq. (S17). The first one is based on a combination of the methods in Ref. [1, 2]. This method leads to the tightest bound but has a high computational cost (potentially exponential in the system size) except in a few simple cases. The second one is based on the differential equation method in Ref. [2], which is slightly looser than the first one, but is much easier to compute, and can also lead to a simple analytic upper bound such as Eq. (6).

CHEN-LUCAS BOUND FOR LR COMMUTATORS

In this section we present the tightest LR bounds for locally interacting systems, obtained by applying the method in Ref. [1] to the commutativity graph introduced in Ref. [2]. The goal is to upper bound $\|[\hat{h}_j, \hat{S}(t)]\|$ which appears in the simple bound in Eq. (4) and $\|[\hat{h}_k, e^{i\mathbf{H}'_k t'}(\hat{S}) - e^{i\mathbf{H}_k t'}(\hat{S})]\|$ which appears in the improved PBC bound in Eq. (S17). We begin with the first one. The bound for the second one is a generalization of the first one and is qualitatively smaller at early times. For simplicity we focus on 1D in this section.

The bound for $\|[\hat{h}_j, \hat{S}(t)]\|$ is obtained by generalizing Thm. 4 of Ref. [1] to the commutativity graph G. The result is (we present the time integrated version for simplicity)

$$\int_0^t \|[\hat{h}_j, \hat{S}(t')]\| dt' \le \|\hat{S}\| \sum_{P\in\mathcal{P}_{jS}} \frac{(2t)^{n(P)-1}}{[n(P)-1]!} \prod_{i\in P, i\neq s} h_i, \tag{S19}$$

where $\mathcal{P}_{jS}$ is the set of all irreducible paths on G from S to j, $n(P)$ is the number of vertices in P, and $h_i = \|\hat{h}_i\|$. An irreducible path P on graph G is a simple path (a path without repeated vertices) in which any two non-consecutive vertices in P are not adjacent in G. That is, let $P = (i_n = j, i_{n-1}, i_{n-2}, \dots, i_2, i_1 = S)$, then we have $(i_m, i_{m-1}) \notin G,\ 2 \le m \le n$. See Fig. S2 for examples of irreducible paths.

The bound for $\|[\hat{h}_j, e^{i\mathbf{H}'_j t'}(\hat{S}) - e^{i\mathbf{H}_j t'}(\hat{S})]\|$ is obtained in a similar way:

$$\int_0^t \|[\hat{h}_j, e^{i\mathbf{H}'_j t'}(\hat{S}) - e^{i\mathbf{H}_j t'}(\hat{S})]\| dt' \le \|\hat{S}\| \sum_{\hat{h}_q\in\hat{H}'_j - \hat{H}_j} \sum_{Y\in\mathcal{Y}_{s,jq}} \binom{n_j(Y)+n_q(Y)-1}{n_q(Y)} \frac{(2t)^{n(Y)-1}}{[n(Y)-1]!} \prod_{i\in Y, i\neq s} h_i, \tag{S20}$$

where the first sum is over all vertices q that appears in $\hat{H}'_j - \hat{H}_j$, $\mathcal{Y}_{s,jq}$ is the set of all irreducible Y-shapes on G with root s and end points j, q, $n_j(Y)$ is the number of vertices on the j-branch of Y and similarly for $n_q(Y)$, so that $n(Y) = n_j(Y) + n_q(Y) + n_s(Y) + 1$. The definition of an irreducible Y-shape with root s and endpoints j, q generalizes that of an irreducible path: it is a three-branch tree with a branch point y (y may coincide with one of s, j, q) such that the three branches P_{sy}, P_{jy}, P_{qy} are irreducible paths, and any vertex in $P_{sy}\backslash\{y\}$ is not linked (with respect to

G) to any vertex in $(P_{jy} \cup P_{qy})\backslash\{y\}$. The binomial coefficient in Eq. (S20) arises due to the different ways of relative time ordering the operators on the j-branch and the q-branch of Y.

We can see that at early times, the improved PBC bound in Eq. (S20) grows like $t^{\min n(Y_s)-1}$, where the minimum is taken over all the L-cell-unembeddable Y-shapes with root s (notice that the set of smallest L-cell-unembeddable Y-shapes always contain an irreducible one). Put it another way, the small-t exponent of the improved PBC bound is equal to the minimum number of Hamiltonian terms needed to be attached to $\hat{S}$ to make the cluster unembeddable (or, the number of Hamiltonian terms in the smallest unembeddable Lie cluster containing S), which agrees with perturbation theory (provided that the expectation value in $|\psi\rangle$ of the leading term doesn't vanish).

In general, the rhs of Eqs. (S19,S20) can only be calculated numerically. Yet there are a few special cases in which we can obtain simple analytic expressions due to the simple structure of the commutativity graph. In the following we show the bound for 1D TFIM as an example. Similar bounds apply to any 1D model whose commutativity graph is a single chain, another example is the FHM in the large-U limit [2].

Example: 1D TFIM in PBC We write the Hamiltonian as

$$\hat{H} = -J\sum_j \hat{Z}_{j,j+1} - h\sum_j \hat{X}_j, \tag{S21}$$

where $\hat{Z}_{j,j+1} \equiv \hat{\sigma}^z_j\hat{\sigma}^z_{j+1}$ and $\hat{X}_j \equiv \hat{\sigma}^x_j$. For illustrative purpose, take $\hat{S} = \hat{\sigma}^x_i$. The commutativity graph G is simply a 1D ring, as shown in Fig. S1. In this case, there are only two irreducible paths between any two points in G. Inserting Eq. (S19) evaluated for the PBC TFIM into Eq. (4) we obtain

$$|\delta\langle\hat{\sigma}^x_j(t)\rangle_\psi| \leq 4\sqrt{\frac{J}{h}}\frac{(2\sqrt{Jh}t)^L}{L!} + 2\sqrt{\frac{J}{h}}\frac{(2\sqrt{Jh}t)^{L+2}}{(L+2)!}, \tag{S22}$$

where we assume for simplicity that L is an odd integer.

The improved PBC error bound for $\delta\langle\hat{\sigma}^x_i(t)\rangle_\psi$ is given by Eq. (S18), which in the current case becomes

$$|\delta\langle\hat{\sigma}^x_i(t)\rangle_\psi| \leq 2\sum_{|j-i|\leq L}\int_0^t dt'\,\|[J\hat{Z}_{j,j+1}, e^{i\mathbf{H}'_j t'}(\hat{X}_i) - e^{i\mathbf{H}_j t'}(\hat{X}_i)]\|, \tag{S23}$$

where $\hat{H}'_j = \hat{H}_{[j+1,\ldots,j+L]}$, $\hat{H}_j = \hat{H}_{[j+1,\ldots,j+L-1]}$ for $j < i$, and we have a similar expression for $j \geq i$. Now we apply Eq. (S20) to bound the rhs. In this case, $\hat{h}_q = JZ_{j+L-1,j+L}$, and since both $\hat{H}'_j, \hat{H}_j$ have open boundary, there is only one irreducible Y-shape with endpoints j, s, q. Eq. (S20) becomes

$$\int_0^t dt'\,\|[J\hat{Z}_{j,j+1}, e^{i\mathbf{H}'_j t'}(\hat{X}_i) - e^{i\mathbf{H}_j t'}(\hat{X}_i)]\| \leq \frac{(2t)^{2L-2}}{(2L-2)!}J^L h^{L-2}\binom{2L-3}{n_j},\;\; n_j = \begin{cases} 2(i-j)-1, & i-L<j<i, \\ 2(j-i)+1, & i\leq j<i+L. \end{cases} \tag{S24}$$

When $|j-i| = L$, we have $e^{i\mathbf{H}_j t'}(\hat{X}_i) = \hat{X}_i$, so we can simply use Eq. (S19). The result is similar to the first term in Eq. (S22) with substitution $L \to 2L-1$. Inserting Eq. (S24) along with the $|j-i| = L$ case into Eq. (S23), we get

$$|\delta\langle\sigma^x_j(t)\rangle| \leq 4\sqrt{\frac{J}{h}}\frac{(2\sqrt{Jh}t)^{2L-1}}{(2L-1)!} + \frac{J}{h}\frac{(4\sqrt{Jh}t)^{2L-2}}{(2L-2)!}. \tag{S25}$$

BOUNDING THE PBC ERROR BOUND BY SOLVING A LINEAR DIFFERENTIAL EQUATION

Apart from a few special cases, the computational complexity of the Chen-Lucas bound, Eq. (S20), grows exponentially with system size, since the number of irreducible paths on G grows exponentially in general. For some models with very complicated G, the computation of the Chen-Lucas bound may take even longer than the quantum dynamics simulation itself. For this reason, in this section we give an alternative method based on Ref. [2], which is slightly looser than the Chen-Lucas bound but whose computational time complexity grows only quadratically with system size. In addition, with some further simplifications this method leads to the simple analytic expression in Eq. (6).

The goal here is to bound the FSE of a dynamics simulation on a periodic cluster of size $L_1 \times L_2 \times \ldots \times L_d$. The first step is to extend the 1D bound to d dimensions. To this end, denote by $\mathcal{C}_j$ a cluster of size $L_1 \times L_2 \times \ldots \times L_j \times \infty \times \ldots \times \infty$, that is, for $i \leq j$, the i-th direction is periodic with size L_i, while for $i > j$ the i-th direction is infinite. Then we have

$$\begin{aligned} |\delta \langle \hat{S}(t) \rangle_{L_1 \times \ldots \times L_d}| &\equiv |\langle \hat{S}(t) \rangle_{\infty \times \ldots \times \infty} - \langle \hat{S}(t) \rangle_{L_1 \times \ldots \times L_d}| \\ &\leq \sum_{j=1}^{d} |\langle \hat{S}(t) \rangle_{\mathcal{C}_{j-1}} - \langle \hat{S}(t) \rangle_{\mathcal{C}_j}| \end{aligned} \tag{S26}$$

Since for each j, the clusters $\mathcal{C}_{j-1}$ and $\mathcal{C}_j$ only differ in the j-th direction, the difference $|\langle \hat{S}(t) \rangle_{\mathcal{C}_{j-1}} - \langle \hat{S}(t) \rangle_{\mathcal{C}_j}|$ can be upper bounded using the 1D method. In the following we first focus on the $j = 1$ term, since other terms can be treated in an almost identical way. As before, we mainly focus on the "nearest-neighbor interacting" case (only allow interactions between neighboring unit cells), as the generalization to non-nearest-neighbor interactions is straightforward. We have

$$|\langle \hat{S}(t) \rangle_{\mathcal{C}_0} - \langle \hat{S}(t) \rangle_{\mathcal{C}_1}| \leq 2 \int_0^t dt' \sum_k \|[\hat{h}_k, e^{i\mathbf{H}'_k t'}(\hat{S}) - e^{i\mathbf{H}_k t'}(\hat{S})]\|. \tag{S27}$$

Notice that

$$\begin{aligned} [\hat{h}_k, e^{i\mathbf{H}'_k t}(\hat{S}) - e^{i\mathbf{H}_k t}(\hat{S})] &= \int_0^t dt' \, \mathbf{h}_k e^{i\mathbf{H}'_k t} \frac{d}{dt'} (\hat{S} - e^{-i\mathbf{H}'_k t'} e^{i\mathbf{H}_k t'} \hat{S}) \\ &= i \int_0^t dt' \, \mathbf{h}_k e^{i\mathbf{H}'_k (t-t')} (\mathbf{H}'_k - \mathbf{H}_k) e^{i\mathbf{H}_k t'}(\hat{S}). \end{aligned} \tag{S28}$$

Ref. [2] introduces a method to bound unequal time commutator of the form $\mathbf{h}_k e^{i\mathbf{H}t}(\hat{S})$ by solving a first order linear differential equation on the commutativity graph G. In the following we extend this method to bound double commutators of the form $\mathbf{h}_k e^{i\mathbf{H}_2(t-t')} \mathbf{h}_j e^{i\mathbf{H}_1 t'}(\hat{S})$, where $\hat{H}_2 = \hat{H}'_k, \hat{H}_1 = \hat{H}_k$, as required for Eq. (S28).

To begin, let us first recall some basic results from Ref. [2] and fix our notations. The thermodynamic limit Hamiltonian with commutativity graph G is written in Eq. (S10) as $\hat{H} = \sum_{j \in G} \hat{h}_j$. Since both $\hat{H}_1$ and $\hat{H}_2$ are sums of subset of terms in $\hat{H}_\infty = \hat{H}$ [see Eq. (S16)], we can write

$$\hat{H}_a = \sum_{j \in G} \hat{h}_j^a, \quad a = 1, 2, \infty, \tag{S29}$$

where $\hat{h}_j^a = \hat{h}_j$ if the term $\hat{h}_j$ is contained in $\hat{H}_a$ and $\hat{h}_j^a = 0$ otherwise. Let $G_{ij}^a(t)$ be the solution to the differential equation

$$\frac{d}{dt} G_{ij}^a(t) = 2 \sum_{k: \langle ki \rangle \in G} \sqrt{h_i^a h_k^a} G_{kj}^a(t) \equiv \sum_{k \in G} M_{ik}^a G_{kj}^a, \quad a = 1, 2, \infty, \tag{S30}$$

with initial condition $G_{ij}^a(0) = \delta_{ij}$, where $h_i^a \equiv \|\hat{h}_i^a\| \geq 0$ and $M_{ik}^a \equiv 2\sqrt{h_i^a h_k^a} \cdot (\langle ik \rangle \in G)$. The solutions can be written formally as $G_{ij}^a(t) = [e^{M^a t}]_{ij}$. Notice that since $0 \leq h_j^1 \leq h_j^2 \leq h_j$ we have $0 \leq M_{ij}^1 \leq M_{ij}^2 \leq M_{ij}$ and therefore $G_{ij}^1(t) \leq G_{ij}^2(t) \leq G_{ij}(t)$ for $t \geq 0$. In translation invariant systems, $G_{ij}(t)$ has a Fourier integral expression

$$G_{ij}(t) = [e^{Mt}]_{ij} = \int_{\vec{k}} [e^{M_{\vec{k}} t}]_{\alpha_i \alpha_j} e^{i\vec{k} \cdot (\vec{r}_i - \vec{r}_j)}, \tag{S31}$$

where $\vec{r}_i$ denotes the lattice translation vector of the unit cell containing vertex i, α_i labels the index of i inside a unit cell, we use the notation $\int_{\vec{k}} = \int \frac{d^d k}{(2\pi)^d}$, and

$$[M_{\vec{k}}]_{\alpha_i \alpha_j} \equiv \sum_{\vec{r}_j} M_{ij} e^{-i\vec{k} \cdot (\vec{r}_i - \vec{r}_j)}. \tag{S32}$$

In the following we first upper bound $\|\mathbf{h}_k e^{i\mathbf{H}_2(t-t')} \mathbf{h}_j e^{i\mathbf{H}_1 t'}(\hat{S})\|$ in terms of $G_{ij}^a(t)$ and then apply Eq. (S31) to get a simple final expression.

First consider the case when $t' = t$. For an arbitrary local operator $\hat{A}$, denote $\hat{A}^i(t) = [\hat{h}_i, \hat{A}(t)]$ and $\hat{A}^{ij}(t) = [\hat{h}_i, [\hat{h}_j, \hat{A}(t)]]$, where $\hat{A}(t) \equiv e^{i\mathbf{H}_1 t}(\hat{A})$. We want to find an upper bound for $\|\hat{S}^{ij}(t)\|$. Taking the time derivative using Heisenberg's equation, we have [note: from Eq. (S33) to Eq. (S38) we write $\hat{h}_j$ to mean $\hat{h}_j^1$ for notational simplicity]

$$\begin{aligned} i\frac{d}{dt}\hat{A}^{ij}(t) &= [\hat{h}_i, [\hat{h}_j, [\hat{A}(t), \sum_{k:\langle kA\rangle \in G} \hat{h}_k(t)]]] \\ &= \sum_{k:\langle kA\rangle \in G} \{[\hat{A}^{ij}(t), \hat{h}_k(t)] + [\hat{A}(t), \hat{h}_k^{ij}(t)] + [\hat{A}^i(t), \hat{h}_k^j(t)] + [\hat{A}^j(t), \hat{h}_k^i(t)]\}. \end{aligned} \tag{S33}$$

We can use the same derivations as in Eqs. (6-8) in Ref. [2] to prove that

$$\|\hat{A}^{ij}(t)\| \le 2 \sum_{k:\langle kA\rangle \in G} \int_0^t \{\|\hat{A}\|\|\hat{h}_k^{ij}(t')\| + \|\hat{A}^i(t')\|\|\hat{h}_k^j(t')\| + \|\hat{A}^j(t')\|\|\hat{h}_k^i(t')\|\}dt'. \tag{S34}$$

The last two terms can be bounded by Eqs. (16,17) of Ref. [2]:

$$\|\hat{A}^i(t)\| \le \bar{A}^i(t) \equiv \sum_{k:\langle kA\rangle \in G} G_{ik}^1(t)\sqrt{h_k h_i} 2\|\hat{A}\|. \tag{S35}$$

Notice that $\frac{d}{dt}\bar{A}^i(t) = \sum_{k:\langle kA\rangle \in G} 2\|A\|\bar{h}_k^i(t)$, so the last two terms in Eq. (S34) can be combined to $\frac{d}{dt'}[\bar{A}^i(t')\bar{A}^i(t')]/\|\hat{A}\|$, and we get

$$\|\hat{A}^{ij}(t)\| \le 2 \sum_{k:\langle kA\rangle \in G} \int_0^t \|\hat{A}\|\|\hat{h}_k^{ij}(t')\|dt' + \bar{A}^i(t)\bar{A}^j(t)/\|\hat{A}\|. \tag{S36}$$

Now take $\hat{A} = \hat{h}_l$, a term in $\hat{H}$. Using Grönwall's inequality, we can prove that $\|\hat{h}_l^{ij}(t)\| \le \bar{h}_l^{ij}(t)$ where $\bar{h}_l^{ij}(t)$ is the solution to the differential equation

$$\frac{d}{dt}\bar{h}_l^{ij}(t) = 2 \sum_{k:\langle kl\rangle \in G} h_l \bar{h}_k^{ij}(t) + \frac{1}{h_l}\frac{d}{dt}[\bar{h}_l^i(t)\bar{h}_l^j(t)], \tag{S37}$$

with initial condition $\bar{h}_l^{ij}(0) = 0$. If we substitute $\bar{\Gamma}_l(t) = \bar{h}_l^{ij}(t)/\sqrt{h_l}$, Eq. (S37) is of the form $\frac{d}{dt}\bar{\Gamma} = M^a \cdot \bar{\Gamma} + B$, which has formal solution $\bar{\Gamma}(t) = \int_0^t dt'\, e^{M^a(t-t')}B(t')dt'$, i.e.

$$\bar{h}_l^{ij}(t) = \sum_k \int_0^t \sqrt{\frac{h_l}{h_k^3}} G_{lk}^1(t-t') d[\bar{h}_k^i(t')\bar{h}_k^j(t')]. \tag{S38}$$

An upper bound for $\|S^{ij}(t)\|$ can be obtained by taking $\hat{A} = \hat{S}$ in Eq. (S36) and inserting Eqs. (S35, S38). Finally, Eq. (15) in Ref. [2] allows us to upper bound $\|\boldsymbol{h}_i e^{i\mathbf{H}_2(t-t')}\boldsymbol{h}_j e^{i\mathbf{H}_1 t'}(\hat{S})\|$ in terms of $\|\hat{S}^{ij}(t)\|$ and $G_{ij}^2(t)$ by taking $\hat{B} = \boldsymbol{h}_j e^{i\mathbf{H}t'}(\hat{S})$:

$$\|\boldsymbol{h}_i e^{i\mathbf{H}_2(t-t')}\boldsymbol{h}_j e^{i\mathbf{H}_1 t'}(\hat{S})\| \le 2\sum_{l\in G} G_{il}^2(t-t')\sqrt{\frac{h_i}{h_l}}\|\hat{S}^{lj}(t')\|. \tag{S39}$$

In summary, to get a bound for FSE $|\delta\langle\hat{S}(t)\rangle_{L_1\times\ldots\times L_d}|$, one need to first solve the differential equation Eq. (S30) to get $G_{ij}^1(t), G_{ij}^2(t)$ [note that since $G_{ij}^1(t) \le G_{ij}^2(t)$, having a bound for $G_{ij}^2(t)$ is enough], then use Eqs. (S35,S36,S38) to get a bound for $\|\hat{S}^{lj}(t')\|$, then insert into Eq. (S39) to get a bound for the double commutator, and finally use Eqs. (S26,S27,S28) to bound $|\delta\langle\hat{S}(t)\rangle_{L_1\times\ldots\times L_d}|$. All steps in this procedure are efficient, with total computational cost scaling at most quadratically with the system size.

Derivation of Eq. (6)

We now derive the simple bound in Eq. (6). We use $G_{ij}^a(t) \le G_{ij}(t)$ and Eq. (S31) to simplify the expression. Eq. (S38) becomes

$$\bar{h}_l^{ij}(t) = \sqrt{h_j h_j h_l} \sum_{m\in G} \int_0^t \frac{1}{\sqrt{h_m}} [e^{M(t-t')}]_{lm}[M^2 e^{Mt'}]_{im}[M e^{Mt'}]_{jm} dt' + (i \leftrightarrow j). \tag{S40}$$

Taking $\hat{A} = \hat{S}$ in Eq. (S36) and inserting Eqs. (S35, S40), we get

$$\bar{S}^{ij}(t_3) = \sqrt{h_i h_j} \sum_{m,l\in G} \int_{t_{1,2}} \frac{S_l}{\sqrt{h_m}} [e^{M(t_2-t_1)}]_{lm} [M^2 e^{Mt_1}]_{im} [M e^{Mt_1}]_{jm} + (i \leftrightarrow j) + \bar{S}^i(t_3)\bar{S}^j(t_3)/S, \tag{S41}$$

where $\int_{t_{1,2}} \equiv \int_{0\le t_1 \le t_2 \le t_3} dt_1 dt_2$ and $S_l \equiv 2\sqrt{h_l}(\langle ls\rangle \in G)\|\hat{S}\|$. Notice that M is symmetric, and so are e^{Mt}, Me^{Mt}, etc. Inserting Eq. (S41) into Eq. (S39), we obtain

$$\begin{aligned}
\|\boldsymbol{h}_i e^{i\mathbf{H}_2(t-t_3)} \boldsymbol{h}_j e^{i\mathbf{H}_1 t_3}(\hat{S})\| \;&\le\; 2\int_{t_{1,2}} \sum_{\substack{m,l\in G\\ a=1,2}} \sqrt{\frac{h_i h_j}{h_m}} [M^{3-a} e^{M(t-t_3+t_2-t_1)}]_{im} [M^a e^{M(t_2-t_1)}]_{jm} [e^{Mt_1}]_{ml} S_l + 2\bar{S}^i(t)\bar{S}^j(t_3)/S \\
&=\; 2\int_{t_{1,2},\vec{k}_{1,2}} \sum_{\substack{\alpha_m,l\\ a=1,2}} \sqrt{\frac{h_i h_j}{h_m}} [M_{\vec{k}_1}^{3-a} e^{M_{\vec{k}_1}(t-t_3+t_2-t_1)}]_{\alpha_i\alpha_m} [M_{\vec{k}_2}^{a} e^{M_{\vec{k}_2}(t_2-t_1)}]_{\alpha_j\alpha_m} \\
&\quad \times [e^{M_{\vec{k}_1+\vec{k}_2} t_1}]_{\alpha_m\alpha_l} e^{i\vec{k}_1\cdot(\vec{r}_i-\vec{r}_l)+i\vec{k}_2\cdot(\vec{r}_j-\vec{r}_l)} S_l + 2\bar{S}^i(t)\bar{S}^j(t_3)/S,
\end{aligned} \tag{S42}$$

where α_m runs over all vertices in a unit cell. Now we insert Eq. (S42) into Eqs. (S28) and (S27) to bound FSE $|\langle\hat{S}(t)\rangle_{\mathcal{C}_0} - \langle\hat{S}(t)\rangle_{\mathcal{C}_1}|$. Eqs. (S28) and (S27) combines to be

$$|\langle\hat{S}(t)\rangle_{\mathcal{C}_0} - \langle\hat{S}(t)\rangle_{\mathcal{C}_1}| \le 2 \sum_{(i,j)\in\mathcal{S}} \int_0^t dt_4 \int_0^{t_4} \|\boldsymbol{h}_i e^{i\mathbf{H}_2(t_4-t_3)} \boldsymbol{h}_j e^{i\mathbf{H}_1 t_3}(\hat{S})\| dt_3, \tag{S43}$$

where

$$\begin{aligned}
\mathcal{S} \;\equiv\; & \{(i,j)| n_i = n_j = 2 \;\wedge\; x_i^{\mathrm{L}} < x_S^{\mathrm{L}} \;\wedge\; x_S^{\mathrm{R}} \le x_i^{\mathrm{R}} + L - 1 \;\wedge\; x_j^{\mathrm{L}} = x_i^{\mathrm{L}} + L - 1\} \\
& \cup \{(i,j)| n_i = n_j = 2 \;\wedge\; x_i^{\mathrm{R}} > x_S^{\mathrm{R}} \;\wedge\; x_S^{\mathrm{L}} \ge x_i^{\mathrm{L}} - (L-1) \;\wedge\; x_j^{\mathrm{R}} = x_i^{\mathrm{R}} - (L-1)\}.
\end{aligned} \tag{S44}$$

The restriction on the summation over (i,j) follows from the discussion above Thm. 2 and the definition of $\hat{H}_i, \hat{H}_i'$ in Eq. (S14), which is essentially the requirement that i is the EUV of some Lie cluster starting from the vertex s, and that $\hat{h}_j$ is a term in $\hat{H}_2 - \hat{H}_1 \equiv \hat{H}_i' - \hat{H}_i$. Notice that the set $\mathcal{S}$ is translation invariant in directions $L_2, \ldots, L_d$. Namely, if $(i,j) \equiv ((\vec{r}_i,\alpha_i),(\vec{r}_j,\alpha_j)) \in \mathcal{S}$, then for any $\vec{r}_{1\perp} \perp \hat{x}, \vec{r}_{2\perp} \perp \hat{x}$, we have $(i',j') \equiv ((\vec{r}_i + \vec{r}_{1\perp},\alpha_i),(\vec{r}_j + \vec{r}_{2\perp},\alpha_j)) \in \mathcal{S}$. Let $\mathcal{T}_\perp$ denote the group of all lattice translation vectors in directions $L_2, \ldots, L_d$, such that $\mathcal{S} \cong \mathcal{S}/\mathcal{T}_\perp \times \mathcal{T}_\perp$. We can therefore decompose the sum over i,j as $\sum_{(i,j)\in\mathcal{S}} = \sum_{(x_i,x_j)\in\mathcal{S}/\mathcal{T}_\perp} \sum_{(\vec{r}_{i\perp},\vec{r}_{j\perp})\in\mathcal{T}_\perp}$. We have (we abbreviate $x_i = x_i^{\mathrm{L}}, x_j = x_j^{\mathrm{L}}$)

$$\begin{aligned}
\sum_{\substack{(\vec{r}_{i\perp},\vec{r}_{j\perp})\\ \in\mathcal{T}_\perp}} \|\boldsymbol{h}_i e^{i\mathbf{H}_2(t-t_3)} \boldsymbol{h}_j e^{i\mathbf{H}_1 t_3}(\hat{S})\| \;&\le\; 2\sqrt{h_{\alpha_i} h_{\alpha_j}} \int_{t_{1,2},k_{1x},k_{2x}} \sum_{\substack{\alpha_m,l\\ a=1,2}} [M_{k_{1x}}^{3-a} e^{M_{k_{1x}}(t-t_3+t_2-t_1)}]_{\alpha_i\alpha_m} [M_{k_{2x}}^{a} e^{M_{k_{2x}}(t_2-t_1)}]_{\alpha_j\alpha_m} \\
&\quad \times [e^{M_{k_{1x}+k_{2x}} t_1}]_{\alpha_m\alpha_l} \frac{1}{\sqrt{h_{\alpha_m}}} e^{ik_{1x}(x_i-x_l)+ik_{2x}(x_j-x_l)} S_l + 2\bar{S}_x^i(t)\bar{S}_x^j(t_3)/S,
\end{aligned} \tag{S45}$$

where $M_{k_x} \equiv M_{\vec{k}=(k_x,0,\ldots,0)}$, and

$$\bar{S}_x^j(t) = \sum_{\vec{r}_{j\perp}\in\mathcal{T}_\perp} \bar{S}^j(t) = \sum_{\langle nS\rangle} \int_{k_x} [e^{M_{k_x} t}]_{\alpha_j\alpha_n} e^{ik_x(x_j-x_n)} 2\sqrt{h_j h_n} S. \tag{S46}$$

We now need to sum over x_i, x_j satisfying restrictions defined in Eq. (S44). Notice that all such (x_i,x_j) satisfy $|x_i - x_j| = L-1$. It turns out to be more convenient to extend the summation to all (x_i,x_j) satisfying $|x_i - x_j| = L-1$. This still gives an upper bound since the rhs of Eq. (S42) is always non-negative. We let $x_j = x_i \pm (L-1)$ and sum over x_i from $-\infty$ to ∞:

$$\begin{aligned}
\sum_{(i,j)\in\mathcal{S}} \|\boldsymbol{h}_i e^{i\mathbf{H}_2(t_4-t_3)} \boldsymbol{h}_j e^{i\mathbf{H}_1 t_3}(\hat{S})\| \;&\le\; 2 \sum_{\substack{\alpha_m,\alpha_i,\alpha_j,l\\ a=1,2\\ \Delta x=\pm(L-1)}} \sqrt{h_{\alpha_i} h_{\alpha_j}} \int_{t_{1,2},k_x} [M_{-k_x}^{3-a} e^{M_{-k_x}(t_4-t_3+t_2-t_1)}]_{\alpha_i\alpha_m} [M_{k_x}^{a} e^{M_{k_x}(t_2-t_1)}]_{\alpha_j\alpha_m} \\
&\quad \times [e^{M_0 t_1}]_{\alpha_m\alpha_l} \frac{1}{\sqrt{h_{\alpha_m}}} e^{ik_x\Delta x} S_l + \sum_{(i,j)\in\mathcal{S}/\mathcal{T}_\perp} 2\bar{S}_x^i(t_4)\bar{S}_x^j(t_3)/S.
\end{aligned} \tag{S47}$$

This is the bound for the $j=1$ term in Eq. (S26). Those $j>1$ terms in Eq. (S26) can be treated in an almost identical way; the only difference is that since the directions $L_1,\dots,L_{j-1}$ are now periodic, the integrals over $\vec{k}$ in those $j-1$ directions have to be replaced by a discrete sum, $k_m \in \{\frac{2\pi n}{L_m}|n=0,1,\dots,L_m-1\}, 1\le m\le j-1$. The result, however, remains completely the same as Eq. (S47). In summary, we have

$$\begin{aligned}|\delta\langle\hat{S}(t)\rangle_{L_1\times\ldots\times L_d}| \;\le\; & 4\sum_{\substack{\alpha_m,\alpha_i,\alpha_j,l\\1\le p\le d,a=1,2\\\Delta x_p=\pm(L_p-1)}}\sqrt{h_{\alpha_i}h_{\alpha_j}}\int_{t_{1,2,3,4},k_p}[M^{3-a}_{-k_p}e^{M_{-k_p}(t_4-t_3+t_2-t_1)}]_{\alpha_i\alpha_m}[M^a_{k_p}e^{M_{k_p}(t_2-t_1)}]_{\alpha_j\alpha_m}\\ & \times[e^{M_0t_1}]_{\alpha_m\alpha_l}\frac{1}{\sqrt{h_{\alpha_m}}}e^{ik_p\Delta x_p}S_l+4\sum_{\substack{(i,j)\in\mathcal{S}_p\\1\le p\le d}}\int_{t_{3,4}}\bar{S}^i_p(t_4)\bar{S}^j_p(t_3)/S,\end{aligned}\tag{S48}$$

where the time integrations are restricted to $0<t_1<t_2<t_3<t_4<t$. We now use the same derivation in Eq. (28) of Ref. [2] to upper bound the k integral by its analytic continuation to $i\kappa$. We focus on the first term, since the second term can be treated in a similar way. We have

$$\begin{aligned}|\delta\langle\hat{S}(t)\rangle_{L_1\times\ldots\times L_d}| \;\le\; & 4\sum_{\substack{\alpha_m,\alpha_i,\alpha_j,l\\1\le p\le d,a=1,2}}\sqrt{h_{\alpha_i}h_{\alpha_j}}\int_{t_{1,2,3,4}}\{[M^{3-a}_{i\kappa_p}e^{M_{i\kappa_p}(t_4-t_3+t_2-t_1)}]_{\alpha_m\alpha_i}[M^a_{i\kappa_p}e^{M_{i\kappa_p}(t_2-t_1)}]_{\alpha_j\alpha_m}+(\kappa_p\to-\kappa_p)\}\\ & \times[e^{M_0t_1}]_{\alpha_m\alpha_l}\frac{1}{\sqrt{h_{\alpha_m}}}e^{-\kappa_p(L_p-1)}S_l+(\text{Term 2})\end{aligned}\tag{S49}$$

$$\begin{aligned}\le\; & 4\sum_{\substack{\alpha_i,\alpha_j,l\\1\le p\le d,a=1,2}}\sqrt{h_{\alpha_i}h_{\alpha_j}}\int_{t_{1,2,3,4}}\{[M^a_{i\kappa_p}e^{M_{i\kappa_p}(t_2-t_1)}DM^{3-a}_{i\kappa_p}e^{M_{i\kappa_p}(t_4-t_3+t_2-t_1)}]_{\alpha_j\alpha_i}+(\kappa_p\to-\kappa_p)\}\\ & \times\|e^{M_0t_1}\|e^{-\kappa_p(L_p-1)}S_l+(\text{Term 2})\\ \le\; & 8\sum_{1\le p\le d}c_Hc_Sc_{\kappa_p}\int_{t_{1,2,3,4}}\omega^3_{i\kappa_p}e^{\omega_{i\kappa_p}(t_4-t_3+2t_2-2t_1)+\omega_0t_1-\kappa_p(L_p-1)}+(\text{Term 2})\\ \le\; & 2\sum_{1\le p\le d}c_Hc_Sc_{\kappa_p}\frac{e^{2\omega_{i\kappa_p}t-\kappa_p(L-1)}}{2\omega_{i\kappa_p}-\omega_0}+(\text{Term 2}),\end{aligned}\tag{S50}$$

where $D=\text{diag}\{\frac{1}{\sqrt{h_{\alpha_m}}}\}$, $c_H=\sum_{\alpha_i}h_{\alpha_i}$, $c_S=\sum_{\langle lS\rangle}2\sqrt{h_l}S$, $c_{\kappa_p}=\|U_{i\kappa_p}\|\|U^{-1}_{i\kappa_p}\|\|U^{-1}_{i\kappa_p}DU_{i\kappa_p}\|+(\kappa_p\to-\kappa_p)$, $\omega_{i\kappa_p}$ is the Perron-Frobenius eigenvalue of $M_{i\kappa_p}$ (i.e. the eigenvalue with the largest magnitude; this must be real and positive by the Perron-Frobenius theorem), and $U_{i\kappa_p}$ is the matrix that diagonalizes $M_{i\kappa_p}$, i.e. $M_{i\kappa_p}=U_{i\kappa_p}\Omega_{i\kappa_p}U^{-1}_{i\kappa_p}$ for some diagonal matrix $\Omega_{i\kappa_p}$. In the third line we use Cauchy-Schwarz inequality $\sum_{i,j}\sqrt{h_i}C_{ij}\sqrt{h_j}\le\sum_i h_i\|C\|$. Combined with the second term, the final result is

$$|\delta\langle\hat{S}(t)\rangle_{L_1\times\ldots\times L_d}|\le\sum_{1\le p\le d}C_{\kappa_p}e^{2\omega_{i\kappa_p}t-\kappa_p(L-1)},\tag{S51}$$

where

$$C_{\kappa_p}=2\frac{c_Hc_Sc_{\kappa_p}}{2\omega_{i\kappa_p}-\omega_0}+8Sc_H\frac{\|U_{i\kappa_p}\|^2\|U^{-1}_{i\kappa_p}\|^2}{\omega^2_{i\kappa_p}}s_{\kappa_p}s_{-\kappa_p},\quad s_{\kappa_p}=\sqrt{\sum_{\langle lS\rangle}h_le^{2\vec{\kappa}_p\cdot(\vec{r}_l-\vec{r}_s)}}.\tag{S52}$$

Notice that $\omega_{i\kappa_p}$ means $\omega_{i\vec{\kappa}_p}$ where the only nonzero component of $\vec{\kappa}_p$ is in the p-th direction equal to κ_p.

With Eq. (S51) we are ready to derive the bound in Eq. (6). The arguments in Sec. IV of Ref. [2] can be generalized to prove the following

Proposition 1. *Let $f(t)$ be a function with Taylor expansion $f(t)=\sum_{n\ge m}f_nt^n$, where m is a positive integer and $f_n\ge0,\forall n\ge m$. If $f(l/v)\le C$, then $f(t)\le C(vt/l)^m$, for $0\le t\le l/v$.*

Now take $f(t)=|\langle\hat{S}(t)\rangle_{\mathcal{C}_{p-1}}-\langle\hat{S}(t)\rangle_{\mathcal{C}_p}|$. Eq. (S51) proves that $f(\frac{L_p}{2v_p})\le C_{\kappa_{p0}}e^{\kappa_{p0}}$ (one has to redo the above derivations for each direction separately), where

$$v_p=\min_{\kappa_p>0}\frac{\omega_{i\kappa_p}}{\kappa_p}\tag{S53}$$

is the LR speed in the p-th direction, and κ_{p0} is the position of the minimum. On the other hand, using the Taylor expansion of $G_{ij}(t)$ in Eq. (S31), one can show that the upper bound for $f(t)$ given in Eqs. (S39) and (S43) has a Taylor series expansion with the same leading term as the Chen-Lucas bound in Eq. (S20) and with non-negative coefficients, i.e. $f(t) = \sum_{n\geq m} f_n t^n$ where $f_n \geq 0$, and $m = \min n_p(Y_S) - 1$ is the number of Hamiltonian terms of the smallest Y-shape starting from S that is L_p-cell unembeddable in the p-th direction. Therefore, Proposition 1 says

$$|\langle \hat{S}(t)\rangle_{\mathcal{C}_0} - \langle \hat{S}(t)\rangle_{\mathcal{C}_1}| \leq C_{\kappa_{p0}} e^{\kappa_{p0}} \left(\frac{2v_p t}{L_p}\right)^{\min n_p(Y_S)-1}. \tag{S54}$$

In summary, we have

$$|\delta\langle \hat{S}(t)\rangle_{L_1\times\ldots\times L_d}| \leq \sum_{1\leq p\leq d} C_p \left(\frac{2v_p t}{L_p}\right)^{\mathcal{L}_p}, \tag{S55}$$

where $C_p \equiv C_{\kappa_{p0}} e^{\kappa_{p0}}$ and $\mathcal{L}_p \equiv \min n_p(Y_S) - 1$. In general, the exponent $\mathcal{L}_p$ is linearly related to L_p, i.e. $\mathcal{L}_p = \eta_p L_p - \mu_{p,S}$. This finishes the proof of Eq. (6).

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