Supplementary Material for
Exponential Hardness of Optimization from the Locality in Quantum Neural Networks

Appendix A: Preliminaries

We start from the definition of a unitary t-design [1]. Consider a ensemble $\mathbb{V}$ of unitaries V on a d-dimensional Hilbert space, and denote $P_{t,t}(V)$ as an arbitrary polynomial of degree at most t in the entries of V and at most t in those of $V^\dagger$. Then $\mathbb{V}$ is a unitary t-design if

$$\frac{1}{|\mathbb{V}|}\sum_{V\in\mathbb{V}} P_{t,t}(V) = \int_{\mathcal{U}(d)} d\mu(V) P_{t,t}(V), \tag{A1}$$

where $|\mathbb{V}|$ is the size of the set $\mathbb{V}$, $\mathcal{U}(d)$ is the unitary group of degree d and $d\mu(V)$ is the Haar measure on $\mathcal{U}(d)$. Namely, $P_{t,t}(V)$ averaging over the t-design $\mathbb{V}$ will yield exactly the same result as averaging over the entire unitary group $\mathcal{U}(d)$. Fortunately, these integrals over polynomials can be analytically solved and expressed into closed forms. For example, the following element-wise identities hold for the first two moments [2, 3]

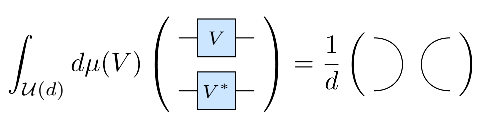
$$\int_{\mathcal{U}(d)} d\mu(V) v_{i,j} v^*_{i',j'} = \frac{\delta_{i,i'}\delta_{j,j'}}{d}, \tag{A2a}$$

$$\begin{aligned}\int_{\mathcal{U}(d)} d\mu(V) v_{i_1,j_1} v_{i_2,j_2} v^*_{i'_1,j'_1} v^*_{i'_2,j'_2} = {} & \frac{1}{d^2-1}\left(\delta_{i_1,i'_1}\delta_{i_2,i'_2}\delta_{j_1,j'_1}\delta_{j_2,j'_2} + \delta_{i_1,i'_2}\delta_{i_2,i'_1}\delta_{j_1,j'_2}\delta_{j_2,j'_1}\right) \\ & - \frac{1}{d\left(d^2-1\right)}\left(\delta_{i_1,i'_1}\delta_{i_2,i'_2}\delta_{j_1,j'_2}\delta_{j_2,j'_1} + \delta_{i_1,i'_2}\delta_{i_2,i'_1}\delta_{j_1,j'_1}\delta_{j_2,j'_2}\right),\end{aligned} \tag{A2b}$$

where $v_{i,j}$ and $v^*_{i',j'}$ denote the entries of V and V^*, respectively, and $\delta_{i,j}$ denotes the Kronecker delta. For practical purposes, these element-wise identities need to be transformed into various matrix forms, during which one will encounter many contraction operations. Here we take advantage of tensor network notations to deal with the contraction operations. For example, if we arrange the indices like

$$v_{i,j} = \left(i \;-\!\boxed{V}\!-\; j \right), \quad v^*_{i',j'} = \left(i' \;-\!\boxed{V^*}\!-\; j' \right), \tag{A3}$$

(A2a) could be represented as the following diagram


(A4)

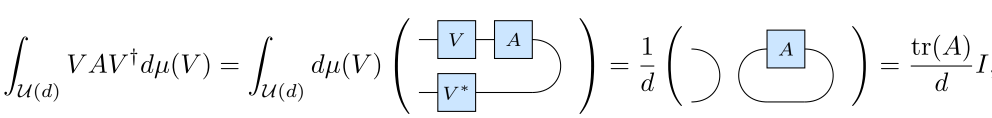
where the arcs on the right hand side of (A4) represent identity matrices, i.e. the Kronecker delta $\delta_{i,i'}$ and $\delta_{j,j'}$. As a simple instance, we first prove Lemma 1 using (A4).

Lemma 1 *For an arbitrary linear operator A on the d-dimensional Hilbert space, the following equality holds*

$$\int_{\mathcal{U}(d)} VAV^\dagger d\mu(V) = \frac{\mathrm{tr}(A)}{d} I, \tag{A5}$$

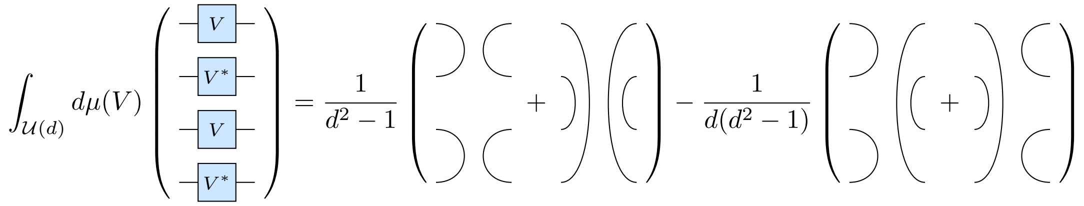
where I is the identity operator on the d-dimensional Hilbert space.

Proof By tensor network notations and (A4), we have


(A6)

which is exactly the same with (A5). ■

Similarly, (A2b) could be represented by tensor network notations as the following diagram


(A7)

Now we utilize (A7) to derive a central identity used in the proof in the next section as Lemma 2.

Lemma 2 *Suppose $V \in \mathbb{V}$ is a unitary on the Hilbert space $\mathcal{H}_A \otimes \mathcal{H}_B$ with $\dim(\mathcal{H}_A) = d_A$ and $\dim(\mathcal{H}_B) = d_B$ where $\mathbb{V}$ is a unitary 2-design. For any linear operators P, Q on $\mathcal{H}_A \otimes \mathcal{H}_B$, the following identity holds*

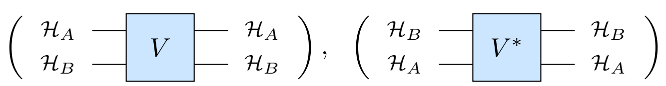
$$\mathbb{E}_V \left[\left\| \operatorname{tr}_B \left(QVPV^\dagger \right) \right\|_2^2 \right] = \frac{1}{d^2-1} \left[\| \operatorname{tr}_B Q \|_2^2 \left(|\operatorname{tr} P|^2 - \frac{\|P\|_2^2)}{d} \right) + d_A \|Q\|_2^2 \left(\|P\|_2^2 - \frac{|\operatorname{tr} P|^2}{d} \right) \right], \tag{A8}$$

where $\|\cdot\|_2$ is the Schatten 2-norm and $d = d_A d_B$ denotes the dimension of the whole Hilbert space $\mathcal{H}_A \otimes \mathcal{H}_B$.

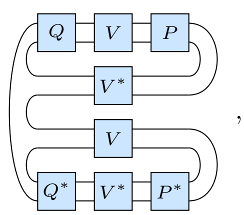
Proof Note that $\mathbb{V}$ is a unitary 2-design and $\left\| \operatorname{tr}_B \left(QVPV^\dagger \right) \right\|_2^2$ is a polynomial of degree at most 2 in the entries of V. By the definition of unitary 2-designs in (A1), the left hand side of (A8) could be rewritten as

$$\mathbb{E}_V \left[\left\| \operatorname{tr}_B \left(QVPV^\dagger \right) \right\|_2^2 \right] = \int_{\mathcal{U}(d)} d\mu(V) \operatorname{tr} \left(\operatorname{tr}_B (QVPV^\dagger) \operatorname{tr}_B (VP^\dagger V^\dagger Q^\dagger) \right). \tag{A9}$$

Since the Hilbert space $\mathcal{H}_A \otimes \mathcal{H}_B$ has a bipartite tensor product structure, the linear operators on $\mathcal{H}_A \otimes \mathcal{H}_B$ could be represented as 4-degree tensors. We take the convention for the arrangement of the indices of V and V^* corresponding to $\mathcal{H}_A, \mathcal{H}_B$ as follows

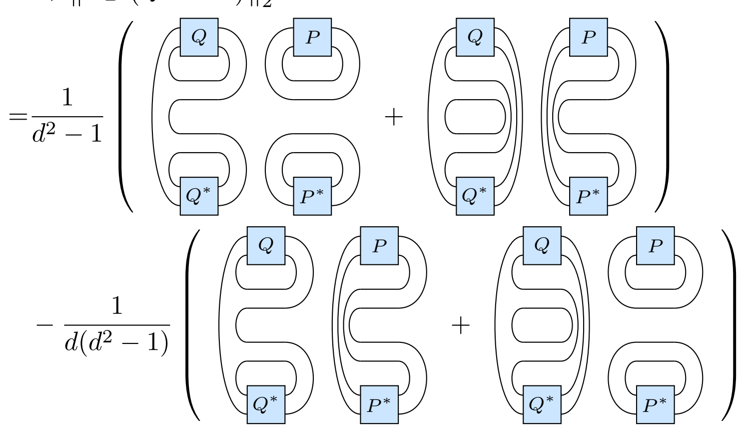

(A10)

The arrangements of indices for P, Q and P^*, Q^* are the same as V and V^*, respectively. The integrand on the right hand side of (A9) could be represented diagrammatically as


(A11)

Combining (A7), (A9) and (A11), the left hand side of (A8) is equal to

$$\mathbb{E}_V \left\| \operatorname{tr}_B \left(QVPV^\dagger \right) \right\|_2^2$$


(A12)

$$= \frac{1}{d^2-1} \left[\operatorname{tr}(\operatorname{tr}_B Q^\dagger \operatorname{tr}_B Q) \left(|\operatorname{tr}(P)|^2 - \frac{\operatorname{tr}(P^\dagger P)}{d} \right) + d_A \operatorname{tr}(Q^\dagger Q) \left(\operatorname{tr}(P^\dagger P) - \frac{|\operatorname{tr} P|^2}{d} \right) \right],$$

which is exactly the desired identity (A8). ■

Then, we will explicitly write down several special cases of Lemma 2 for the sake of convenience.

Corollary 3 *Suppose $V \in \mathbb{V}$ is a unitary on the Hilbert space $\mathcal{H}_A \otimes \mathcal{H}_B$ with $\dim(\mathcal{H}_A) = d_A$ and $\dim(\mathcal{H}_B) = d_B$ where $\mathbb{V}$ is a unitary 2-design. Let ρ be an arbitrary density matrix on $\mathcal{H}_A \otimes \mathcal{H}_B$ and $\rho_A = \operatorname{tr}_B(V\rho V^\dagger)$ be the reduced density matrix on $\mathcal{H}_A$ from $V\rho V^\dagger$. The expectation of the purity of ρ_A is*

$$\mathbb{E}_V\left[\operatorname{tr}\left(\rho_A^2\right)\right] = \frac{(d_A^2-1)d_B}{d^2-1}\operatorname{tr}(\rho^2) + \frac{(d_B^2-1)d_A}{d^2-1}. \tag{A13}$$

where $d = d_A d_B$ denotes the dimension of the whole Hilbert space $\mathcal{H}_A \otimes \mathcal{H}_B$. Since pure states satisfy $\operatorname{tr}(\rho^2) = 1$, (A13) can be further simplified for pure states as

$$\mathbb{E}_V\left[\operatorname{tr}\left(\rho_A^2\right)\right] = \frac{d_A + d_B}{d_A d_B + 1}. \tag{A14}$$

Proof This is a special case of Lemma 2 by taking $P = \rho$ and $Q = I_A \otimes I_B$. ■

Corollary 4 *Suppose $V \in \mathbb{V}$ is a unitary on the Hilbert space $\mathcal{H}_A \otimes \mathcal{H}_B$ with $\dim(\mathcal{H}_A) = d_A$ and $\dim(\mathcal{H}_B) = d_B$ where $\mathbb{V}$ is a unitary 2-design. Let ρ be an arbitrary density matrix on $\mathcal{H}_A \otimes \mathcal{H}_B$. For any traceless operator O_B on $\mathcal{H}_B$, the following identity holds*

$$\mathbb{E}_V\left[\left\|\operatorname{tr}_B\left(I_A \otimes O_B V\rho V^\dagger\right)\right\|_2^2\right] = \frac{d_A^2\|O_B\|_2^2}{d^2-1}\left(\operatorname{tr}(\rho^2) - \frac{1}{d}\right), \tag{A15}$$

where $d = d_A d_B$ denotes the dimension of the whole Hilbert space $\mathcal{H}_A \otimes \mathcal{H}_B$ and I_A is the identity on $\mathcal{H}_A$.

Proof This is a special case of Lemma 2 by taking $P = \rho$, $Q = I_A \otimes O_B$ with $\operatorname{tr}(O_B) = 0$. ■

Corollary 5 *Suppose $V \in \mathbb{V}$ is a unitary on the Hilbert space $\mathcal{H}_A \otimes \mathcal{H}_B$ with $\dim(\mathcal{H}_A) = d_A$ and $\dim(\mathcal{H}_B) = d_B$ where $\mathbb{V}$ is a unitary 2-design. For any traceless operator P on $\mathcal{H}_A \otimes \mathcal{H}_B$ and any linear operators O_A, O_B on $\mathcal{H}_A$, $\mathcal{H}_B$ respectively, the following identity holds*

$$\mathbb{E}_V\left[\left\|\operatorname{tr}_B\left(O_A \otimes O_B V P V^\dagger\right)\right\|_2^2\right] = \frac{\|O_A\|_2^2\|P\|_2^2}{d^2-1}\left[d_A\|O_B\|_2^2 - \frac{|\operatorname{tr} O_B|^2}{d}\right], \tag{A16}$$

where $d = d_A d_B$ denotes the dimension of the whole Hilbert space $\mathcal{H}_A \otimes \mathcal{H}_B$.

Proof This is a special case of Lemma 2 by taking $\operatorname{tr}(P) = 0$ and $Q = O_A \otimes O_B$. ■

In the end of this section, we recall several fundamental inequalities in linear algebra and probability theory to make our proofs in the next section more self-contained.

Lemma 6 (Hölder's inequality for tracial matrices) *For any linear operators X, Y, the following inequality holds*

$$\left|\operatorname{tr}(X^\dagger Y)\right| \le \|X\|_p \|Y\|_q, \tag{A17}$$

where p, q satisfy $\frac{1}{p} + \frac{1}{q} = 1$ and $\|\cdot\|_p$ denotes the Schatten p-norm defined by $\|A\|_p = (\operatorname{tr}|A|^p)^{1/p}$, $|A| = \sqrt{A^\dagger A}$.

Lemma 7 (Partial trace monotonicity) *For any linear operator H on the Hilbert space $\mathcal{H}_A \otimes \mathcal{H}_B$ with $\dim \mathcal{H}_B = d_B$, the following inequality holds* [4]

$$\|\operatorname{tr}_B H\|_p \le d_B^{(p-1)/p}\|H\|_p. \tag{A18}$$

Namely, the Schatten p-norm is non-increasing under partial tracing up to a constant coefficient. Specially, we have

$$\|\operatorname{tr}_B H\|_1 \le \|H\|_1, \quad \|\operatorname{tr}_B H\|_2 \le \sqrt{d_B}\|H\|_2, \quad \|\operatorname{tr}_B H\|_\infty \le d_B\|H\|_\infty. \tag{A19}$$

Lemma 8 (Markov's inequality) *Let X be a random variable taking non-negative real value. For any $\epsilon > 0$, the following inequality holds*

$$\Pr[X \ge \epsilon] \le \frac{\mathbb{E}[X]}{\epsilon}, \tag{A20}$$

where $\Pr[X \ge \epsilon]$ denotes the probability of $X \ge \epsilon$ and $\mathbb{E}[X]$ denotes the expectation of the random variable X.

Lemma 9 (Jensen's inequality) *Let X be a random variable and $f : \mathbb{R} \to \mathbb{R}$ is a convex function. The following inequality holds*

$$f(\mathbb{E}[X]) \leq \mathbb{E}[f(X)]. \tag{A21}$$

Lemma 10 *Suppose that X is a random variable taking real values in $[0, a]$. The following inequality holds*

$$\mathrm{Var}[X] \leq a \cdot \mathbb{E}[X]. \tag{A22}$$

Proof According to the relation $x^2 \leq ax$, we have

$$\mathrm{Var}[X] \leq \mathbb{E}[X^2] \leq \mathbb{E}[aX] = a \cdot \mathbb{E}[X]. \tag{A23}$$

■

Appendix B: Proof of Theorem 1

To make the proof easy to read and emphasize important intermediate results, we prove Lemma 11-16 first and derive Theorem 1 by use of these lemmas.

Lemma 11 *Suppose $V \in \mathbb{V}$ is a unitary on the Hilbert space $\mathcal{H}_A \otimes \mathcal{H}_B$ with $\dim(\mathcal{H}_A) = d_A$ and $\dim(\mathcal{H}_B) = d_B$ where $\mathbb{V}$ is a unitary 2-design. Let ρ be an arbitrary density matrix on $\mathcal{H}_A \otimes \mathcal{H}_B$ and $\rho_A = \mathrm{tr}_B(V\rho V^\dagger)$ be the reduced density matrix on $\mathcal{H}_A$ from $V\rho V^\dagger$. The expectation of the 2-norm distance between ρ_A and the maximally mixed state I_A/d_A satisfies*

$$\mathbb{E}_V \left\| \rho_A - \frac{I_A}{d_A} \right\|_2 \leq \sqrt{\frac{1}{d_B}}. \tag{B1}$$

Proof According to the concavity of the square root function and Jensen's inequality in Lemma 9, we have

$$\mathbb{E}_V \left\| \rho_A - \frac{I_A}{d_A} \right\|_2 \leq \sqrt{\mathbb{E}_V \left[\left\| \rho_A - \frac{I_A}{d_A} \right\|_2^2 \right]}. \tag{B2}$$

Using Corollary 3, the expectation under the square root on the right hand side of (B2) can be exactly calculated as

$$\begin{aligned} \mathbb{E}_V \left[\left\| \rho_A - \frac{I_A}{d_A} \right\|_2^2 \right] &= \mathbb{E}_V \,\mathrm{tr} \left[\left(\rho_A - \frac{I_A}{d_A} \right)^2 \right] = \mathbb{E}_V \,\mathrm{tr} \left(\rho_A^2 - \frac{2}{d_A}\rho_A + \frac{I_A}{d_A^2} \right) \\ &= \frac{(d_A^2 - 1)d_B}{d^2 - 1} \,\mathrm{tr}(\rho^2) + \frac{(d_B^2 - 1)d_A}{d^2 - 1} - \frac{1}{d_A}. \end{aligned} \tag{B3}$$

By the upper bound of the purity $\mathrm{tr}(\rho^2) \leq 1$, (B3) could be further relaxed to

$$\begin{aligned} \mathbb{E}_V \left[\left\| \rho_A - \frac{I_A}{d_A} \right\|_2^2 \right] &\leq \frac{(d_A^2 - 1)d_B}{d^2 - 1} + \frac{(d_B^2 - 1)d_A}{d^2 - 1} - \frac{1}{d_A} \\ &= \frac{d_A + d_B}{d_A d_B + 1} - \frac{1}{d_A} \leq \frac{1}{d_B}. \end{aligned} \tag{B4}$$

Combining (B2) and (B4), we arrive at (B1). ■

Lemma 12 *Suppose $V \in \mathbb{V}$ is a unitary on the Hilbert space $\mathcal{H}_A \otimes \mathcal{H}_B$ with $\dim(\mathcal{H}_A) = d_A$ and $\dim(\mathcal{H}_B) = d_B$ where $\mathbb{V}$ is a unitary 2-design. For any density matrix ρ on $\mathcal{H}_A \otimes \mathcal{H}_B$ and any traceless operator O_B on $\mathcal{H}_B$, the following inequality holds*

$$\mathbb{E}_V \left\| \mathrm{tr}_B \left((I_A \otimes O_B) V\rho V^\dagger \right) \right\|_2 \leq \|O_B\|_\infty \sqrt{\frac{1}{d_B}}. \tag{B5}$$

Proof According to the concavity of the square root function and Jensen's inequality in Lemma 9, we have

$$\mathbb{E}_V \left\|\mathrm{tr}_B\left((I_A\otimes O_B)V\rho V^\dagger\right)\right\|_2 \leq \sqrt{\mathbb{E}_V\left[\left\|\mathrm{tr}_B\left((I_A\otimes O_B)V\rho V^\dagger\right)\right\|_2^2\right]}. \tag{B6}$$

Using Corollary 4, the expectation under the square root in (B6) can be exactly calculated as

$$\mathbb{E}_V\left[\left\|\mathrm{tr}_B\left((I_A\otimes O_B)V\rho V^\dagger\right)\right\|_2^2\right] = \frac{d_A^2\|O_B\|_2^2}{d^2-1}\left(\mathrm{tr}(\rho^2)-\frac{1}{d}\right), \tag{B7}$$

By the upper bound of the purity $\mathrm{tr}(\rho^2)\leq 1$, (B7) could be further relaxed to

$$\mathbb{E}_V\left[\left\|\mathrm{tr}_B\left((I_A\otimes O_B)V\rho V^\dagger\right)\right\|_2^2\right] \leq \frac{d_A^2\|O_B\|_2^2}{d^2-1}\left(1-\frac{1}{d}\right) = \frac{d_A^2\|O_B\|_2^2}{d(d+1)} \leq \frac{\|O_B\|_2^2}{d_B^2}. \tag{B8}$$

Considering $\|O_B\|_2\leq\sqrt{d_B}\|O_B\|_\infty$, we further obtain

$$\mathbb{E}_V\left[\left\|\mathrm{tr}_B\left((I_A\otimes O_B)V\rho V^\dagger\right)\right\|_2^2\right] \leq \frac{\|O_B\|_\infty^2}{d_B}. \tag{B9}$$

Combining (B6) and (B9), we arrive at (B5). ■

Lemma 13 *Suppose $V\in\mathbb{V}$ is a unitary on the Hilbert space $\mathcal{H}_A\otimes\mathcal{H}_B$ with $\dim(\mathcal{H}_A)=d_A$ and $\dim(\mathcal{H}_B)=d_B$ where $\mathbb{V}$ is a unitary 2-design. Let O_A be an arbitrary traceless operator on $\mathcal{H}_A$ and O_B be either an arbitrary traceless operator or a homothety cI_B on $\mathcal{H}_B$, where I_B is the identity operator on $\mathcal{H}_B$ and $c\in\mathbb{C}$ is an arbitrary complex number. Denote $U_A\in\mathcal{U}(d_A)$ as a unitary operator on $\mathcal{H}_A$. For any density matrix ρ on $\mathcal{H}_A\otimes\mathcal{H}_B$, the following inequality holds*

$$\mathbb{E}_V\left[\max_{U_A}\left|\mathrm{tr}\left[(O_A\otimes O_B)(U_A\otimes I_B)V\rho V^\dagger(U_A^\dagger\otimes I_B)\right]\right|\right] \leq \|O_A\|_\infty\|O_B\|_\infty\sqrt{\frac{d_A}{d_B}}. \tag{B10}$$

Proof The trace expression on the left hand side of (B10) can be rewritten as

$$\mathrm{tr}\left[(O_A\otimes O_B)(U_A\otimes I_B)V\rho V^\dagger(U_A^\dagger\otimes I_B)\right] = \mathrm{tr}\left[(U_A^\dagger O_A U_A)\,\mathrm{tr}_B\left((I_A\otimes O_B)V\rho V^\dagger\right)\right]. \tag{B11}$$

On the one hand, if O_B is traceless, by using Hölder's inequality in Lemma 6, we obtain

$$\begin{aligned}\left|\mathrm{tr}\left[(U_A^\dagger O_A U_A)\,\mathrm{tr}_B\left((I_A\otimes O_B)V\rho V^\dagger\right)\right]\right| &\leq \left\|U_A^\dagger O_A U_A\right\|_2\left\|\mathrm{tr}_B\left((I_A\otimes O_B)V\rho V^\dagger\right)\right\|_2\\ &\leq \sqrt{d_A}\,\|O_A\|_\infty\left\|\mathrm{tr}_B\left((I_A\otimes O_B)V\rho V^\dagger\right)\right\|_2,\end{aligned} \tag{B12}$$

where we have used the unitary invariance of the Schatten norms to eliminate U_A. Since (B12) holds for any U_A, it certainly holds when taking the maximum, i.e.

$$\max_{U_A}\left|\mathrm{tr}\left[(U_A^\dagger O_A U_A)\,\mathrm{tr}_B\left((I_A\otimes O_B)V\rho V^\dagger\right)\right]\right| \leq \sqrt{d_A}\,\|O_A\|_\infty\left\|\mathrm{tr}_B\left((I_A\otimes O_B)V\rho V^\dagger\right)\right\|_2. \tag{B13}$$

Together with Lemma 12, we arrive at

$$\begin{aligned}&\mathbb{E}_V\left[\max_{U_A}\left|\mathrm{tr}\left[(O_A\otimes O_B)(U_A\otimes I_B)V\rho V^\dagger(U_A^\dagger\otimes I_B)\right]\right|\right]\\ &\leq \sqrt{d_A}\,\|O_A\|_\infty\,\mathbb{E}_V\left\|\mathrm{tr}_B\left((I_A\otimes O_B)V\rho V^\dagger\right)\right\|_2 \leq \|O_A\|_\infty\|O_B\|_\infty\sqrt{\frac{d_A}{d_B}}.\end{aligned} \tag{B14}$$

On the other hand, if $O_B=cI_B$, the right hand side of (B11) can be further rewritten as

$$\mathrm{tr}\left[(U_A^\dagger O_A U_A)\,\mathrm{tr}_B\left((I_A\otimes O_B)V\rho V^\dagger\right)\right] = c\cdot\mathrm{tr}\left[U_A^\dagger O_A U_A\rho_A\right] = c\cdot\mathrm{tr}\left[U_A^\dagger O_A U_A\left(\rho_A-\frac{I_A}{d_A}\right)\right]. \tag{B15}$$

where we have used the traceless condition of O_A and $\rho_A = \mathrm{tr}_B(V\rho V^\dagger)$ is the reduced density matrix on $\mathcal{H}_A$ from $V\rho V^\dagger$. Again, by Hölder's inequality in Lemma 6, we obtain

$$\begin{aligned}\left|c\cdot\mathrm{tr}\left[U_A^\dagger O_A U_A\left(\rho_A-\frac{I_A}{d_A}\right)\right]\right| &\le |c|\left\|U_A^\dagger O_A U_A\right\|_2\left\|\rho_A-\frac{I_A}{d_A}\right\|_2\\ &\le\sqrt{d_A}\left\|O_B\right\|_\infty\left\|O_A\right\|_\infty\left\|\rho_A-\frac{I_A}{d_A}\right\|_2.\end{aligned}\tag{B16}$$

Since (B16) holds for any U_A, it certainly holds when taking the maximum. Together with (B11), (B15) and Lemma 11, we arrive at

$$\begin{aligned}&\mathbb{E}_V\left[\max_{U_A}\left|\mathrm{tr}\left[(O_A\otimes O_B)(U_A\otimes I_B)V\rho V^\dagger(U_A^\dagger\otimes I_B)\right]\right|\right]\\ &\le\sqrt{d_A}\left\|O_B\right\|_\infty\left\|O_A\right\|_\infty\mathbb{E}_V\left\|\rho_A-\frac{I_A}{d_A}\right\|_2\le\left\|O_B\right\|_\infty\left\|O_A\right\|_\infty\sqrt{\frac{d_A}{d_B}}.\end{aligned}\tag{B17}$$

Combining (B14) and (B17), we know that (B10) holds whether O_B is traceless or $O_B = cI_B$, $c\in\mathbb{C}$. ■

Lemma 14 *Suppose $V\in\mathbb{V}$ is a unitary on the Hilbert space $\mathcal{H}_A\otimes\mathcal{H}_B$ with $\dim(\mathcal{H}_A)=d_A$ and $\dim(\mathcal{H}_B)=d_B$ where $\mathbb{V}$ is a unitary 2-design. Let O_A,O_B be arbitrary linear operators on $\mathcal{H}_A$,$\mathcal{H}_B$, respectively. Denote $U_A\in\mathcal{U}(d_A)$ as a unitary operator on $\mathcal{H}_A$. For any traceless matrix H on $\mathcal{H}_A\otimes\mathcal{H}_B$, the following inequality holds*

$$\mathbb{E}_V\left\|\mathrm{tr}\left((O_A\otimes O_B)VHV^\dagger\right)\right\|_2\le\|O_A\|_2\|O_B\|_2\|H\|_\infty\sqrt{\frac{d_A}{d-1}},\tag{B18}$$

where $d=d_Ad_B$ denotes the dimension of the whole Hilbert space $\mathcal{H}_A\otimes\mathcal{H}_B$.

Proof According to the concavity of the square root function and Jensen's inequality in Lemma 9, we have

$$\mathbb{E}_V\left\|\mathrm{tr}_B\left((O_A\otimes O_B)VHV^\dagger\right)\right\|_2\le\sqrt{\mathbb{E}_V\left[\left\|\mathrm{tr}_B\left((O_A\otimes O_B)VHV^\dagger\right)\right\|_2^2\right]}.\tag{B19}$$

Using Corollary 5, the expectation under the square root in (B19) can be exactly calculated as

$$\mathbb{E}_V\left[\left\|\mathrm{tr}_B\left((O_A\otimes O_B)VHV^\dagger\right)\right\|_2^2\right]=\frac{\|O_A\|_2^2\|H\|_2^2}{d^2-1}\left[d_A\|O_B\|_2^2-\frac{|\,\mathrm{tr}\,O_B|^2}{d}\right].\tag{B20}$$

Combining (B19), (B20) and $\|H\|_2\le\sqrt{d}\|H\|_\infty$, we arrive at

$$\begin{aligned}\mathbb{E}_V\left\|\mathrm{tr}_B\left((O_A\otimes O_B)VHV^\dagger\right)\right\|_2&\le\sqrt{\frac{1}{d^2-1}}\|O_A\|_2\|H\|_2\sqrt{d_A\|O_B\|_2^2-\frac{|\,\mathrm{tr}\,O_B|^2}{d}}\\ &\le\sqrt{\frac{d_A}{d^2-1}}\|O_A\|_2\|O_B\|_2\|H\|_2\le\sqrt{\frac{d_A}{d-1}}\|O_A\|_2\|O_B\|_2\|H\|_\infty,\end{aligned}\tag{B21}$$

which is exactly the same as (B18). ■

Lemma 15 (Local unitary behind 2-design circuit) *Suppose $V\in\mathbb{V}$ is a unitary on the Hilbert space $\mathcal{H}_A\otimes\mathcal{H}_B$ with $\dim(\mathcal{H}_A)=d_A$ and $\dim(\mathcal{H}_B)=d_B$ where $\mathbb{V}$ is a unitary 2-design. Denote $U_A\in\mathcal{U}(d_A)$ as a unitary operator on $\mathcal{H}_A$. For any density matrix ρ and any traceless Hermitian operator H on $\mathcal{H}_A\otimes\mathcal{H}_B$, the following inequality holds*

$$\mathbb{E}_V\left[\max_{U_A}\left[\mathrm{tr}\left(H(U_A\otimes I_B)V\rho V^\dagger(U_A^\dagger\otimes I_B)\right)\right]\right]\le\|H\|_\infty(2d_A^2-1)\sqrt{\frac{d_A}{d_B}},\tag{B22}$$

Proof Any traceless Hermitian operator H could be expanded as

$$H=H^A+H^B+H^{AB},\tag{B23a}$$

$$H^A:=\mathrm{tr}_B(H)\otimes\frac{I_B}{d_B},\tag{B23b}$$

$$H^B:=\frac{I_A}{d_A}\otimes\mathrm{tr}_A(H),\tag{B23c}$$

$$H^{AB}:=H-H^A-H^B,\tag{B23d}$$

where H^A, H^B only act on $\mathcal{H}_A$, $\mathcal{H}_B$ non-trivially, respectively. H^{AB} acts on $\mathcal{H}_A$ and $\mathcal{H}_B$ both non-trivially. Here a linear operator acting $H^A(H^B)$ non-trivially means that the operator can not be decomposed to the tensor product form of $I_A \otimes Q_B(Q_A \otimes I_B)$ where $Q_B(Q_A)$ is an arbitrary operator on $\mathcal{H}_B(\mathcal{H}_A)$. Denote $\{\Lambda_j^A\}_{j=0}^{d_A^2-1}$ is the set of clock-and-shift matrices [5] on $\mathcal{H}_A$ which is an orthogonal basis in the linear operator space with respect to the Hilbert-Schmidt inner product. Λ_j^A are all unitary and hence $\|\Lambda_j^A\|_\infty = 1$. We assume $\Lambda_0^A = I_A$ without loss of generality. Then Λ_j^A are all traceless except Λ_0^A. Thus, H^{AB} could be further expanded in terms of Λ_j^A as

$$H^{AB} = \sum_{j=1}^{d_A^2-1} \Lambda_j^A \otimes O_j^B. \tag{B24}$$

where the explicit expression of O_j^B could be derived from (B23d) as

$$\begin{aligned} O_j^B &= \frac{1}{d_A} \operatorname{tr}_A \left(\left(\Lambda_j^{A\dagger} \otimes I_B \right) H^{AB} \right) \\ &= \frac{1}{d_A} \operatorname{tr}_A((\Lambda_j^{A\dagger} \otimes I_B)H) - \frac{1}{d_A} \operatorname{tr}_A[(\Lambda_j^{A\dagger} \otimes I_B)H^A] \\ &= \frac{1}{d_A} \operatorname{tr}_A((\Lambda_j^{A\dagger} \otimes I_B)H) - \frac{1}{d_A d_B} \operatorname{tr}_A(\Lambda_j^{A\dagger} \operatorname{tr}_B(H)) \otimes I_B. \end{aligned} \tag{B25}$$

By definition, O_j^B are all traceless. Combining (B23a) and (B24), we expand H as a summation of bipartite tensor product operators. Next, we will take the maximum for each term in the summation to obtain the desired bound, i.e.

$$\mathbb{E}_V \left[\max_{U_A} \left[\operatorname{tr} \left(H(U_A \otimes I_B) V \rho V^\dagger (U_A^\dagger \otimes I_B) \right) \right] \right] \tag{B26a}$$

$$\leq \mathbb{E}_V \left[\max_{U_A} \left[\operatorname{tr} \left(H^A(U_A \otimes I_B) V \rho V^\dagger (U_A^\dagger \otimes I_B) \right) \right] \right] \tag{B26b}$$

$$+ \mathbb{E}_V \left[\max_{U_A} \left[\operatorname{tr} \left(H^B(U_A \otimes I_B) V \rho V^\dagger (U_A^\dagger \otimes I_B) \right) \right] \right] \tag{B26c}$$

$$+ \sum_{j=1}^{d_A^2-1} \mathbb{E}_V \left[\max_{U_A} \left| \operatorname{tr} \left((\Lambda_j^A \otimes O_j^B)(U_A \otimes I_B) V \rho V^\dagger (U_A^\dagger \otimes I_B) \right) \right| \right]. \tag{B26d}$$

For (B26b) involving H^A from (B23b), Lemma 13 together with $\|\operatorname{tr}_B(H)\|_\infty \leq d_B \|H\|_\infty$ from Lemma 7 gives

$$\mathbb{E}_V \left[\max_{U_A} \left[\operatorname{tr} \left(\left(\operatorname{tr}_B(H) \otimes \frac{I_B}{d_B} \right) (U_A \otimes I_B) V \rho V^\dagger (U_A^\dagger \otimes I_B) \right) \right] \right] \leq \frac{\|\operatorname{tr}_B(H)\|_\infty}{d_B} \sqrt{\frac{d_A}{d_B}} \leq \|H\|_\infty \sqrt{\frac{d_A}{d_B}}. \tag{B27}$$

For (B26c) involving H^B from (B23c), Lemma 1 together with the given condition $\operatorname{tr}(H) = 0$ gives

$$\begin{aligned} &\mathbb{E}_V \left[\max_{U_A} \left[\operatorname{tr} \left((\frac{I_A}{d_A} \otimes \operatorname{tr}_A H)(U_A \otimes I_B) V \rho V^\dagger (U_A^\dagger \otimes I_B) \right) \right] \right] \\ = &\mathbb{E}_V \left[\operatorname{tr} \left((\frac{I_A}{d_A} \otimes \operatorname{tr}_A H) V \rho V^\dagger \right) \right] = \frac{\operatorname{tr}(\rho)}{d} \operatorname{tr}(H) = 0. \end{aligned} \tag{B28}$$

For each term in (B26d) involving O_j^B from (B23d) and (B24), Lemma 13 gives

$$\mathbb{E}_V \left[\max_{U_A} \left[\operatorname{tr} \left((\Lambda_j^A \otimes O_j^B)(U_A \otimes I_B) V \rho V^\dagger (U_A^\dagger \otimes I_B) \right) \right] \right] \leq \|\Lambda_j^A\|_\infty \|O_j^B\|_\infty \sqrt{\frac{d_A}{d_B}} = \|O_j^B\|_\infty \sqrt{\frac{d_A}{d_B}}, \tag{B29}$$

Here $\|O_j^B\|_\infty$ can be bounded using Lemma 7 as

$$\begin{aligned} \|O_j^B\|_\infty &= \left\| \frac{1}{d_A} \operatorname{tr}_A((\Lambda_j^{A\dagger} \otimes I_B)H) - \frac{1}{d_A d_B} \operatorname{tr}_A(\Lambda_j^{A\dagger} \operatorname{tr}_B(H)) \otimes I_B \right\|_\infty \\ &\leq \frac{1}{d_A} \left\| \operatorname{tr}_A((\Lambda_j^{A\dagger} \otimes I_B)H) \right\|_\infty + \frac{1}{d_A d_B} \left\| \operatorname{tr}_A(\Lambda_j^{A\dagger} \operatorname{tr}_B(H)) \otimes I_B \right\|_\infty \\ &\leq \left\| (\Lambda_j^{A\dagger} \otimes I_B)H \right\|_\infty + \frac{1}{d_B} \left\| \Lambda_j^{A\dagger} \operatorname{tr}_B(H) \right\|_\infty \\ &= \|H\|_\infty + \frac{1}{d_B} \|\operatorname{tr}_B(H)\|_\infty \leq \|H\|_\infty + \|H\|_\infty = 2\|H\|_\infty, \end{aligned} \tag{B30}$$

where we have used the unitarity of Λ_j^A and the unitary invariance of the Schatten norms. (B29) and (B30) are summarized as

$$\mathbb{E}_V\left[\max_{U_A}\left|\mathrm{tr}\left((\Lambda_j^A\otimes O_j^B)(U_A\otimes I_B)V\rho V^\dagger(U_A^\dagger\otimes I_B)\right)\right|\right]\leq 2\|H\|_\infty\sqrt{\frac{d_A}{d_B}}. \tag{B31}$$

Finally, combining (B27), (B28) and (B31), we obtain

$$\begin{aligned}&\mathbb{E}_V\left[\max_{U_A}\left[\mathrm{tr}\left(H(U_A\otimes I_B)V\rho V^\dagger(U_A^\dagger\otimes I_B)\right)\right]\right]\\&\leq\|H\|_\infty\sqrt{\frac{d_A}{d_B}}+(d_A^2-1)\cdot 2\|H\|_\infty\sqrt{\frac{d_A}{d_B}}=(2d_A^2-1)\|H\|_\infty\sqrt{\frac{d_A}{d_B}},\end{aligned} \tag{B32}$$

which is exactly the desired inequality (B22). ■

Lemma 16 (Local unitary before 2-design circuit) *Suppose $V\in\mathbb{V}$ is a unitary on the Hilbert space $\mathcal{H}_A\otimes\mathcal{H}_B$ with $\dim(\mathcal{H}_A)=d_A$ and $\dim(\mathcal{H}_B)=d_B$ where $\mathbb{V}$ is a unitary 2-design. Denote $U_A\in\mathcal{U}(d_A)$ as a unitary operator on $\mathcal{H}_A$. For any density matrix ρ and any traceless Hermitian operator H on $\mathcal{H}_A\otimes\mathcal{H}_B$, the following inequality holds*

$$\mathbb{E}_V\left[\max_{U_A}\left[\mathrm{tr}\left(HV(U_A\otimes I_B)\rho(U_A^\dagger\otimes I_B)V^\dagger\right)\right]\right]\leq\|H\|_\infty\frac{d_A^2}{\sqrt{d_Ad_B-1}}. \tag{B33}$$

Proof Similar with the proof of Lemma 15, we denote $\{\Lambda_j^A\}_{j=0}^{d_A^2-1}$ is the set of clock-and-shift matrices [5]. Any density matrix ρ can be expanded in terms of Λ_j^A as

$$\rho=\sum_{j=0}^{d_A^2-1}\Lambda_j^A\otimes O_j^B, \tag{B34}$$

where O_j^B can be explicitly expressed as

$$O_j^B=\frac{1}{d_A}\mathrm{tr}_A((\Lambda_j^{A\dagger}\otimes I_B)\rho). \tag{B35}$$

Next, we will take the maximum for each term in the summation in (B34) to obtain the desired bound, i.e.

$$\begin{aligned}&\mathbb{E}_V\left[\max_{U_A}\left[\mathrm{tr}\left(HV(U_A\otimes I_B)\rho(U_A^\dagger\otimes I_B)V^\dagger\right)\right]\right] &\text{(B36a)}\\&\leq\sum_{j=0}^{d_A^2-1}\mathbb{E}_V\left[\max_{U_A}\left|\mathrm{tr}\left(HV(U_A\otimes I_B)(\Lambda_j^A\otimes O_j^B)(U_A^\dagger\otimes I_B)V^\dagger\right)\right|\right] &\text{(B36b)}\\&=\sum_{j=0}^{d_A^2-1}\mathbb{E}_V\left[\max_{U_A}\left|\mathrm{tr}\left(U_A\Lambda_j^AU_A^\dagger\,\mathrm{tr}_B(V^\dagger HV(I_A\otimes O_j^B))\right)\right|\right] &\text{(B36c)}\end{aligned}$$

For each term in (B36c), we employ Hölder's inequality in Lemma 6 to obtain

$$\begin{aligned}\left|\mathrm{tr}\left(U_A\Lambda_j^AU_A^\dagger\,\mathrm{tr}_B(V^\dagger HV(I_A\otimes O_j^B))\right)\right|&\leq\|U_A\Lambda_j^AU_A^\dagger\|_2\left\|\mathrm{tr}_B(V^\dagger HV(I_A\otimes O_j^B))\right\|_2\\&\leq\sqrt{d_A}\left\|\mathrm{tr}_B(V^\dagger HV(I_A\otimes O_j^B))\right\|_2.\end{aligned} \tag{B37}$$

Since (B37) holds for any U_A, it certainly holds when taking the maximum, i.e.

$$\max_{U_A}\left|\mathrm{tr}\left(U_A\Lambda_j^AU_A^\dagger\,\mathrm{tr}_B(V^\dagger HV(I_A\otimes O_j^B))\right)\right|\leq\sqrt{d_A}\left\|\mathrm{tr}_B(V^\dagger HV(I_A\otimes O_j^B))\right\|_2. \tag{B38}$$

Together with Lemma 14, we obtain

$$\begin{aligned}\mathbb{E}_V\left[\max_{U_A}\left|\mathrm{tr}\left(U_A\Lambda_j^AU_A^\dagger\,\mathrm{tr}_B(V^\dagger HV(I_A\otimes O_j^B))\right)\right|\right]&\leq\sqrt{d_A}\mathbb{E}_V\left\|\mathrm{tr}_B(V^\dagger HV(I_A\otimes O_j^B))\right\|_1\\&\leq\frac{d_A}{\sqrt{d_Ad_B-1}}\|O_j^B\|_2\|H\|_\infty,\end{aligned} \tag{B39}$$

where $\|O_B\|_2$ can be bounded using (B35) and Lemma 7 as

$$\|O_B\|_2 \le \|O_B\|_1 = \frac{1}{d_A}\|\operatorname{tr}_A((\Lambda_j^{A\dagger}\otimes I_B)\rho)\|_1 \le \frac{1}{d_A}\|(\Lambda_j^{A\dagger}\otimes I_B)\rho\|_1 = \frac{1}{d_A}\|\rho\|_1 = \frac{1}{d_A}, \tag{B40}$$

where we have used the unitarity of Λ_j^A and the unitary invariance of the Schatten norms. Combining (B36), (B39) and (B40), we arrive at

$$\mathbb{E}_V\left[\max_{U_A}\left|\operatorname{tr}\left(HV(U_A\otimes I_B)\rho(U_A^\dagger\otimes I_B)V^\dagger\right)\right|\right] \le d_A^2\cdot\frac{d_A}{\sqrt{d_Ad_B-1}}\cdot\frac{1}{d_A}\|H\|_\infty = \|H\|_\infty\frac{d_A^2}{\sqrt{d_Ad_B-1}}, \tag{B41}$$

which is exactly the same as (B33). ■

In fact, in the proofs of Lemma 15 and 16 above, the clock-and-shift matrices could be replaced by Pauli strings specially for qubit systems. Finally, we provide a proof for Theorem 1, which we recall for convenience. Note that compared to Theorem 1 in the manuscript, here we prove a more general version where the Hilbert space dimension is no more restricted to qubit systems.

Theorem 1 *Suppose $V_1\in\mathbb{V}_1, V_2\in\mathbb{V}_2$ are unitaries on the Hilbert space $\mathcal{H}_A\otimes\mathcal{H}_B$ with $\dim(\mathcal{H}_A)=d_A$ and $\dim(\mathcal{H}_B)=d_B$. Denote $U_A\in\mathcal{U}(d_A)$ as a unitary on $\mathcal{H}_A$. If either $\mathbb{V}_1$ or $\mathbb{V}_2$, or both are unitary 2-designs, then for any density matrix ρ and any Hermitian operator H on $\mathcal{H}_A\otimes\mathcal{H}_B$, then the following inequality holds*

$$\mathbb{E}_{V_1,V_2}[\Delta_{H,\rho}(V_1,V_2)] \le 4w(H)d_A^2\sqrt{\frac{d_A}{d_B}}. \tag{B42}$$

where $\mathbb{E}_{V_1,V_2}$ denotes the expectation over $\mathbb{V}_1,\mathbb{V}_2$ independently. $w(H)=\lambda_{\max}(H)-\lambda_{\min}(H)$ denotes the spectral width of H, where $\lambda_{\max}(H)$ is the maximum eigenvalue of H and $\lambda_{\min}(H)$ is the minimum.

Proof By definition, we have $\mathbf{U}=V_2(U_A\otimes I_B)V_1$ and

$$\Delta_{H,\rho}(V_1,V_2) = \max_{U_A}\left[\operatorname{tr}\left(H\mathbf{U}\rho\mathbf{U}^\dagger\right)\right] - \min_{U_A}\left[\operatorname{tr}\left(H\mathbf{U}\rho\mathbf{U}^\dagger\right)\right], \tag{B43}$$

where the maximum and minimum with respect to U_A are taken over the entire unitary group $\mathcal{U}(d_A)$ of degree d_A. Without loss of generality, we assume that H is traceless since (B42) is invariant if H is added by a homothety $H\to H+cI$, $c\in\mathbb{R}$. Moreover, considering that the minimization term in (B43) could be written as

$$-\min_{U_A}\left[\operatorname{tr}\left(H\mathbf{U}\rho\mathbf{U}^\dagger\right)\right] = \max_{U_A}\left[\operatorname{tr}\left((-H)\mathbf{U}\rho\mathbf{U}^\dagger\right)\right], \tag{B44}$$

and $w(H)=w(-H)$, in order to prove (B42), we only need to prove that

$$\mathbb{E}_{V_1,V_2}\left[\max_{U_A}\left[\operatorname{tr}\left(H\mathbf{U}\rho\mathbf{U}^\dagger\right)\right]\right] \le 2w(H)d_A^2\sqrt{\frac{d_A}{d_B}}, \tag{B45}$$

holds for any traceless Hermitian operator H. On the one hand, if $\mathbb{V}_1$ is a unitary 2-design, Lemma 15 gives

$$\begin{aligned}\mathbb{E}_{V_1,V_2}\left[\max_{U_A}\left[\operatorname{tr}\left(H\mathbf{U}\rho\mathbf{U}^\dagger\right)\right]\right] &= \mathbb{E}_{V_2}\left\{\mathbb{E}_{V_1}\left[\max_{U_A}\left[\operatorname{tr}\left(V_2^\dagger HV_2(U_A\otimes I_B)V_1\rho V_1^\dagger(U_A^\dagger\otimes I_B)\right)\right]\right]\right\}\\ &\le \mathbb{E}_{V_2}\left[\|V_2^\dagger HV_2\|_\infty(2d_A^2-1)\sqrt{\frac{d_A}{d_B}}\right] = \|H\|_\infty(2d_A^2-1)\sqrt{\frac{d_A}{d_B}}.\end{aligned} \tag{B46}$$

where we have used the unitary invariance of the Schatten norms and the normalization condition $\mathbb{E}_{V_2}[1]=1$. On the other hand, if $\mathbb{V}_2$ is a unitary 2-design, Lemma 16 gives

$$\begin{aligned}\mathbb{E}_{V_1,V_2}\left[\max_{U_A}\left[\operatorname{tr}\left(H\mathbf{U}\rho\mathbf{U}^\dagger\right)\right]\right] &= \mathbb{E}_{V_1}\left\{\mathbb{E}_{V_2}\left[\max_{U_A}\left[\operatorname{tr}\left(HV_2(U_A\otimes I_B)V_1\rho V_1^\dagger(U_A^\dagger\otimes I_B)V_2^\dagger\right)\right]\right]\right\}\\ &\le \mathbb{E}_{V_1}\left\{\|H\|_\infty\frac{d_A^2}{\sqrt{d_Ad_B-1}}\right\} = \|H\|_\infty\frac{d_A^2}{\sqrt{d_Ad_B-1}}.\end{aligned} \tag{B47}$$

where we have used the fact that $V_1\rho V_1^\dagger$ is also a density matrix and the normalization condition $\mathbb{E}_{V_1}[1]=1$. Note that for any traceless Hermitian operator H, we have $\lambda_{\max}(H)\ge 0$, $\lambda_{\min}(H)\le 0$ and

$$\|H\|_\infty = \max\{\lambda_{\max}(H),-\lambda_{\min}(H)\} \le \lambda_{\max}(H)-\lambda_{\min}(H) = w(H). \tag{B48}$$

Combining (B46), (B47), (B48) and

$$
\begin{aligned}
&(2d_A^2-1)\sqrt{\frac{d_A}{d_B}} < 2d_A^2\sqrt{\frac{d_A}{d_B}},\\
&\frac{d_A^2}{\sqrt{d_Ad_B-1}} < \frac{d_A^2}{\sqrt{(d_A-1)d_B}} < 2d_A^2\sqrt{\frac{d_A}{d_B}},
\end{aligned}
\tag{B49}
$$

for $d_A \geq 2$, we know that the inequality

$$
\mathbb{E}_{V_1,V_2}\left[\max_{U_A}\left[\mathrm{tr}\left(H\mathbf{U}\rho\mathbf{U}^\dagger\right)\right]\right] \leq 2w(H)d_A^2\sqrt{\frac{d_A}{d_B}},
\tag{B50}
$$

holds if either $\mathbb{V}_1$ or $\mathbb{V}_2$ is a unitary 2-design. Certainly, (B50) also holds if both $\mathbb{V}_1$ and $\mathbb{V}_2$ are 2-designs. Together with (B44), we arrive at (B42). ■

Note that for qubit systems where $d_A = 2^m$ and $d_B = 2^{n-m}$, the upper bound in (B42) reduces to that in the manuscript, i.e.

$$
\mathbb{E}_{V_1,V_2}[\Delta_{H,\rho}(V_1,V_2)] \leq \frac{w(H)}{2^{n/2-3m-2}}.
\tag{B51}
$$

Although Theorem 1 only establish an upper bound on the expectation of $\Delta_{H,\rho}(V_1,V_2)$, we can derive the upper bound on the variance of $\Delta_{H,\rho}(V_1,V_2)$ from Theorem 1 with the non-negativity and boundedness of $\Delta_{H,\rho}(V_1,V_2)$. Namely, since $\Delta_{H,\rho}(V_1,V_2) \in [0, w(H)]$, Lemma 10 gives

$$
\mathrm{Var}_{V_1,V_2}[\Delta_{H,\rho}(V_1,V_2)] \leq w(H)\cdot\mathbb{E}_{V_1,V_2}[\Delta_{H,\rho}(V_1,V_2)] \leq 4w^2(H)d_A^2\sqrt{\frac{d_A}{d_B}}.
\tag{B52}
$$

Furthermore, Theorem 1 together with the non-negativity of $\Delta_{H,\rho}(V_1,V_2)$ can also provide an upper bound of the probability that $\Delta_{H,\rho}(V_1,V_2)$ deviates from zero. Specifically, according to Theorem 1 and Markov's inequality in Lemma 8, the following concentration inequality

$$
\Pr\left[\Delta_{H,\rho}(V_1,V_2) \geq \epsilon\right] \leq \frac{\mathbb{E}_{V_1,V_2}[\Delta_{H,\rho}(V_1,V_2)]}{\epsilon} \leq \frac{4w(H)d_A^2}{\epsilon}\sqrt{\frac{d_A}{d_B}},
\tag{B53}
$$

holds for any $\epsilon > 0$. It is worth noticing that the upper bound in (B42) only involves $w(H)$ and does not depend on any detail of the Hermitian operator H. In order to derive this compact and general upper bound in (B42), we perform many relaxations such as in (B24), (B48) and (B49). Otherwise, if some specific structures about H are known, a more complicated but tighter bound could be obtained as

$$
\mathbb{E}_{V_1,V_2}[\Delta_{H,\rho}(V_1,V_2)] \leq \max\{N_A + 2N_{AB}, d_A\sqrt{\frac{d}{d-1}}\}\cdot\left\|H - \mathrm{tr}(H)\frac{I}{d}\right\|_\infty\sqrt{\frac{d_A}{d_B}},
\tag{B54}
$$

where $N_A \leq 1$ denotes the number of non-vanishing terms in (B23b) and $N_{AB} \leq (d_A^2-1)$ denotes the number of non-vanishing terms in (B24), which can be seen as a "coupling rank" or say "coupling complexity" between subsystem A and B of the Hamiltonian H. The variational quantum eigensolver (VQE) example of the Heisenberg model $\hat{H}$ in the main text has $N_A = 0$, $N_{AB} = 3$ and that of quantum autoencoder (QAE) has $N_A = 1$, $N_{AB} = 0$. Therefore, we have two tighter bound for these two examples as

$$
\begin{aligned}
\text{Heisenberg:}\quad &\mathbb{E}_{V_1,V_2}[\Delta_{\mathrm{VQE}}(V_1,V_2)] \leq 24\cdot w(\hat{H})\cdot\frac{1}{2^{n/2}},\\
\text{Autoencoder:}\quad &\mathbb{E}_{V_1,V_2}[\Delta_{\mathrm{QAE}}(V_1,V_2)] \leq \frac{8}{\sqrt{3}}\cdot\frac{1}{2^{n/2}},
\end{aligned}
\tag{B55}
$$

which are used in the figure of the numerical simulation section in the main text.

Appendix C: Proof of Proposition 2

In this section, we prove Lemma 17-19 first and derive Proposition 2 by use of these lemmas.

Lemma 17 *For any density matrices ρ and σ we have*

$$F(\rho,\sigma) \leq \operatorname{rank}(\rho\sigma)\operatorname{tr}(\rho\sigma), \tag{C1}$$

where $F(\rho,\sigma) = \left(\operatorname{tr}\sqrt{\rho^{1/2}\sigma\rho^{1/2}}\right)^2$ denotes the Bures fidelity.

Proof Let λ_i be the i-th eigenvalue of $\sqrt{\rho^{1/2}\sigma\rho^{1/2}}$ in the non-increasing order. Note that $\lambda_i \geq 0$ holds for any i due to the positive semi-definite property of $\sqrt{\rho^{1/2}\sigma\rho^{1/2}}$. By definition, the square root of the Bures fidelity can be represented as

$$\sqrt{F(\rho,\sigma)} = \sum_i \lambda_i, \tag{C2}$$

while the square root of the Hilbert-Schmidt inner product of ρ and σ can be represented as

$$\sqrt{\operatorname{tr}(\rho\sigma)} = \sqrt{\operatorname{tr}(\rho^{1/2}\sigma\rho^{1/2})} = \sqrt{\sum_i \lambda_i^2}. \tag{C3}$$

According to the inequality between the vector 1-norm and 2-norm $\|\mathbf{x}\|_1 \leq \sqrt{n}\|\mathbf{x}\|_2$ for any n-dimensional vector $\mathbf{x}$, (C2) and (C3) lead to

$$\sqrt{F(\rho,\sigma)} \leq \sqrt{\operatorname{rank}(\rho\sigma)}\sqrt{\operatorname{tr}(\rho\sigma)}. \tag{C4}$$

Take the square of both sides and we arrive at (C1). ∎

Lemma 18 *Suppose $V \in \mathbb{V}$ is a unitary on the Hilbert space $\mathcal{H}_A \otimes \mathcal{H}_B$ with $\dim(\mathcal{H}_A) = d_A$ and $\dim(\mathcal{H}_B) = d_B$ where $\mathbb{V}$ is a unitary 1-design. Denote $U_A \in \mathcal{U}(d_A)$ as a unitary operator on $\mathcal{H}_A$. For any density matrices ρ and σ on $\mathcal{H}_A \otimes \mathcal{H}_B$, the following inequality holds*

$$\mathbb{E}_V\left[\max_{U_A} F((U_A\otimes I_B)V\rho V^\dagger(U_A\otimes I_B)^\dagger,\sigma)\right] \leq \frac{d_A}{d_B}. \tag{C5}$$

where F denotes the Bures fidelity.

Proof According to the monotonicity of the Bures fidelity under the action of quantum channels [6], we have

$$F((U_A\otimes I_B)V\rho V^\dagger(U_A\otimes I_B)^\dagger,\sigma) \leq F(\operatorname{tr}_A\left((U_A\otimes I_B)V\rho V^\dagger(U_A\otimes I_B)^\dagger\right),\operatorname{tr}_A\sigma) = F(\operatorname{tr}_A\left(V\rho V^\dagger\right),\operatorname{tr}_A\sigma). \tag{C6}$$

Since (C6) holds for any U_A, it certainly holds when taking the maximum. Together with Lemma 17, it holds that

$$\max_{U_A} F((U_A\otimes I_B)V\rho V^\dagger(U_A\otimes I_B)^\dagger,\sigma) \leq F(\operatorname{tr}_A\left(V\rho V^\dagger\right),\operatorname{tr}_A\sigma) \leq d_A\operatorname{tr}(\operatorname{tr}_A\left(V\rho V^\dagger\right)\operatorname{tr}_A\sigma). \tag{C7}$$

Because $\mathbb{V}$ is a unitary 1-design, we can apply Lemma 1 to obtain

$$\mathbb{E}_V\left[\operatorname{tr}(\operatorname{tr}_A\left(V\rho V^\dagger\right)\operatorname{tr}_A\sigma)\right] = \operatorname{tr}\left(\operatorname{tr}_A\left(\frac{\operatorname{tr}(\rho)}{d}I\right)\operatorname{tr}_A\sigma\right) = \operatorname{tr}(\rho)\operatorname{tr}(\sigma)\frac{1}{d_B} \leq \frac{1}{d_B}, \tag{C8}$$

where $d = d_A d_B$ denotes the dimension of $\mathcal{H}_A \otimes \mathcal{H}_B$. Combining (C7) and (C8), we arrive at (C5). ∎

Lemma 19 *Suppose $V_1 \in \mathbb{V}_1, V_2 \in \mathbb{V}_2$ are independent unitaries on the Hilbert space $\mathcal{H}_A \otimes \mathcal{H}_B$ with $\dim(\mathcal{H}_A) = d_A$ and $\dim(\mathcal{H}_B) = d_B$. Denote $U_A \in \mathcal{U}(d_A)$ as a unitary operator on $\mathcal{H}_A$. If either $\mathbb{V}_1$ or $\mathbb{V}_2$, or both are unitary 1-designs, then for any density matrix ρ and σ on $\mathcal{H}_A \otimes \mathcal{H}_B$, the following inequality holds*

$$\mathbb{E}_{V_1,V_2}\left[\max_{U_A} F\left(\mathbf{U}\rho\mathbf{U}^\dagger,\sigma\right)\right] \leq \frac{d_A}{d_B}, \tag{C9}$$

where $\mathbf{U} = V_2(U_A\otimes I_B)V_1$ and F is the Bures fidelity.

Proof On the one hand, if $\mathbb{V}_1$ is a unitary 1-design, Lemma 18 gives

$$\begin{aligned}\mathbb{E}_{V_1,V_2}\left[\max_{U_A} F\left(\mathbf{U}\rho\mathbf{U}^\dagger,\sigma\right)\right] &= \mathbb{E}_{V_2}\left\{\mathbb{E}_{V_1}\left[\max_{U_A} F\left((U_A\otimes I_B)V_1\rho V_1^\dagger(U_A\otimes I_B)^\dagger, V_2^\dagger\sigma V_2\right)\right]\right\}\\ &\le \mathbb{E}_{V_2}\left[\frac{d_A}{d_B}\right] = \frac{d_A}{d_B},\end{aligned} \tag{C10}$$

where we have used the unitary invariance of the fidelity and the normalization condition $\mathbb{E}_{V_2}[1] = 1$. Note that in this case there is no restriction on $\mathbb{V}_2$. On the other hand, if $\mathbb{V}_2$ is a unitary 1-design, similarly, Lemma 18 gives

$$\begin{aligned}\mathbb{E}_{V_1,V_2}\left[\max_{U_A} F\left(\mathbf{U}\rho\mathbf{U}^\dagger,\sigma\right)\right] &= \mathbb{E}_{V_1}\left\{\mathbb{E}_{V_2}\left[\max_{U_A} F\left(V_1\rho V_1^\dagger, (U_A\otimes I_B)^\dagger V_2^\dagger\sigma V_2(U_A\otimes I_B)\right)\right]\right\}\\ &\le \mathbb{E}_{V_1}\left[\frac{d_A}{d_B}\right] = \frac{d_A}{d_B},\end{aligned} \tag{C11}$$

where we have used the unitary invariance of the fidelity again and the normalization condition $\mathbb{E}_{V_1}[1] = 1$. Combining (C10) and (C11), we know that (C9) holds if either $\mathbb{V}_1$ or $\mathbb{V}_2$ is a unitary 1-design. Certainly, (C9) also holds if both $\mathbb{V}_1$ and $\mathbb{V}_2$ are 1-designs. ■

Finally, we provide a proof for Proposition 2. Compared to Proposition 2 in the manuscript, here we prove a more general version where the Hilbert space dimension is no more restricted to qubit systems.

Proposition 2 *Suppose $V_1 \in \mathbb{V}_1, V_2 \in \mathbb{V}_2$ are independent unitaries on the Hilbert space $\mathcal{H}_A \otimes \mathcal{H}_B$ with $\dim(\mathcal{H}_A) = d_A$ and $\dim(\mathcal{H}_B) = d_B$. Denote $U_A \in \mathcal{U}(d_A)$ as a unitary operator on $\mathcal{H}_A$. If either V_1 or V_2, or both are from unitary 1-designs, then for any density matrices ρ and σ, the following inequality holds*

$$\mathbb{E}_{V_1,V_2}\left[\Delta_{\mathrm{QSL}}(V_1,V_2)\right] \le \frac{d_A}{d_B}, \tag{C12}$$

where $\mathbb{E}_{V_1,V_2}$ denotes the expectation over $\mathbb{V}_1, \mathbb{V}_2$ independently.

Proof By definition, we have $\mathbf{U} = V_2(U_A \otimes I_B)V_1$ and

$$\Delta_{\mathrm{QSL}}(V_1,V_2) = \max_{U_A} F\left(\mathbf{U}\rho\mathbf{U}^\dagger,\sigma\right) - \min_{U_A} F\left(\mathbf{U}\rho\mathbf{U}^\dagger,\sigma\right). \tag{C13}$$

According to Lemma 19 and the non-negativity of the fidelity, it holds that

$$\mathbb{E}_{V_1,V_2}\left[\Delta_{\mathrm{QSL}}(V_1,V_2)\right] \le \mathbb{E}_{V_1,V_2}\left[\max_{U_A} F\left(\mathbf{U}\rho\mathbf{U}^\dagger,\sigma\right)\right] \le \frac{d_A}{d_B}, \tag{C14}$$

if either V_1 or V_2, or both are from unitary 1-designs. ■

For qubit systems where $d_A = 2^m$ and $d_B = 2^{n-m}$, the upper bound in (C12) reduces to that in the manuscript, i.e.

$$\mathbb{E}_{V_1,V_2}[\Delta_{\mathrm{QSL}}(V_1,V_2)] \le \frac{1}{2^{n-2m}}. \tag{C15}$$

Importantly, due to the non-negativity and boundedness of $\Delta_{\mathrm{QSL}}(V_1,V_2)$, we can derive the upper bound on the variance and the probability tail from Proposition 2 using Lemma 10 and Markov's inequality in Lemma 8, i.e.

$$\begin{aligned}&\mathrm{Var}_{V_1,V_2}[\Delta_{\mathrm{QSL}}(V_1,V_2)] \le 1\cdot\mathbb{E}_{V_1,V_2}[\Delta_{\mathrm{QSL}}(V_1,V_2)] \le \frac{d_A}{d_B},\\ &\Pr\left[\Delta_{\mathrm{QSL}}(V_1,V_2) \ge \epsilon\right] \le \frac{\mathbb{E}_{V_1,V_2}[\Delta_{\mathrm{QSL}}(V_1,V_2)]}{\epsilon} \le \frac{1}{\epsilon}\frac{d_A}{d_B},\quad \forall\, \epsilon > 0.\end{aligned} \tag{C16}$$

Appendix D: Numerical simulation with varying layers

This section provides some experimental results on how the variation range of the cost function caused by a local unitary varies with the number of circuit layers. We construct circuits of V_1 with different numbers of layers to perform experiments with other settings the same as those in the manuscript. As shown in Fig. 1, different lines with markers represent the average

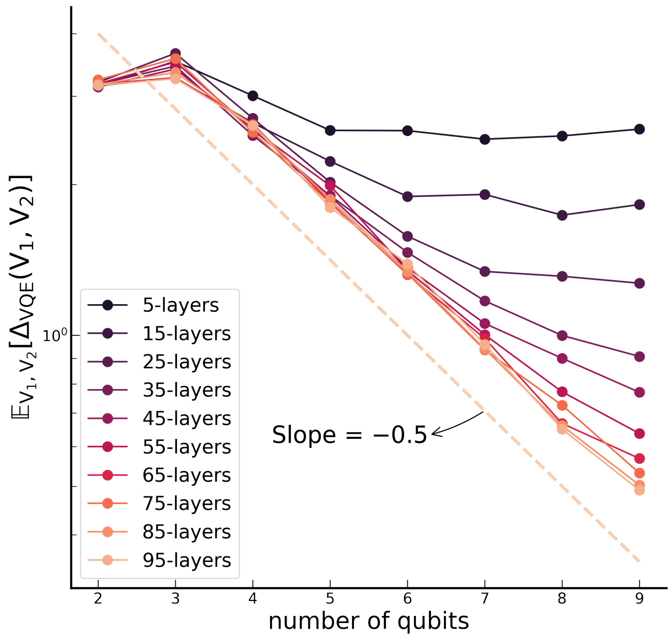


FIG. 1. The semi-log plot of the average value of the variation range $\Delta_{\mathrm{VQE}}(V_1, V_2)$ vs. the number of qubits. The cost function used here is the energy expectation of the 1-dimensional antiferromagnetic Heisenberg model. Different lines represent different numbers of circuit layers from 5 to 95 with step length 10, with the line for 5 layers on the top and 95 layers on the bottom. And the dashed line, as a guide to the eye, has a slope of -0.5, which is the exponential decay rate we derived in Theorem 1.

value of $\Delta_{\mathrm{VQE}}(V_1, V_2)$ over samples vs. the number of qubits n corresponding to different numbers of layers we laid in V_1. We can see that as the number of layers increases, these lines become more and more parallel to the dashed reference line, which has a slope of -0.5, i.e., the exponential decay rate we derived in Theorem 1. Thus there is a transition to 2-design where $\mathbb{E}_{V_1,V_2}[\Delta_{H,\rho}(V_1, V_2)]$ converges. This implies that Theorem 1 is valid when the circuit is sufficiently deep, practically with depth around $10 \times n$.

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