1 Represent $\alpha_{S,d}$ in tensor network

Connect the beginning part with the previous text.

In this section, we represent the variance of Fermionic classical shadow in the form of a tensor network. The variance is bounded by $1/\alpha_{S,d}$, where

$$\alpha_{S,d} = \int_{Q\sim O_d} \mathrm{d}\mu(Q) \left| \langle 0| U_Q \gamma_S U_Q^\dagger |0\rangle \right|^2 \tag{1}$$

$$= \int_{Q\sim O_d} \mathrm{d}\mu(Q) \langle 0| U_Q \gamma_S U_Q^\dagger |0\rangle \langle 0| U_Q \gamma_S^\dagger U_Q^\dagger |0\rangle . \tag{2}$$

The subscript d denotes the layer number of the matchgate circuit. The expression could be simplified by substituting the relationship between $\gamma_S^\dagger$ and γ_S, which is

$$\gamma_S^\dagger = (-1)^{\frac{|S|(|S|-1)}{2}} \gamma_S. \tag{3}$$

The relation is true because of the anti-commutation relation of Majorana operators $\{\gamma_i, \gamma_j\} = 2\delta_{ij}$. The anti-commutation relation produces a coefficient of $(-1)^{|S|-1}$ when γ_{l_1} is moved to the first place. Then, the $\gamma_S^\dagger$ could be calculated by

$$\gamma_S^\dagger =(-1)^{|S|-1} \gamma_{l_1}\gamma_{l_{|S|}}\gamma_{l_{|S|-1}}\cdots\gamma_{l_2} \tag{4}$$

$$=(-1)^{|S|-1+|S|-2} \gamma_{l_1}\gamma_{l_2}\gamma_{l_{|S|}}\gamma_{l_{|S|-1}}\cdots\gamma_{l_3} \tag{5}$$

$$=(-1)^{\frac{|S|(|S|-1)}{2}} \gamma_S. \tag{6}$$

By substituting Eq. 6, the $\alpha_{S,d}$ could be expressed as

$$\alpha_{S,d} =(-1)^{\frac{|S|(|S|-1)}{2}} \int_{Q\sim O_d} \mathrm{d}\mu(Q) \langle 0| U_Q \gamma_S U_Q^\dagger |0\rangle^2 \tag{7}$$

$$=(-1)^{\frac{|S|(|S|-1)}{2}} \int_{Q\sim O_d} \mathrm{d}\mu(Q) \operatorname{tr}\Big(U_Q \gamma_S U_Q^\dagger |0\rangle\langle 0| \Big)^2 \tag{8}$$

$$=(-1)^{\frac{|S|(|S|-1)}{2}} 2^{2n} \int_{Q\sim O_d} \mathrm{d}\mu(Q) \langle\langle 0,0| \mathcal{U}_Q \otimes \mathcal{U}_Q |\gamma_S,\gamma_S\rangle\rangle \tag{9}$$

$$=(-1)^{\frac{|S|(|S|-1)}{2}} 2^{2n} \langle\langle 0,0| \int_{Q\sim O_d} \mathrm{d}\mu(Q) \mathcal{U}_Q^{\otimes 2} |\gamma_S,\gamma_S\rangle\rangle. \tag{10}$$

In the third line, we rewrite the formula regarding super vectors and super operators. The integral of the form $\int \mathrm{d}\mu(Q)\mathcal{U}_Q^{\otimes k}$ is known as the twirling. Sometimes we will use the terminology *twirling* for simplification.

The d-layers matchgate circuit is composed of interweaving stacking two-qubits matchgates. Thus, to calculate the integral $\int_{Q\sim O_d} \mathrm{d}\mu(Q)\mathcal{U}_Q^{\otimes 2}$, we could independently calculate the integral of each 2 qubits matchgates. The result of the integral of the 2 qubits matchgates is given by Lemma 1

$$\int_{Q\sim M_2} \mathrm{d}\mu(Q)\mathcal{U}_Q^{\otimes 2} =|\gamma_\emptyset\rangle\rangle|\gamma_\emptyset\rangle\rangle\langle\langle\gamma_\emptyset|\langle\langle\gamma_\emptyset| + \frac{1}{4}\sum_{i,j} |\gamma_i\rangle\rangle|\gamma_i\rangle\rangle\langle\langle\gamma_j|\langle\langle\gamma_j| \tag{11}$$

$$+ \frac{1}{6}\sum_{\substack{i_1\neq i_2\\ j_1\neq j_2}} |\gamma_{i_1}\gamma_{i_2}\rangle\rangle|\gamma_{i_1}\gamma_{i_2}\rangle\rangle\langle\langle\gamma_{j_1}\gamma_{j_2}|\langle\langle\gamma_{j_1}\gamma_{j_2}| \tag{12}$$

$$+ \frac{1}{4}\sum_{\substack{i_1\neq i_2, j_1\neq j_2\\ i_1\neq i_3, j_1\neq j_3\\ i_2\neq i_3, j_2\neq j_3}} |\gamma_{i_1}\gamma_{i_2}\gamma_{i_3}\rangle\rangle|\gamma_{i_1}\gamma_{i_2}\gamma_{i_3}\rangle\rangle\langle\langle\gamma_{j_1}\gamma_{j_2}\gamma_{j_3}|\langle\langle\gamma_{j_1}\gamma_{j_2}\gamma_{j_3}| \tag{13}$$

$$+ |\gamma_1\gamma_2\gamma_3\gamma_4\rangle\rangle|\gamma_1\gamma_2\gamma_3\gamma_4\rangle\rangle\langle\langle\gamma_1\gamma_2\gamma_3\gamma_4|\langle\langle\gamma_1\gamma_2\gamma_3\gamma_4|, \tag{14}$$

where i, j are index ranged from 1 to 4.

To calculate the interweaving stacking of two-qubits matchgates, we represent the super vectors $|\gamma_S\rangle\rangle$ using the Pauli basis through the Jordan-Wigner transformation. Due to the transformation, the γ_S is corresponded to a Pauli basis with a phase $\pm \mathrm{i}^{\lfloor |S|/2 \rfloor}$. Thus, the super vector $|\gamma_S, \gamma_S\rangle\rangle$ could be represented as

$$|\gamma_S, \gamma_S\rangle\rangle = (-1)^{\lfloor \frac{|S|}{2} \rfloor} |P^S, P^S\rangle\rangle, \tag{15}$$

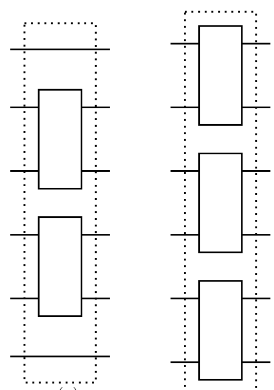
where P^S is the Pauli operator that corresponding to the γ_S. Therefore, due to the Lemma 2, the net phase of the $\alpha_{S,d}$ is 1.

We also represent the integral of the 2 qubits matchgates with Pauli basis by applying Jordan-Wigner transformation to Eq. 11. Denote the twirling as a 4-bond tensor as the following rule,

$$T^{\sigma_1,\sigma_2}_{\sigma_3,\sigma_4} = \langle\langle \sigma_1, \sigma_2 | \langle\langle \sigma_1, \sigma_2 | \int_{Q\sim M_2} \mathrm{d}\mu(Q) \mathcal{U}_Q^{\otimes 2} | \sigma_3, \sigma_4 \rangle\rangle | \sigma_3, \sigma_4 \rangle\rangle, \tag{16}$$

where $\sigma_1, \sigma_2, \sigma_3, \sigma_4$ are two-qubits Pauli operators. The concrete elements of the tensor T is shown in the Table 1. For example, due to Eq. 11 and Eq. 16, T^{XY}_{YZ} is equal to $\frac{1}{6}$.

To build the tensor network, we will define some notation. Let $T^{(o)}$ represent the odd-layer of T gates, and $T^{(e)}$ represent the even-layer of T gates, which are shown in the following circuits.



The whole tensor network $T^{(\mathrm{whole})}$ could be expressed by alternately apply $T^{(o)}$ and $T^{(e)}$ gates,

$$T^{(\mathrm{whole})}(t, b_1, b_2) = {T^{(o)}}^{b_2} \left(\prod_{i=0}^{t} T^{(e)} T^{(o)} \right) {T^{(e)}}^{b_1}, \tag{17}$$

where $b_1, b_2 \in \{0, 1\}$, $t + b_1 + b_2$ stands for the number of layers.

The calculation of $\alpha_{S,d}$ could be represented by the tensor network contraction. Notice the matrix identity

$$|0\rangle\langle 0| = \frac{1}{2^n} \sum_{\Lambda \subset [2n]} \prod_{i\in\Lambda} Z_i, \tag{18}$$

where Z_i denotes the application of the Pauli Z operator to the i-th qubit. Specially, let $\prod_{i\in\emptyset} Z_i = \mathbb{I}_n$. Then, the super vector of $|0, 0\rangle\rangle$ could be expressed as

$$|0, 0\rangle\rangle = \frac{1}{2^{2n}} \sum_{\Lambda, \Lambda' \subset [2n]} |\prod_{i\in\Lambda} Z_i, \prod_{j\in\Lambda'} Z_j\rangle\rangle. \tag{19}$$

By transforming all the super vectors and the super operators in the Pauli basis, the evolution of $\mathcal{U}_Q|\gamma_S\rangle\rangle$ could be equivalently expressed by

$$\int \mathrm{d}\mu(Q) \mathcal{U}_Q^{\otimes 2} |\gamma_S, \gamma_S\rangle\rangle = T^{(\mathrm{whole})} |P^S\rangle\rangle. \tag{20}$$

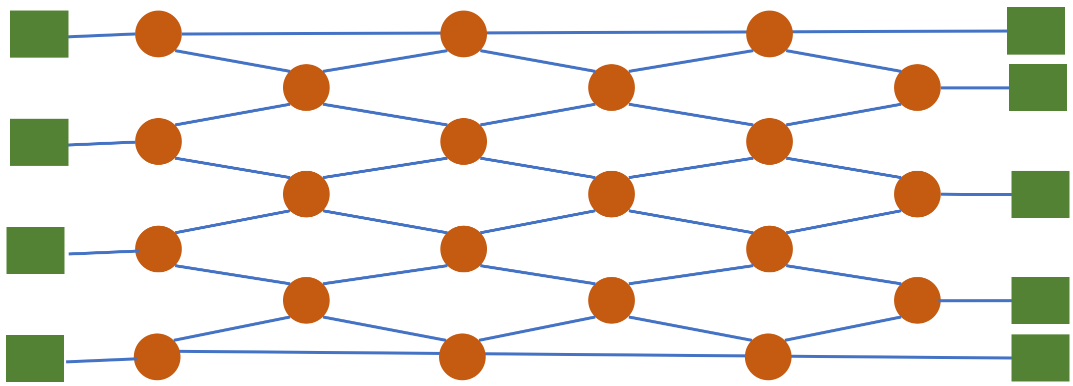


Figure 1: Tensor network representation of the twirled d-layers matchgate circuit.

In the equation, for simplicity, we slightly abuse the notation $|P^S\rangle\rangle$ to represent the tensor of Pauli basis $|P^S, P^S\rangle\rangle$. Formally, $|P^S\rangle\rangle$ is the tensor δ_S^R, where $\delta_S^R = 1$ if and only if $R = S$, otherwise, $\delta_S^R = 0$. In this representation, The tensor contraction $T^{(\text{whole})}(t, b_1, b_2)P^S$ is equivalent to the evolution $\int \mathrm{d}\mu(Q)\mathcal{U}_Q^{\otimes 2}|\gamma_S, \gamma_S\rangle\rangle$. Thus, the calculation of $\alpha_{S,d}$ could be expressed as the tensor network contraction, as illustrated in Fig. 1. polish the figure

Lemma 1 (Theorem 1 in [1])**.** *Let Q be a matrix uniformly randomly sampled from orthogonal group $\mathcal{O}(n)$, then*

$$\int_{Q\sim M_n} \mathrm{d}\mu(Q)\mathcal{U}_Q = |\mathbb{I}\rangle\rangle\langle\langle\mathbb{I}| \tag{21}$$

$$\int_{Q\sim M_n} \mathrm{d}\mu(Q)\mathcal{U}_Q^{\otimes 2} = \sum_{k=0}^{2n} |\mathcal{R}_k^{(2)}\rangle\rangle\langle\langle\mathcal{R}_k^{(2)}| \tag{22}$$

$$\int_{Q\sim M_n} \mathrm{d}\mu(Q)\mathcal{U}_Q^{\otimes 3} = \sum_{\substack{k_1,k_2,k_3\geq 0\\ k_1+k_2+k_3\leq 2n}} |\mathcal{R}_{k_1,k_2,k_3}^{(3)}\rangle\rangle\langle\langle\mathcal{R}_{k_1,k_2,k_3}^{(3)}|. \tag{23}$$

where

$$|\mathcal{R}_k^{(2)}\rangle\rangle = \binom{2n}{k}^{-1/2} \sum_{S\subseteq[2n],|S|=k} |\gamma_S\rangle\rangle|\gamma_S\rangle\rangle \tag{24}$$

$$|\mathcal{R}_k^{(3)}\rangle\rangle = \binom{2n}{k_1, k_2, k_3, 2n-k_1-k_2-k_3}^{-1/2} \sum_{\substack{S_1,S_2,S_3\subseteq[2n] disjoint\\ |S_j|=k_j, 1\leq j\leq 3}} |\gamma_{S_1}\gamma_{S_2}\rangle\rangle|\gamma_{S_2}\gamma_{S_3}\rangle\rangle|\gamma_{S_3}\gamma_{S_1}\rangle\rangle \tag{25}$$

Lemma 2. *The net phase of $\alpha_{S,d}$ is 1.*

Proof. The net phase of $\alpha_{S,d}$ is 1 is $(-1)^{\frac{|S|(|S|-1)}{2}}(-1)^{\lfloor |S|/2\rfloor}$. We categorize the discussion of the parity of $|S|$.

1. $|S|$ **is an odd number.** Let $|S| = 2q+1$, $q \in \mathbb{N}$, $q \geq 0$. And then

$$(-1)^{\frac{|S|(|S|-1)}{2}}(-1)^{\lfloor |S|/2\rfloor} = (-1)^{q(2q+1)+q} = 1. \tag{26}$$

2. $|S|$ **is an even number.** Let $|S| = 2q$, $q \in \mathbb{N}$, $q \geq 0$. And then

$$(-1)^{\frac{|S|(|S|-1)}{2}}(-1)^{\lfloor |S|/2\rfloor} = (-1)^{(2q-1)q+q} = 1. \tag{27}$$

□

T	II	IX	IY	IZ	XI	XX	XY	XZ	YI	YX	YY	YZ	ZI	ZX	ZY	ZZ
II	1															
IX		1/4	1/4					1/4				1/4				
IY		1/4	1/4					1/4				1/4				
IZ				1/6		1/6	1/6			1/6	1/6		1/6			
XI					1/4				1/4					1/4	1/4	
XX				1/6		1/6	1/6			1/6	1/6		1/6			
XY				1/6		1/6	1/6			1/6	1/6		1/6			
XZ		1/4	1/4					1/4				1/4				
YI					1/4				1/4					1/4	1/4	
YX				1/6		1/6	1/6			1/6	1/6		1/6			
YY				1/6		1/6	1/6			1/6	1/6		1/6			
YZ		1/4	1/4					1/4				1/4				
ZI				1/6		1/6	1/6			1/6	1/6		1/6			
ZX					1/4				1/4					1/4	1/4	
ZY					1/4				1/4					1/4	1/4	
ZZ																1

Table 1: Values of tensor T. The head of columns represents the input of T while the head of rows represents the output of T. For example, the value in row 'XY' and column 'YZ' represent the value $T^{XY}_{\ \ \ YZ}$. The blank space of the table stands for 0.

2 Simplify the tensor contraction for the case $|S| = 2$

We have changed the evaluation of the variance to focus on the tensor contraction of $\alpha_{S,d}$. Our main goal is to analyze how the order of $\alpha_{S,d}$ varies with the number of layers. However, estimating this order using tensor network contraction is challenging. Therefore, we will examine a specific case where $|S| = 2$, which is the smallest non-trivial scenario. This simplification allows us to streamline the calculation of contraction and map the calculation to a different model.

The evolution of $\mathcal{U}_Q|\gamma_S\rangle\rangle$ is limited to a subspace of the whole Hilbert space because the matchgate circuit conserves the cardinal number $|S|$. Thus, due to Eq. 20, the results of tensor contraction should obey the cardinal conservation as well

$$T^{(\text{whole})}(t, b_1, b_2)|P^S\rangle\rangle = \sum_{|S'|=|S|} \xi_{S'}|P^{S'}\rangle\rangle, \tag{28}$$

where $S, S' \subset [2n]$, and $\xi_{S'}$ are real coefficient. Thus, its equivalent to study the tensor in the sub-representation of the space $\operatorname{span}\{\gamma_{S'} \mid |S'| = |S|\}$. This simplification can significantly reduce the complexity of the calculations.

Here, we focus on a specific circuit configuration that starts with an even-layer $T^{(e)}$ and ends with an odd-layer $T^{(o)}$, which means $b_1 = 1$ and $b_2 = 0$. The number of qubits in the circuit is set to be an even number. Additionally, the observable γ_S is restricted to $|S| = 2$. From the discussion about Eq. 28, the evolution could be restricted to the subspace $\operatorname{span}\{\gamma_i\gamma_j \mid i \neq j, 1 \leq i, j \leq 2n\}$. By Jordan-Wigner transformation, the basis $\gamma_i\gamma_j$ obtains the form

$$\begin{aligned} Z_l, \quad X_l\left(\prod_{k=l+1}^{m-1} Z_k\right)X_m, \qquad X_l\left(\prod_{k=l+1}^{m-1} Z_k\right)Y_m, \\ Y_l\left(\prod_{k=l+1}^{m-1} Z_k\right)X_m, \qquad Y_l\left(\prod_{k=l+1}^{m-1} Z_k\right)Y_m, \end{aligned} \tag{29}$$

where $1 \leq l, m \leq 2n$.

The representation $\operatorname{span}\{\gamma_i\gamma_j \mid i \neq j, 1 \leq i, j \leq 2n\}$ could be reduced to a smaller subspace. From Table 1, we found that the value of tensor $T^{X\cdot}_{\ \ \cdot\cdot}$ and $T^{Y\cdot}_{\ \ \cdot\cdot}$ are always be the same. In other words, in the output of $T^{(\text{whole})}(t, b_1, b_2)|P^S\rangle\rangle$, the basis $|\cdot, X, \cdot\rangle\rangle$ and $|\cdot, Y, \cdot\rangle\rangle$ always simultaneously appear and have the same coefficients. Let

$$M_i := \frac{1}{\sqrt{2}}(X_i + Y_i), \tag{30}$$

$$
\begin{tikzcd}
\mathrm{span}\{\gamma_i\gamma_j\} \arrow[r] \arrow[d, "T^{(\mathrm{whole})}"'] & V_P \arrow[r] \arrow[d, "T^{(\mathrm{whole})}_{V_P}"'] & \mathcal{P}_n \arrow[r] \arrow[d, "T^{(\mathrm{whole})}_{\mathcal{P}_n}"'] & \mathcal{P}_N \arrow[d, "T^{(\mathrm{whole})}_{\mathcal{P}_N}"'] \\
\mathrm{span}\{\gamma_i\gamma_j\} \arrow[r] & V_P \arrow[r] & \mathcal{P}_n \arrow[r] & \mathcal{P}_N
\end{tikzcd}
$$

Figure 2: The diagram shows how we simplify the calculation step by step. The horizontal arrows point from a high-dimensional space to a relatively low-dimensional space. The vertical arrows stand for the corresponding operators of $T^{(\mathrm{whole})}(t, b_1, b_2)$ in different representations. Finally, we reduce it to the N-elementary polynomial of the 2nd degree polynomial space.

then, the subspace

$$V_P := \mathrm{span}\{|Z_i\rangle\rangle, |M_i(\prod Z_k)M_j\rangle\rangle\} \tag{31}$$

is a sub-representation of $T^{(\mathrm{whole})}$. In more precise, group representation theory language, $T^{(e)}V_P$ is a representation of the free group with generator $T^{(e)}T^{(o)}$. We interpret $T_V^{(\mathrm{whole})}(t)(v)$ as the group element $(T_V^{(e)}T_V^{(o)})^t$ acts on the vector space $T_V^{(e)}(V)$, and $T_V^{(e)}(V) = V$ in specific cases. For simplicity, we will use informal language when there is no ambiguity. Finally, the estimation of $\alpha_{S,d}$ could be simplified to calculate the tensor contraction in the space V_P.

3 Reduce the calculation to polynomial space

We represent $T^{(\mathrm{whole})}$ using polynomial space because it provides the essential properties we require, such as multiplication and addition, which will be important for our later work.

Notice that the space V_P is isometric to the n-elementary polynomial of the 2nd degree polynomial space $\mathcal{P}_n$. The isometric could be constructed by the following

$$\begin{aligned} \phi : V_P &\to \mathcal{P}_n \\ |M_i(\prod Z_k)M_j\rangle\rangle &\mapsto x_i x_j \\ |Z_i\rangle\rangle &\mapsto x_i^2. \end{aligned} \tag{32}$$

The linear map ϕ is a homomorphism with inverse, which means it is an isometric between V_P and $\mathcal{P}_n$. The equivalent representation of $T^{(\mathrm{whole})}$ could be constructed by

$$T^{(\mathrm{whole})}_{\mathcal{P}_n}(t)(\cdot) := \phi \circ T^{(\mathrm{whole})}(t, 1, 0) \circ \phi^{-1}(\cdot). \tag{33}$$

We could also transfer the input of $T^{(\mathrm{whole})}$ to space $\mathcal{P}_n$,

$$\gamma_{ij} \longrightarrow |M_i(\prod Z_k)M_j\rangle\rangle \xrightarrow{\phi} x_i x_j. \tag{34}$$

Thus, the action of d-layer matchgate circuit on the γ_{ij} is equivalent to the action of $T^{(\mathrm{whole})}_{\mathcal{P}_n}(t)$ on the term $x_i x_j$. Due to Lemma 3, the action could be further simplify by finding a sub-representation $\mathcal{P}_N$ of representation $\mathcal{P}_n$, where N equals to $\frac{n}{2}$. Recall that n is an even number so N is an integer.

Certain hidden patterns are revealed by reducing the representation to the polynomial space $\mathcal{P}_N$. Most of the main results are been proved in the $\mathcal{P}_N$.

Lemma 3. *The space $\mathcal{P}_N$ isometric to a sub-representation of $\mathcal{P}_n$.*

Proof. Define the map ϕ as

$$\begin{aligned} \phi : \mathcal{P}_N &\to \mathcal{P}_n \\ y_i^2 &\mapsto x_{2i-1}^2 + 4x_{2i-1}x_{2i} + x_{2i}^2 \\ y_i y_j &\mapsto \left(x_{2i-1} + x_{2i}\right)\left(x_{2j-1} + x_{2j}\right). \end{aligned} \tag{35}$$

We define the ϕ as a linear function so that the definition of mapping on a basis induces the mapping on any element of the space

$$\phi(\sum \xi_{ij} y_i y_j) = \sum \xi_{ij} \phi(y_i y_j). \tag{36}$$

Thus, the space $\phi(\mathcal{P}_N)$ is a linear subspace of $\mathcal{P}_n$. Because ϕ is an injection, there is a map $\phi' : \mathcal{P}_n \to \mathcal{P}_N$ such that $\phi' \circ \phi$ is identity. Define the group action $T_{\mathcal{P}_N}^{(\text{whole})}$ as

$$T_{\mathcal{P}_N}^{(\text{whole})}(y_i y_j) := \phi' \circ T_{\mathcal{P}_n}^{(\text{whole})} \circ \phi(y_i y_j). \tag{37}$$

Based on the definition of representation, we know that the space $\mathcal{P}_N$ with the group action $T_{\mathcal{P}_N}^{(\text{whole})}$ is a representation.

The next step is to show that such a representation $T_{\mathcal{P}_N}^{(\text{whole})}$ does not lose information. Formally, we need to prove that the representation $\mathcal{P}_n$ could be reduced to a sub-representation isometrics to $\mathcal{P}_N$. Naturally, we will consider whether the subspace $\phi(\mathcal{P}_N)$ will constitute a sub-representation. If it is true, the proof is done because $\phi(\mathcal{P}_N) \simeq \mathcal{P}_N$.

By the definition of sub-representation, we need to prove

$$T_{\mathcal{P}_n}^{(\text{whole})}(t)(\phi(\mathcal{P}_N)) \subset \phi(\mathcal{P}_N), \quad \forall t. \tag{38}$$

The readers may recall that the formal representation is $T_{\mathcal{P}_n}^{(e)}\phi(\mathcal{P}_N)$ rather than $\phi(\mathcal{P}_N)$. Here, we remove the ambiguity by proving $T_{\mathcal{P}_n}^{(e)}\phi(\mathcal{P}_N) = \phi(\mathcal{P}_N)$. By expanding the definition of $T_{\mathcal{P}_n}^{(e)}$, we could get the calculation of $T_{\mathcal{P}_n}^{(e)}\phi(y_i y_j)$ backs to the space V_P. Then, we will find that $T_{\mathcal{P}_n}^{(e)}\phi(y_i y_j) = \phi(y_i y_j)$ from the Table 1. Thus, we have $T_{\mathcal{P}_n}^{(e)}\phi(\mathcal{P}_N) = \phi(\mathcal{P}_N)$.

The statement 38 will be proved by induction.

When $t = 0$, $T_{\mathcal{P}_n}^{(e)}\phi(\mathcal{P}_N) \subset \phi(\mathcal{P}_N)$ is true. Suppose the statement is true for t^*, then we have

$$T_{\mathcal{P}_n}^{(\text{whole})}(t^*)(\phi(y_i y_j)) = \sum \xi_{lm} \phi(y_l y_m). \tag{39}$$

And then

$$T_{\mathcal{P}_n}^{(\text{whole})}(t^* + 1)(\phi(y_i y_j)) = T_{\mathcal{P}_n}^{(e)} T_{\mathcal{P}_n}^{(o)}(\sum \xi_{lm} \phi(y_l y_m)) \tag{40}$$

$$= \sum \xi_{lm} \delta_{lm} T_{\mathcal{P}_n}^{(e)} T_{\mathcal{P}_n}^{(o)}(x_{2i-1}^2 + 4x_{2i-1}x_{2i} + x_{2i}^2) \tag{41}$$

$$+ \sum \xi_{lm}(1 - \delta_{lm}) T_{\mathcal{P}_n}^{(e)} T_{\mathcal{P}_n}^{(o)}\left(\left(x_{2i-1} + x_{2i}\right)\left(x_{2j-1} + x_{2j}\right)\right) \tag{42}$$

We will prove Eq. 41 is in the space $\phi(\mathcal{P}_N)$, while the same result of Eq. 42 can be proved by the same method.

Now, we will directly calculate this expression

$$\begin{aligned}
&T^{(e)}_{\mathcal{P}_n}T^{(o)}_{\mathcal{P}_n}(x^2_{2i-1}+4x_{2i-1}x_{2i}+x^2_{2i})\\
=&T^{(e)}_{\mathcal{P}_n}(\frac{1}{6}x^2_{2i-2}+\frac{2}{3}x_{2i-2}x_{2i-1}+x_{2i-2}x_{2i}+x_{2i-2}x_{2i+1}\\
&+\frac{1}{6}x^2_{2i-1}+x_{2i-1}x_{2i}+x_{2i-1}x_{2i+1}\\
&+\frac{1}{6}x^2_{2i}+\frac{2}{3}x_{2i}x_{2i+1}+\frac{1}{6}x^2_{2i+1})\\
=&\frac{1}{36}x^2_{2i-3}+\frac{1}{9}x_{2i-3}x_{2i-2}+\frac{5}{12}x_{2i-3}x_{2i-1}+\frac{5}{12}x_{2i-3}x_{2i}+\frac{1}{4}x_{2i-3}x_{2i+1}+\frac{1}{4}x_{2i-3}x_{2i+2}\\
&+\frac{1}{36}x^2_{2i-2}+\frac{5}{12}x_{2i-2}x_{2i-1}+\frac{5}{12}x_{2i-2}x_{2i}+\frac{1}{4}x_{2i-2}x_{2i+1}+\frac{1}{4}x_{2i-2}x_{2i+2}\\
&+\frac{2}{9}x^2_{2i-1}+\frac{8}{9}x_{2i-1}x_{2i}+\frac{5}{12}x_{2i-1}x_{2i+1}+\frac{5}{12}x_{2i-1}x_{2i+2}\\
&+\frac{2}{9}x^2_{2i}+\frac{5}{12}x_{2i}x_{2i+1}+\frac{5}{12}x_{2i}x_{2i+2}\\
&+\frac{1}{36}x^2_{2i+1}+\frac{1}{9}x_{2i+1}x_{2i+2}\\
&+\frac{1}{36}x^2_{2i+2}
\end{aligned} \tag{43}$$

The result expression is in $\phi(\mathcal{P}_N)$ because we could find a polynomial y in $\mathcal{P}_N$ such that $\phi(y)$ equals the result expression,

$$y=\frac{1}{6}y^2_{i-1}+\frac{5}{3}y_{i-1}y_i+y_{i-1}y_{i+1}+\frac{4}{3}y^2_i+\frac{5}{3}y_{i-1}y_{i+1}+\frac{1}{6}y^2_{i+1} \tag{44}$$

$$\phi(y)=T^{(e)}_{\mathcal{P}_n}T^{(o)}_{\mathcal{P}_n}(x^2_{2i-1}+4x_{2i-1}x_{2i}+x^2_{2i}) \tag{45}$$

Thus, we get that

$$T^{(e)}_{\mathcal{P}_n}T^{(o)}_{\mathcal{P}_n}(x^2_{2i-1}+4x_{2i-1}x_{2i}+x^2_{2i})\subset\phi(\mathcal{P}_N). \tag{46}$$

Thus, Eq. 43 is contained in the space $\phi(\mathcal{P}_N)$, which completes the proof. □

4 Mapping the action of tensors to random walk

The action of layers is the lazy-symmetry random walk on a 2D square lattice in most sites. To illustrate this point, we will begin with a specific example. Considering $1<i<N-1$ and $i+1<j\leq N$, the action of $T^{(e)}_{\mathcal{P}_N}T^{(o)}_{\mathcal{P}_N}$ is

$$T^{(e)}_{\mathcal{P}_N}T^{(o)}_{\mathcal{P}_N}(y_iy_j)=\left(\frac{1}{4}y_{i-1}+\frac{1}{2}y_i+\frac{1}{4}y_{i-1}\right)\left(\frac{1}{4}y_{j-1}+\frac{1}{2}y_j+\frac{1}{4}y_{j-1}\right). \tag{47}$$

In this case, the action of $T^{(e)}_{\mathcal{P}_N}T^{(o)}_{\mathcal{P}_N}$ can be viewed as first independently evolving y_i and y_j in a one-dimensional lattice, and then combining them,

$$\begin{aligned}
y_i&\to\frac{1}{4}y_{i-1}+\frac{1}{2}y_i+\frac{1}{4}y_{i-1}\\
y_j&\to\frac{1}{4}y_{j-1}+\frac{1}{2}y_j+\frac{1}{4}y_{j-1}.
\end{aligned} \tag{48}$$

We observe that this pattern appears in most sites y_iy_j. Therefore, we can analyze the evolving behavior separately in one-dimensional polynomial space (one-dimensional lattice). Afterward, we can examine the differences between the true evolved polynomial and the combined polynomial. This approach is the skeleton of estimating the order of tensor contraction. Now, we will make the above concepts more specific and more concrete.

We introduce the lazy-symmetry random walk in polynomial space, or the one-dimensional lattice, to describe the separate evolution behavior. A lazy-symmetry random walk is a type of Markov process, which is shown in Fig. 3. In this process, consider a point located at a site y_i. In the next time interval, this point has a probability

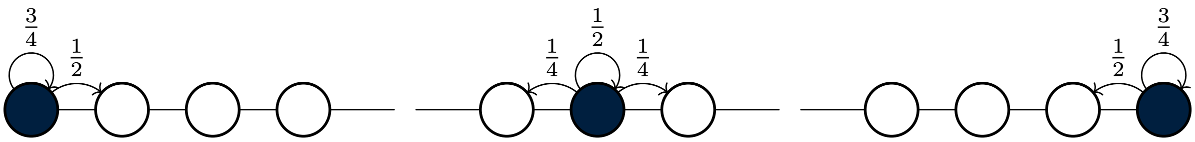


Figure 3: Cases of lazy random walk. The circles represent the sites of the lattice $\{y_1, y_2, \cdots, y_n\}$, while the black circle stands for the starting site y_i, and the numbers over arrows are transition probability.

of 0.25 moving to one of its neighboring sites y_{i-1} or y_{i+1}, and it has a probability of 0.5 staying in place. If the origin site is on the ends of the lattice, it has a probability of 0.75 staying in place and has a probability of 0.25 moving around. The probability transition relation could be expressed by

$$L(y_i) = \begin{cases} \frac{3}{4}y_1 + \frac{1}{4}y_2, & i = 1 \\ \frac{1}{4}y_{i-1} + \frac{1}{2}y_i + \frac{1}{4}y_{i+1}, & 1 < i < N \\ \frac{3}{4}y_N + \frac{1}{4}y_{N-1}, & i = N. \end{cases} \tag{49}$$

We could see that the separate evolution in Eq. 48 fits the form of lazy-symmetry random walk.

In Eq. 47, we showed the result of how $y_i y_j$ transfers in one specific situation. Now, we will show all possible results in any situation in Table 2. The table lists all the possible transition results no matter what inputs it receives. It was created in a similar way to the previous example in Eq. 43.

In Table 2, we can see that in most cases

$$T^{(e)}_{\mathcal{P}_N} T^{(o)}_{\mathcal{P}_N}(y_i y_j) = L(y_i)L(y_j) \tag{50}$$

except for the cases when $|i-j| \leq 1$. Moreover, the coefficients of remainder terms $T^{(e)}_{\mathcal{P}_N} T^{(o)}_{\mathcal{P}_N}(y_i y_j) - L(y_i)L(y_j)$ are small. Refs. [2] gives the analytical solution of lazy-symmetry random walk,

$$L^t(y_i) = \sum_{\mu} \mathcal{L}_i(\mu, t) y_\mu, \tag{51}$$

where $L^t(y_i)$ represents the outcome of random walking t steps from y_i according to the propagation rule L in Eq. 49, and the $\mathcal{L}_i(\mu, t)$ represents the probability of stopping at y_μ after t-steps random walking,

$$\mathcal{L}_i(\mu, t) = \frac{1}{N} + \frac{2}{N} \sum_{k=1}^{N-1} \cos\left(\left(\mu - \frac{1}{2}\right)\frac{\pi k}{N}\right) \cos\left(\left(i - \frac{1}{2}\right)\frac{\pi k}{N}\right) \cos^{2t}\left(\frac{\pi k}{2N}\right). \tag{52}$$

Thus, for the evolution that could be separated by $T^{(e)}_{\mathcal{P}_N} T^{(o)}_{\mathcal{P}_N}(y_i y_j) = L(y_i)L(y_j)$, we could get the analytical solution results

$$T^{(\text{whole})}_{\mathcal{P}_N}(t)(y_i y_j) = (T^{(e)}_{\mathcal{P}_N} T^{(o)}_{\mathcal{P}_N})^t (y_i y_j) \tag{53}$$
$$= L^t(y_i)L^t(y_j) + R(y_i y_j) \tag{54}$$
$$= \sum_{\mu,\nu} \left(\mathscr{L}_{ij}(\mu, \nu, t) y_\mu y_\nu + \mathscr{R}_{ij}(\mu, \nu, t) y_\mu y_\nu\right), \tag{55}$$

where

$$\mathscr{L}_{ij}(\mu, \nu, t) := \mathcal{L}_i(\mu, t)\mathcal{L}_j(\nu, t). \tag{56}$$

The R stands for the remind terms caused by the near-diagonal terms $y_i y_j$, $|i-j| \leq 1$ in Table 2.

The calculation of α could be separated into two parts. The first part is contributed by the lazy-symmetry random walk, and the second part is contributed by the remind terms. Recall that the $\alpha_{S,d}$ can be calculated by the tensor contraction of $T^{(\text{whole})}$, $|P^S\rangle\rangle$ and $|0,0\rangle\rangle$. We have mapped the $T^{(\text{whole})}$ and $|P^S\rangle\rangle$ into polynomial space.

y_iy_j	$T^{(e)}_{\mathcal{P}_N}T^{(o)}_{\mathcal{P}_N}(y_iy_j)$
$i=j=1$	$L(y_i)L(y_j)-\frac{5}{144}y_1y_1-\frac{5}{144}y_2y_2+\frac{5}{72}y_1y_2$
$1<i<N, j=i$	$L(y_i)L(y_j)-\frac{5}{144}y_{i-1}y_{i-1}+\frac{1}{36}y_{i-1}y_i+\frac{1}{24}y_{i-1}y_{i+1}-\frac{1}{36}y_iy_i+\frac{1}{36}y_iy_{i+1}-\frac{5}{144}y_{i+1}y_{i+1}$
$1\le i<N, j=i+1$	$L(y_i)L(y_j)-\frac{1}{48}y_iy_i-\frac{1}{48}y_{i+1}y_{i+1}+\frac{1}{24}y_iy_{i+1}$
$i=j=N$	$L(y_i)L(y_j)-\frac{5}{144}y_Ny_N-\frac{5}{144}y_{N-1}y_{N-1}+\frac{5}{72}y_{N-1}y_N$
other case	$L(y_i)L(y_j)$

Table 2: The transition result of $T^{(e)}_{\mathcal{P}_N}T^{(o)}_{\mathcal{P}_N}$ with input y_iy_j in different condition. Notice that $y_iy_j=y_jy_i$, the indices of the two factors i and j in term y_iy_j can always be arranged in ascending order $i\le j$.

And the $|0,0\rangle\rangle$ mapped into the polynomial space as well. Eq. 19 has transformed $|0,0\rangle\rangle$ into Pauli basis. Notice that $\langle\langle Z_i|$ is a linear function which takes a super vector to a number. Especially, it takes $|Z_i\rangle\rangle$ to 1 and takes the other Pauli basis to 0. As we known, the $|Z_i\rangle\rangle$ is mapped to x_i^2 in $\mathcal{P}_n$. The derivative operators $\frac{\partial^2}{\partial x_i^2}$ satisfy all these properties. In another word, The space of derivative operators is the dual space of polynomial space. Thus, we find the mapping from $|Z_i\rangle\rangle$ to $\mathcal{P}_n$

$$|Z_i\rangle\rangle \to \frac{\partial^2}{\partial x_i^2}. \tag{57}$$

After some algebras, we map the $|0,0\rangle\rangle$ to $\mathcal{P}_N$ when $|S|=2$

$$|0,0\rangle\rangle \to \frac{1}{2^{2n}}\frac{1}{3}\sum_{i,j}\frac{\partial^2}{\partial y_i^2}. \tag{58}$$

Thus, the $\alpha_{S,2t+1}$ could be expressed as

$$\alpha_{\{\gamma_i\gamma_j\},2t+1}=\frac{1}{3}\sum_{\mu}\frac{\partial^2}{\partial y_\mu^2}T^{(\text{whole})}_{\mathcal{P}_N}(t)(y_iy_j). \tag{59}$$

Then, we could calculate $\alpha_{S,d}$ in $\mathcal{P}_N$ via combining Eq. 55

$$\alpha_{\{\gamma_i\gamma_j\},2t+1} =\frac{1}{3}\sum_{\mu}\mathscr{L}_{ij}(\mu,\mu,t)+\frac{1}{3}\sum_{\mu}\mathscr{R}_{ij}(\mu,\mu,t) \tag{60}$$

$$=: \alpha^{\mathscr{L}}_{\{\gamma_i\gamma_j\},2t+1}+\alpha^{\mathscr{R}}_{\{\gamma_i\gamma_j\},2t+1}. \tag{61}$$

5 Estimate the order of $\alpha^{\mathscr{L}}_{\{\gamma_i\gamma_j\},2t+1}$

We have separated the calculation of $\alpha_{\{\gamma_i\gamma_j\},2t+1}$ into two parts in Sec. 4. In this section, we aim to estimate the order of the first part, $\alpha^{\mathscr{L}}_{\{\gamma_i\gamma_j\},2t+1}$.

Theorem 1. *The $\alpha^{\mathscr{L}}_{\{\gamma_i\gamma_j\},2t+1}$ could be estimated by the following formula*

$$3\alpha^{\mathscr{L}}_{\{\gamma_i\gamma_j\},2t+1}=\frac{N}{\sqrt{2\pi t}}(e^{-\frac{a^2}{2t}}+e^{-\frac{b^2}{2t}})+\frac{2N}{\sqrt{2\pi t}}(e^{-\frac{a^2+2N(N-a)}{2t}}+e^{-\frac{b^2+2N(N-b)}{2t}})+\mathcal{O}\left(e^{-\frac{\pi^2}{2}t}\right), \tag{62}$$

where a is defined as $|i-j|$ and b is defined as $i+j-1$.

Proof. By Lemma 4, we could simplify the expression of $\alpha^{\mathscr{L}}_{\{\gamma_i\gamma_j\},2t+1}$ into Eq. 68. Then, we absorb the $k=0$ into the summation

$$
\begin{aligned}
3\alpha^{\mathscr{L}}_{\{\gamma_i\gamma_j\},2t+1} &= \frac{1}{N} + \frac{1}{N}\sum_{k=1}^{N-1}\left[\cos\left((i-j)\frac{k\pi}{N}\right) + \cos\left((i+j-1)\frac{k\pi}{N}\right)\right]\cos^{4t}\left(\frac{\pi k}{2N}\right) \\
&= -\frac{1}{N} + \frac{1}{N}\sum_{k=0}^{N-1}\left[\cos\left((i-j)\frac{k\pi}{N}\right) + \cos\left((i+j-1)\frac{k\pi}{N}\right)\right]\cos^{4t}\left(\frac{\pi k}{2N}\right).
\end{aligned} \tag{63}
$$

In this way, the summation over k will go through a complete cycle/period. This will allow us to utilize some useful properties regarding trigonometric summations.

We want to express this summation as a better-handled integral for computation and analysis purposes. To achieve this, we need to take the following two steps. First, we find that directly turning this into an integral is still not easy to calculate, so we need to replace the term $\cos^{4t}\left(\frac{\pi k}{2N}\right)$ to make the integral of the whole expression easier to calculate. Secondly, we need to estimate the error of this integral approximation.

Notice that the e^{-2tx^2} is a good estimation of $\cos^{4t}(x)$

$$
\begin{aligned}
&e^{-2tx^2} - \cos^{4t}(x) \\
=&e^{-2tx^2} - e^{-2tx^2+O\left(tx^4\right)} \\
=&e^{-2tx^2}\left(1-e^{O\left(tx^4\right)}\right) \\
\sim&\mathcal{O}\left(tx^4 e^{-2tx^2}\right).
\end{aligned} \tag{64}
$$

Substitute $\cos^{4t}\left(\frac{\pi k}{2N}\right)$ with $e^{-\frac{k^2\pi^2 t}{2N^2}}$ in Eq. 76, we have

$$
3\alpha^{\mathscr{L}}_{\{\gamma_i\gamma_j\},2t+1} = -\frac{1}{N} + \frac{1}{N}\sum_{k=0}^{N-1} e^{-\frac{k^2\pi^2 t}{2N^2}}\left[\cos\left((i-j)\frac{k\pi}{N}\right) + \cos\left((i+j-1)\frac{k\pi}{N}\right)\right] + \mathcal{O}\left(e^{-\frac{\pi^2}{2}t}\right) \tag{65}
$$

$$
= -\frac{1}{N} + \frac{1}{N}\sum_{k=0}^{\infty} e^{-\frac{k^2\pi^2 t}{2N^2}}\left[\cos\left((i-j)\frac{k\pi}{N}\right) + \cos\left((i+j-1)\frac{k\pi}{N}\right)\right] + \mathcal{O}\left(e^{-\frac{\pi^2}{2}t}\right). \tag{66}
$$

In the second line, we expand the summation to infinity, and it will not introduce much of errors because

$$
\begin{aligned}
\sum_{k=N}^{\infty} e^{-\frac{k^2\pi^2 t}{2N^2}} =& e^{-\frac{\pi^2}{2}t}\sum_{k=0}^{\infty} e^{-\frac{k^2\pi^2 t}{2N^2}} \\
\leq& e^{-\frac{\pi^2}{2}t}\sum_{k=0}^{\infty} e^{-\frac{k\pi^2 t}{2N^2}} \\
=& e^{-\frac{\pi^2}{2}t}\frac{e^{\frac{\pi^2 t}{2N^2}}}{e^{\frac{\pi^2 t}{2N^2}}-1} \\
=& \mathcal{O}\left(e^{-\frac{\pi^2}{2}t}\right)
\end{aligned}
$$

Lemma 5 did the second job, which turns the summation to the integral and evaluate the errors. Then, we could calculate the summation of series in Eq. 66 via Lemma 5

$$
3\alpha^{\mathscr{L}}_{\{\gamma_i\gamma_j\},2t+1} = \frac{N}{\sqrt{2\pi t}}\left(e^{-\frac{a^2}{2t}} + e^{-\frac{b^2}{2t}}\right) + \frac{2N}{\sqrt{2\pi t}}\left(e^{-\frac{a^2+2N(N-a)}{2t}} + e^{-\frac{b^2+2N(N-b)}{2t}}\right) + \mathcal{O}\left(e^{-\frac{\pi^2}{2}t}\right), \tag{67}
$$

where a is defined as $|i-j|$ and b is defined as $i+j-1$. Here we absorb the error term given by Lemma 5 into the $\mathcal{O}\left(e^{-\frac{\pi^2}{2}t}\right)$ in Eq. 66.

□

We can therefore conclude that the value of $\alpha^{\mathscr{L}}_{\{\gamma_i\gamma_j\},2t+1}$ will be on the order of $\frac{1}{\mathrm{poly}(n)}$ if t is of the same order magnitude as a^2, $t = \Theta(a^2)$. Alternatively, if t is considered to be of lower order than a^2, as denoted by the little-o notation $t = o(a^2)$, then there exists an additional exponentially small term $e^{-\frac{a^2}{2t}}$ present in the expression for $\alpha^{\mathscr{L}}_{\{\gamma_i\gamma_j\},2t+1}$.

Lemma 4. *The expression of $\alpha^{\mathscr{L}}_{\{\gamma_i\gamma_j\},2t+1}$ could be simplified to the following form*

$$3\alpha^{\mathscr{L}}_{\{\gamma_i\gamma_j\},2t+1} = \frac{1}{N} + \frac{1}{N}\sum_k \left[\cos\left((i-j)\frac{k\pi}{N}\right) + \cos\left((i+j-1)\frac{k\pi}{N}\right)\right]\cos^{4t}\left(\frac{\pi k}{2N}\right). \tag{68}$$

Proof. The lemma will be proved by directly calculation.

$$\begin{aligned}
3\alpha^{\mathscr{L}}_{\{\gamma_i\gamma_j\},2t+1} =& \sum_\mu \left[\frac{1}{N} + \frac{2}{N}\sum_{k=1}^{N-1}\cos\left(\left(i-\frac{1}{2}\right)\frac{\pi k}{N}\right)\cos\left(\left(\mu-\frac{1}{2}\right)\frac{\pi k}{N}\right)\cos^{2t}\left(\frac{\pi k}{2N}\right)\right] \\
&\times \left[\frac{1}{N} + \frac{2}{N}\sum_{l=1}^{N-1}\cos\left(\left(j-\frac{1}{2}\right)\frac{\pi l}{N}\right)\cos\left(\left(\mu-\frac{1}{2}\right)\frac{\pi l}{N}\right)\cos^{2t}\left(\frac{\pi l}{2N}\right)\right] \\
=& 1/N + \frac{2}{N^2}\sum_k\left[\sum_\mu \cos\left(\left(\mu-\frac{1}{2}\right)\frac{\pi k}{N}\right)\right]\cos\left(\left(i-\frac{1}{2}\right)\frac{\pi k}{N}\right)\cos^{2t}\left(\frac{\pi k}{2N}\right) \qquad (69)\\
&+ \frac{2}{N^2}\sum_l\left[\sum_\mu \cos\left(\left(\mu-\frac{1}{2}\right)\frac{\pi l}{N}\right)\right]\cos\left(\left(i-\frac{1}{2}\right)\frac{\pi l}{N}\right)\cos^{2t}\left(\frac{\pi l}{2N}\right) \qquad (70)\\
&+ \frac{4}{N^2}\sum_{k,l=1}^{N-1}\sum_{\mu=1}^{N}\cos\left(\left(i-\frac{1}{2}\right)\frac{\pi k}{N}\right)\cos\left(\left(\mu-\frac{1}{2}\right)\frac{\pi k}{N}\right)\cos^{2t}\left(\frac{\pi k}{2N}\right) \\
&\times \cos\left(\left(j-\frac{1}{2}\right)\frac{\pi l}{N}\right)\cos\left(\left(\mu-\frac{1}{2}\right)\frac{\pi l}{N}\right)\cos^{2t}\left(\frac{\pi l}{2N}\right) \qquad (71)
\end{aligned}$$

Notice that the summation of cosin function is zero

$$\begin{aligned}
\sum_{\mu=1}^{N}\cos\left(\left(\mu-\frac{1}{2}\right)\frac{\pi k}{N}\right) &= -\frac{1}{2}\cos\left(\frac{1}{2}\pi(2k+1)\right)\csc\left(\frac{\pi k}{2N}\right) \\
&= \sin(k\pi)\csc\left(\frac{\pi k}{2N}\right) \\
&= 0.
\end{aligned} \tag{72}$$

Substitute this identity into Eq. 71, we could eliminate the terms in line 69 and 70.

Also, notice that

$$\begin{aligned}
&\sum_{\mu=1}^{N}\cos\left(\frac{\pi\left(\mu-\frac{1}{2}\right)i}{N}\right)\cos\left(\frac{\pi\left(\mu-\frac{1}{2}\right)j}{N}\right) \\
=&\frac{1}{2}\sum_{\mu=1}^{N}\cos\left(\frac{\pi\left(\mu-\frac{1}{2}\right)i}{N} - \frac{\pi\left(\mu-\frac{1}{2}\right)j}{N}\right) + \cos\left(\frac{\pi\left(\mu-\frac{1}{2}\right)i}{N} + \frac{\pi\left(\mu-\frac{1}{2}\right)j}{N}\right) \\
=&\frac{1}{2}\sum_{\mu=1}^{N}\cos\left(\frac{\pi(2\mu-1)(i-j)}{2N}\right) + \cos\left(\frac{\pi(2\mu-1)(i+j)}{2N}\right) \\
=&\frac{1}{4}\left(\sin(\pi(i+j))\csc\left(\frac{\pi(i+j)}{2N}\right) - \sin(\pi(j-i))\csc\left(\frac{\pi(i-j)}{2N}\right)\right).
\end{aligned} \tag{73}$$

This result gets value 0 when $\frac{\pi(i+j)}{2N} \neq a\pi$ or $\frac{\pi(i-j)}{2N} \neq b\pi$ for some integer a and b, because $\sin(\pi m) = 0$. The term $\sin(\pi m)\csc\left(\frac{\pi m}{2N}\right)$ gets non-zero only when $\csc\left(\frac{\pi m}{2N}\right)$ gets infinity. Then, we could write down the conditions that i and j satisfy

$$\begin{cases} i + j = 2aN \text{ or } |i - j| = 2bN \\ a, b \in \mathbb{Z} \\ 1 < i, j < N - 1. \end{cases} \tag{74}$$

The equation shows that the result is $j = k$. We can use L'Hôpital's rule to calculate the term

$$\lim_{x\to 0} \sin(\pi x)\csc\left(\frac{\pi x}{2N}\right) = 2N \tag{75}$$

when i and j satisfy the condition $i = j$. Plugin Eq. 75 and Eq. 73 into Eq. 71, we have

$$\alpha^{\mathscr{L}}_{\{\gamma_i\gamma_j\},2t+1} = \frac{1}{N} + \frac{2}{N}\sum_k \cos\left(\left(i - \frac{1}{2}\right)\frac{\pi k}{N}\right)\cos\left(\left(j - \frac{1}{2}\right)\frac{\pi k}{N}\right)\cos^{4t}\left(\frac{\pi k}{2N}\right). \tag{76}$$

Finally, we use trigonometric identities to expand this equation, thereby completing this proof

$$3\alpha^{\mathscr{L}}_{\{\gamma_i\gamma_j\},2t+1} = \frac{1}{N} + \frac{1}{N}\sum_k \left[\cos\left((i - j)\frac{k\pi}{N}\right) + \cos\left((i + j - 1)\frac{k\pi}{N}\right)\right]\cos^{4t}\left(\frac{\pi k}{2N}\right). \tag{77}$$

□

Lemma 5. *The result of summing the infinite series is*

$$\sum_0^\infty e^{-\frac{k^2\pi^2 t}{2N^2}}\cos\left(a\frac{\pi k}{N}\right) = \frac{N}{\sqrt{2\pi t}}e^{-\frac{a^2}{2t}}\left(1 + 2e^{-\frac{2N(N-a)}{t}} + \mathcal{O}(e^{-\frac{6N^2}{t}})\right) + \frac{1}{2} \tag{78}$$

when $t < N^2$.

Proof. To aid analysis, we define a new function $f(k)$ that captures the pattern of each term, where $f(k) = e^{-\frac{1}{2}\beta^2k^2t}\cos(a\beta k)$ and $\beta := \frac{\pi}{N}$. To determine the value of this infinite series, we invoke the Euler-Maclaurin formula. This formula relates the summation of a function to its integral representation, along with correction terms.

Specifically, the Euler-Maclaurin formula gives

$$\sum_{k=0}^\infty f(k) = \int_0^\infty f(x)dx + \frac{1}{2} + \int_0^\infty P_1(x)f'(x)\mathrm{d}x, \tag{79}$$

where $P_1(x) = B_1(x - \lfloor x\rfloor)$, and B_1 is the first order Bernoulli polynomial

$$B_1 = x - \frac{1}{2}. \tag{80}$$

By applying this formula, we can express the infinite series summation in terms of integrals, facilitating further analysis and solution of the problem.

Substitute the definition of B_1 into the Euler-Maclaurin expansion 79, we have

$$\sum_{k=0}^\infty f(k) = \int_0^\infty f(x)\mathrm{d}x + \frac{1}{2} - \frac{1}{2}\int_0^\infty f'(x)\mathrm{d}x + \int_0^\infty (x - \lfloor x\rfloor)f'(x)\mathrm{d}x \tag{81}$$

Integrating an serrate shape function can be relatively difficult. Therefore, we perform a Fourier transform on it,

$$x - \lfloor x\rfloor = \frac{1}{2} - \frac{1}{\pi}\sum_{k=1}^\infty \frac{1}{k}\sin(2\pi kx). \tag{82}$$

changing the integral of the serrate shape function into an integral of trigonometric functions. This makes the calculation simpler.

By the definition of function f, the derivative of f could be calculated

$$f'(x) = -e^{-\frac{1}{2}tx^2\beta^2} tx\beta^2 \cos[ax\beta] - ae^{-\frac{1}{2}tx^2\beta^2}\beta \sin[ax\beta] \tag{83}$$

$$= -tx\beta^2 f(x) - a\beta \tan(ax\beta) f(x). \tag{84}$$

We utilize the symbolic computation platform Wolfram Mathematica to calculate the integral of $f(x)$

$$\int_0^\infty f(x)\mathrm{d}x = \frac{N}{\sqrt{2\pi t}} e^{-\frac{a^2}{2t}} \tag{85}$$

and the integral of sin multiplied with $f'(x)$

$$\int_0^\infty \sin(2\pi kx) f'(x)\mathrm{d}x = -\frac{e^{-\frac{(2k\pi+a\beta)^2}{2t\beta^2}}\left(1+e^{\frac{4ak\pi}{t\beta}}\right)k\pi^{\frac{3}{2}}}{\sqrt{2t\beta^2}}. \tag{86}$$

Plugin Eq. 84, Eq. 86, and Eq. 85 to Eq. 81, we have

$$\sum_0^\infty f(n) = \int_0^\infty f(x)\mathrm{d}x + \frac{1}{2} + \sqrt{\frac{\pi}{2}}\sum_{k=1}^\infty \frac{e^{-\frac{(2k\pi+a\beta)^2}{2t\beta^2}}\left(1+e^{\frac{4ak\pi}{t\beta}}\right)}{\sqrt{t\beta^2}} \tag{87}$$

$$= \frac{N}{\sqrt{2\pi t}} e^{-\frac{a^2}{2t}} + \frac{1}{2} + N\sqrt{\frac{1}{2\pi t}}\left(\sum_{k=1}^\infty e^{-\frac{(2k\pi+a\beta)^2}{2t\beta^2}} + \sum_{k=1}^\infty e^{-\frac{(2k\pi-a\beta)^2}{2t\beta^2}}\right). \tag{88}$$

Now, we want to estimate the order of the third term in Eq. 88

$$\sum_{k=1}^\infty e^{-\frac{(2k\pi+a\beta)^2}{2t\beta^2}} + \sum_{k=1}^\infty e^{-\frac{(2k\pi-a\beta)^2}{2t\beta^2}} \leq 2\sum_{k=1}^\infty e^{-\frac{(2k\pi-a\beta)^2}{2t\beta^2}} \tag{89}$$

$$= 2e^{-\frac{a^2}{2t}} \sum_{k=1}^\infty e^{-\frac{2k^2N^2-2kaN}{t}} \tag{90}$$

$$\leq 2e^{-\frac{a^2}{2t}+\frac{2aN}{t}} \sum_{k=1}^\infty e^{-\frac{2k^2N^2}{t}} \tag{91}$$

$$= 2e^{-\frac{a^2}{2t}+\frac{2aN}{t}}\left(e^{-\frac{2N^2}{t}} + \mathcal{O}(e^{-\frac{6N^2}{t}})\right). \tag{92}$$

If we consider t to be smaller in order than $\mathcal{O}(N^2)$, then we can view $e^{-\frac{6N^2}{t}}$ as a small number. Thus, the summation of $f(n)$ obtains the value

$$\sum_0^\infty f(n) = \frac{N}{\sqrt{2\pi t}} e^{-\frac{a^2}{2t}}\left(1 + 2e^{-\frac{2N(N-a)}{t}} + \mathcal{O}(e^{-\frac{6N^2}{t}})\right) + \frac{1}{2}. \tag{93}$$

□

6 The relation between $\alpha^{\mathscr{L}}_{\{\gamma_i\gamma_j\},2t+1}$ and $\alpha^{\mathscr{R}}_{\{\gamma_i\gamma_j\},2t+1}$

Recall that we have divided the calculation of $\alpha_{\{\gamma_i\gamma_j\},2t+1}$ into two parts. One is the $\alpha^{\mathscr{L}}_{\{\gamma_i\gamma_j\},2t+1}$ and the other is $\alpha^{\mathscr{R}}_{\{\gamma_i\gamma_j\},2t+1}$. Theorem 1 gives the order of $\alpha^{\mathscr{L}}_{\{\gamma_i\gamma_j\},2t+1}$. In this section, we aim to bound the $\alpha^{\mathscr{R}}_{\{\gamma_i\gamma_j\},2t+1}$ by $\alpha^{\mathscr{L}}_{\{\gamma_i\gamma_j\},2t+1}$, so that the order of $\alpha_{\{\gamma_i\gamma_j\},2t+1}$ could be given by the $\alpha^{\mathscr{L}}_{\{\gamma_i\gamma_j\},2t+1}$.

We begin with the polynomial in Eq. 55

$$T^{(\text{whole})}_{\mathcal{P}_N}(t)(y_iy_j) = \sum_{\mu,\nu}\left(\mathscr{L}_{ij}(\mu,\nu,t)y_\mu y_\nu + \mathscr{R}_{ij}(\mu,\nu,t)y_\mu y_\nu\right). \tag{94}$$

Then, we let the polynomial transform one time-interval step, and we get

$$
\begin{aligned}
&T^{(\text{whole})}_{\mathcal{P}_N}(t+1)(y_i y_j) && (95)\\
=&T^{(e)}_{\mathcal{P}_N} T^{(o)}_{\mathcal{P}_N}\left(T^{(\text{whole})}_{\mathcal{P}_N}(t)(y_i y_j)\right) && (96)\\
=&\sum_{\mu,\nu}\left(\mathscr{L}_{ij}(\mu,\nu,t)(L(y_\mu)L(y_\nu)+R(y_\mu,y_\nu))+\mathscr{R}_{ij}(\mu,\nu,t)(L(y_\mu)L(y_\nu)+R(y_\mu,y_\nu))\right) && (97)\\
=&\sum_{\mu,\nu}\left(\mathscr{L}_{ij}(\mu,\nu,t)(L(y_\mu)L(y_\nu)+R(y_\mu,y_\nu))+\mathscr{R}_{ij}(\mu,\nu,t)(L(y_\mu)L(y_\nu)+R(y_\mu,y_\nu))\right) && (98)\\
=&\sum_{\mu,\nu}\mathscr{L}_{ij}(\mu,\nu,t+1)y_\mu y_\nu+\sum_{\mu,\nu}\mathscr{L}_{ij}(\mu,\nu,t)R(y_\mu,y_\nu)\\
&+\sum_{\mu,\nu}\mathscr{R}_{ij}(\mu,\nu,t)(L(y_\mu)L(y_\nu)+R(y_\mu,y_\nu)). && (99)
\end{aligned}
$$

Deduce from Eq. 94, we have

$$
T^{(\text{whole})}_{\mathcal{P}_N}(t+1)(y_i y_j)=\sum_{\mu,\nu}\left(\mathscr{L}_{ij}(\mu,\nu,t+1)y_\mu y_\nu+\mathscr{R}_{ij}(\mu,\nu,t+1)y_\mu y_\nu\right). \tag{100}
$$

Compare Eq. 99 and Eq. 100, we have

$$
\sum_{\mu,\nu}\mathscr{R}_{ij}(\mu,\nu,t+1)y_\mu y_\nu=\sum_{\mu,\nu}\mathscr{L}_{ij}(\mu,\nu,t)R(y_\mu,y_\nu)+\sum_{\mu,\nu}\mathscr{R}_{ij}(\mu,\nu,t)(L(y_\mu)L(y_\nu)+R(y_\mu,y_\nu)) \tag{101}
$$

$$
\mathscr{R}_{ij}(l,k,t+1)=\sum_{\mu,\nu}\mathscr{R}_{ij}(\mu,\nu,t)\frac{\partial^2 L(y_\mu)L(y_\nu)}{\partial y_l\partial y_k}+\sum_{\mu,\nu}\left(\mathscr{L}_{ij}(\mu,\nu,t)+\mathscr{R}_{ij}(\mu,\nu,t)\right)\frac{\partial^2 R(y_\mu,y_\nu)}{\partial y_l\partial y_k}. \tag{102}
$$

Eq. 102 describes the strict relationship between $\mathscr{R}_{ij}$ and $\mathscr{L}_{ij}$ in a recursive form, thereby giving the relationship between $\alpha^{\mathscr{L}}_{\{\gamma_i\gamma_j\},2t+1}$ and $\alpha^{\mathscr{R}}_{\{\gamma_i\gamma_j\},2t+1}$. However, deriving the general term formula from this recursive formula is difficult. Therefore, we hope to use some inequalities to simplify this recursive relationship and thus bound $\alpha^{\mathscr{R}}_{\{\gamma_i\gamma_j\},2t+1}$ by $\alpha^{\mathscr{L}}_{\{\gamma_i\gamma_j\},2t+1}$.

We will first define some auxiliary variables,

$$
\begin{aligned}
\alpha_k(t)&:=\frac{1}{2}\sum_{\mu=1}^{N-k}\left(\mathcal{L}_i(\mu,t)\mathcal{L}_j(\mu+k,t)+\mathcal{L}_i(\mu+k,t)\mathcal{L}_j(\mu,t)\right)\\
\beta_k(t)&:=\frac{1}{2}\sum_{\mu=1}^{N-k}\left(\mathscr{R}_{i,j}(\mu,\mu+k,t)+\mathscr{R}_{i,j}(\mu+k,\mu,t)\right)\\
a(t)&:=\begin{pmatrix}\alpha_0(t)\\ \alpha_1(t)\end{pmatrix},\quad b(t):=\begin{pmatrix}\beta_0(t)\\ \beta_1(t)\end{pmatrix}.
\end{aligned}
$$

Notice that $\alpha^{\mathscr{L}}_{\{\gamma_i\gamma_j\},2t+1}=\alpha_0(t)$, $\alpha^{\mathscr{R}}_{\{\gamma_i\gamma_j\},2t+1}=\beta_0(t)$. Because $\mathscr{L}_{i,j}(\mu,\nu,t)+\mathscr{R}_{i,j}(\mu,\nu,t)$ represents the probability of being in site y_iy_j during a random walk, it satisfies the property that the summation across all sites is 1. Meanwhile, the summation of all $\mathscr{L}_{i,j}(\mu,\nu,t)$ is 1. The two things deduce that

$$
\sum_{\mu,\nu}\mathscr{R}_{i,j}(\mu,\nu,t)=0. \tag{103}
$$

Especially, in numerical simulation, we observe that all β_k are greater than 0 except for β_0. Under this assumption, we have the following theory:

Theorem 2. *Assume that $\beta_0<0$, and $\forall k>0$, $\beta_k>0$. $-\beta_0(t)\leq$.*

Theorem 2 establishes the mathematical relationship between the two components $\alpha^{\mathscr{L}}_{\{\gamma_i\gamma_j\},2t+1}$ and $\alpha^{\mathscr{R}}_{\{\gamma_i\gamma_j\},2t+1}$. By combining this theoretical relationship with the equality described in Eq. 61, we are able to deduce the order of magnitude of the $\alpha_{\{\gamma_i\gamma_j\},2t+1}$. Bringing these pieces together allows us to systematically determine the scale or size of $\alpha_{\{\gamma_i\gamma_j\},2t+1}$ based on the other defined quantities.

proof of theorem 2. From the recursive relationship in Eq. 102 and Table 2, we could write down the recursive relationship of β_k

$$\beta_0(t+1) = \frac{6}{16}\beta_0(t) + \frac{1}{4}\beta_1(t) - \frac{14}{144}\left(\beta_0(t) - \alpha_0(t)\right) - \frac{1}{24}\left(\beta_1(t) - \alpha_1(t)\right) + O\left(\frac{1}{N^2}\right) \tag{104}$$

$$= \frac{5}{18}\beta_0(t) + \frac{5}{24}\beta_1(t) + \frac{7}{72}\alpha_0(t) + \frac{1}{12}\alpha_1(t) + O\left(\frac{1}{N^2}\right) \tag{105}$$

$$\beta_1(t+1) \leq \frac{5}{9}\beta_0(t) + \frac{5}{12}\beta_1(t) - \frac{1}{18}\alpha_0(t) - \frac{1}{24}\alpha_1(t) \tag{106}$$

□

7 Efficiency when the distance of set is short

Now, we are ready to show a simple result. Suppose the elements of S are $i_1, i_2, \cdots, i_{|S|}$ which satisfies $i_1 < i_2 < \cdots < i_{|S|}$. Define the distance of $|S|$ as

$$d(S) := \max(|i_{2j-1} - i_{2j}| \mid j \in \{1, 2, \cdots \frac{|S|}{2}\}). \tag{107}$$

The number $\frac{|S|}{2}$ is an integer because

$$\alpha_{S',d} = 0 \tag{108}$$

when $|S'|$ is an odd number [1]. Intuitively, Eq. 108 is true because we measure the state in the computational basis. The computational basis can only consist of operators γ_S. Thus, we only care about the set S with even cardinal number. Then, we have the following theorem:

Theorem 3. *The expectation value of* $\mathrm{tr}(\rho\gamma_S)$ *can be obtained by using* $\mathrm{polylog}(n)$*-layers matchgate circuit within the Fermionic classical shadows protocol, when the distance of* S *is* $\mathcal{O}(\log n)$ *and the cardinal number* $|S|$ *is a constant* $2c$.

Proof. Let the initial tensor be P^S, and apply $T^{(\text{whole})}$ to the tensor P^S. Each $T^{(e)}T^{(o)}$ in $T^{(\text{whole})}$ will transform the P^S to the superposition of a series of Pauli tensors

$$T^{(e)}T^{(o)}P^S = \sum_{|S'|=|S|} \xi_{S'}|P^{S'}\rangle\rangle, \tag{109}$$

where $\xi_{S'}$ are real coefficients that satisfy $\sum \xi_{S'} = 1$. Now, we only preserve the branches S' which has smaller distance $d(S') < d(S)$ unless $d(S) = 1$. The condition $d(S) = 1$ means that

$$P^S = \prod_{i\in\Lambda} Z_i \tag{110}$$

via Jordan-Wigner transformation. Only the Pauli basis in the form of $\prod_{i\in\Lambda} Z_i$ have non-zero inner product with $|0,0\rangle\rangle$, which we explain it in Sec. 4.

Table 1 tells us that summation of the coefficients of remained branches is greater than $\frac{1}{9^{|S|}}$. explain why is 1/9

We apply $T^{(e)}T^{(o)}$ $d(S)/2$-times, and in each step, only remain the branches with smaller cardinal numbers. Afterward, the summation of coefficients of remained branches is greater than $\frac{1}{9^{|S|d(S)}/2}$. Notice that $|S|$ is a constant number and $d(S) = \mathcal{O}(\log(n))$, the summation number is

$$\sum_{S''} \xi_{S''} \geq \frac{1}{9^{\mathcal{O}(\log(n))}} = \frac{1}{\mathcal{O}(\mathrm{poly}(n))}, \tag{111}$$

where S'' are the remained branches. □

References

[1] Kianna Wan, William J. Huggins, Joonho Lee, and Ryan Babbush. Matchgate shadows for fermionic quantum simulation, 2022.

[2] Luca Giuggioli. Exact spatiotemporal dynamics of confined lattice random walks in arbitrary dimensions: a century after smoluchowski and pólya. *Physical Review X*, 10(2):021045, 2020.