On spectral gaps of locally random one-dimensional nearest-neighbor quantum circuits

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Introduction: Random quantum circuits have played an important role in quantum computation and quantum information sciences. Their study has allowed researchers to find experiments capable of achieving a quantum advantage by offering classically-hard to simulate sampling experiments [1–6], providing insights into quantum chaos [7–9] and entanglement transitions [10–12], as well as improving the study of the trainability of variational quantum algorithms [13–19]. In particular, random quantum circuits composed of local unitary gates sampled independently and identically distributed (i.i.d.) according to the Haar measure over the standard representation of $\mathbb{U}(4)$, and acting on neighboring pairs of qubits in a one-dimensional lattice, have received considerable attention. While several works [20–23] have provided bounds for their spectral gap–the absolute value of the largest non-one eigenvalue of the t-th moment operator of the random circuit's unitary distribution–its exact value has not been reported. In this work we contribute to the body of knowledge of random quantum circuits by exactly computing the $t=2$ spectral gap for unitary circuits in a line (open boundary conditions) and in a circle (closed boundary conditions), showcasing that the latter is exactly the square root of the former for all system sizes. Moreover, we also numerically compare such spectral gaps to those obtained from random circuits with local gates sampled from the orthogonal and symplectic groups.

Framework: Let $\mathcal{H}=(\mathbb{C}^d)^{\otimes n}$ be the Hilbert space of n qudits. In this work we study random circuits $U:\mathcal{H}\rightarrow\mathcal{H}$ in a one-dimensional lattice composed of local gates acting on alternating pairs of nearest neighboring qudits. As such, the circuit U can be expressed as a product of layers of the form

$$U=\prod_{l=1}^{L}U_l\,,\quad \text{where}\quad U_l=(U_{n,1}^l)^{\Delta}U_{2,3}^lU_{4,5}^l\cdots U_{n-2,n-1}^lU_{1,2}^lU_{3,4}^l\cdots U_{n-1,n}^l\,. \tag{1}$$

Here, $U_{j,j'}$ is a local unitary that acts on qudits j and j', and $\Delta=0$ for open boundary conditions (unitaries acting in a line), while $\Delta=1$ for closed boundary conditions (unitaries acting in a circle). We show such a circuit in Fig. 1. We assume that each $U_{j,j'}$ is sampled i.i.d. according to the Haar measure over some local group $G_{j,j'}^l$. Specifically, we will consider the cases when $G_{j,j'}^l=\mathbb{U}(d^2)$, $\mathbb{O}(d^2)$ or $\mathbb{SP}(d^2/2)$. Crucially, it is known that in the large number of layers limit (i.e., as $L\rightarrow\infty$), the distribution of unitaries will converge to that of some global group $\mathbb{G}\subseteq\mathbb{U}(d^n)$ that is determined by the local groups from which the gates are sampled.

Here, one may ask the question: *How fast does the distribution of unitaries $\mathcal{E}_L$ obtained from a shallow circuit U converges to the Haar measure over $\mathbb{G}$?* To answer this question, one defines the t-th moment operator

$$\mathcal{A}_L^{(t)}=\mathcal{T}_{\mathbb{G}}^{(t)}-\mathcal{T}_{\mathcal{E}_L}^{(t)}\,,\quad\text{with}\quad \mathcal{T}_{\mathbb{G}}^{(t)}=\int_{\mathbb{G}}d\mu U^{\otimes t}\otimes(U^*)^{\otimes t}\,,\quad\text{and}\quad \mathcal{T}_{\mathcal{E}_L}^{(t)}=\int_{\mathcal{E}_L}dU U^{\otimes t}\otimes(U^*)^{\otimes t}\,, \tag{2}$$

where $\int_{\mathbb{G}}d\mu$ denotes the Haar measure over $\mathbb{G}$, and $\int_{\mathcal{E}_L}dU$ the average over the set of unitaries $\mathcal{E}_L$ (and the associated distribution dU) obtained from an L-layered circuit U as in Eq. (1). As such, the matrix $\mathcal{A}_L^{(t)}$ quantifies how much the t-th moment of the distributions differ, and we say that $\mathcal{E}_L$ forms an ε-approximate t-design if $|\mathcal{A}_L^{\otimes t}|_\infty\leqslant\varepsilon$. Crucially, given that the moment operator over the Haar measure of a group is a projector onto its t-th order commutant (i.e., onto the set of operators that commute with $U^{\otimes t}$ for any unitary in the group) [24], then we know that $\mathcal{T}_{\mathbb{G}}^{(t)}$ can only have eigenvalues which are equal to one or zero. Moreover, it is well known that $\mathcal{T}^{(t)}_{\mathcal{E}_L}$ must share exactly the same eigenvectors with eigenvalue equal to one as $\mathcal{T}^{(t)}_{\mathbb{G}}$. Hence, we can study how many layers are needed for the distribution of unitaries to become an ε-approximate t-design by quantifying the largest non-one eigenvalue, or the spectral gap, of $\mathcal{T}^{(t)}_{\mathcal{E}_L}$, which we denote as $\lambda^{(n)}_{max}$.

Theoretical Results: Our main theoretical result is an exact characterization of the spectral gap for the $t = 2$ case when $G^l_{j,j'} = \mathbb{U}(d^2)\ \forall j, j'$ in Eq. (1) (the spectral gap for $t = 1$ can be trivially found to be zero, indicating that for all L, the circuit forms a 1-design). Clearly, the distribution of unitaries of such a circuit will converge to the group $\mathbb{G} = \mathbb{U}(d^n)$, for which it is known that $\mathcal{T}^{(t)}_{\mathbb{U}(d^n)}$ has only two non-zero eigenvalues [25]. Below we describe our proof technique, which consists of a series of dimensionality reductions and simplifications.

- We first note that the operator $\mathcal{T}^{(2)}_{\mathcal{E}_L}$ can be expressed as $\mathcal{T}^{(2)}_{\mathcal{E}_L} = \prod_l \mathcal{T}^{(2)}_{\mathcal{E}_l} = (\mathcal{T}^{(2)}_{\mathcal{E}})^L$, where $\mathcal{T}^{(2)}_{\mathcal{E}}$ is the single-layer 2-nd moment operator $\mathcal{T}^{(2)}_{\mathcal{E}} = (\mathcal{T}^{(2)}_{n,1})^{\Delta}\mathcal{T}^{(2)}_{2,3}\mathcal{T}^{(2)}_{4,5}\cdots\mathcal{T}^{(2)}_{n-2,n-1}\mathcal{T}^{(2)}_{1,2}\mathcal{T}^{(2)}_{3,4}\cdots\mathcal{T}^{(2)}_{n-1,n}$, and with the $\mathcal{T}^{(2)}_{j,j'}$ being 2-nd moment operators for the local gates in the circuit. Therefore, instead of computing the eigenvalues of $\mathcal{T}^{(2)}_{\mathcal{E}_L}$, we can study those of $\mathcal{T}^{(2)}_{\mathcal{E}}$.

- Next, we use the fact that each $\mathcal{T}^{(2)}_{j,k'}$ is a projector into the local two-dimensional commutant of $\mathbb{U}(d^2)$ [25, 26]. Hence, for all qudit dimensions d, one can evaluate the effective action of $\mathcal{T}^{(2)}_{\mathcal{E}}$ as a $2^n \times 2^n$ matrix where each $\mathcal{T}^{(2)}_{j,j'}$ is replaced by the 4×4 projector A presented below in Eq. (3). That is, we need to compute the eigenvalues of the $2^n \times 2^n$ matrix $P = L_2 L_1$ with $L_2 = (A_{n,1})^{\Delta} A_{2,3}A_{4,5}\cdots A_{n-2,n-1}$ and $L_1 = A_{1,2}A_{3,4}\cdots A_{n-1,n}$, and where $A_{j,j'}$ indicates that a 4×4 projector A acts on the qubits j and j'.

- Since each $A_{j,j'}$ is a projector, one can verify that L_2 is a projector, indicating that any eigenvector of P must also be an eigenvector of L_2 with eigenvalue one (this follows from the fact that $(L_2)^k P = P$ for all k). Such simplification allows us to note that the eigenvectors of P can only span a $2^{n/2}$ dimensional space. Taking $\Delta = 0$ (open boundary conditions), we find that an appropriate selection of basis allows us to express the action of P as the $2^{n/2} \times 2^{n/2}$ upper-triangular block matrix $\widetilde{P}$ given in Eq. (3).

$$A = \begin{pmatrix} 1 & \frac{d^3-d}{d^4-1} & \frac{d^3-d}{d^4-1} & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & \frac{d^3-d}{d^4-1} & \frac{d^3-d}{d^4-1} & 1 \end{pmatrix}, \quad \widetilde{P} = \begin{pmatrix} 1 & 0 & \cdots & \cdots & \cdots \\ 0 & 1 & \cdots & \cdots & \cdots \\ 0 & 0 & \boxed{B_1} & \cdots & \cdots \\ & 0 & & \boxed{B_2} & \cdots \\ & 0 & & 0 & \ddots \end{pmatrix}, \quad B_1 = \left(\frac{d^3-d}{d^4-1}\right)^2 \begin{pmatrix} 2 & 1 & 0 & 0 & \dots & 0 \\ 1 & 2 & 1 & 0 & \dots & 0 \\ 0 & 1 & 2 & 1 & \dots & 0 \\ \vdots & & \ddots & \ddots & \ddots & \vdots \\ 0 & \dots & 0 & 1 & 2 & 1 \\ 0 & \dots & 0 & 0 & 1 & 2 \end{pmatrix}. \tag{3}$$

- From Eq. (3) we know that the eigenvalues of $\widetilde{P}$ are those of each block in the diagonal. First we find two eigenvalues equal to one (whose associated eigenvectors are verified to be those of $\mathcal{T}^{(t)}_{\mathbb{U}(d^n)}$). Next, we show that the maximum eigenvalue of the k-th block is upper bounded by $\left(\frac{2(d^3-d)}{d^4-1}\right)^{2k}$. Then, the B_1 submatrix (of size $\frac{n-2}{2} \times \frac{n-2}{2}$) shown in Eq. (3) is Toeplitz and tridiagonal, meaning that an exact formula for its eigenvalues can be derived. As such, we can prove that the largest eigenvalue of B_1 is larger than any eigenvalue of $B_k\ \forall k \geqslant 2$, leading to the analytical expression $\lambda^{(n)}_{max} = (\frac{d^3-d}{d^4-1})^2(2 + 2cos(\frac{2\pi}{n}))$. In the large n limit $\lambda^{(n)}_{max} \xrightarrow[n\to\infty]{} (\frac{d^3-d}{d^4-1})^2$ or $\lambda^{(n)}_{max} \xrightarrow[n\to\infty]{} \frac{16}{25} = .64$ for the qubit $d = 2$ case.

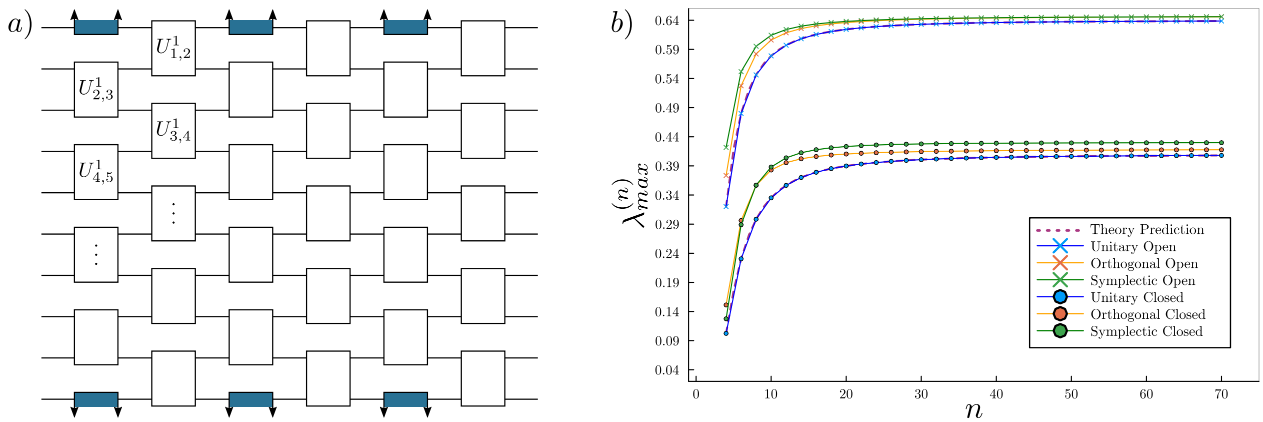

Figure 1. a) We study random quantum circuits where local random gates act on alternating pairs of neighboring qudits. The colored gates are removed (added) with open (closed) boundary conditions. b) We numerically show the spectral gap versus n for a single layer of circuits composed of local unitary, orthogonal and symplectic gates; as detailed in the main text. We show, as a dashed curved, the theoretical predictions for the unitary case with open and closed boundaries.

- For the closed boundary conditions, we follow a similar procedure and find that the important sub-matrix is now pentadiagonal and not Toeplitz. In fact, the form of the matrix ends up being the exact square of the open boundary case so that $\lambda^{(n)}_{max} = \left(\frac{d^3-d}{d^4-1}\right)^4 (2+2cos(\frac{2\pi}{n}))^2$ and $\lambda^{(n)}_{max} \xrightarrow[n\to\infty]{} \frac{256}{625} = .4096$ if $d=2$.

Numerical Results: Here we compare the spectral gap of the unitary case with that of a single layer for the following cases: (i) All local gates are sampled from the orthogonal group $G^l_{j,j'} = \mathbb{O}(d^2)\ \forall j, j'$, so that the ensuing unitary distribution converges in the large number of layers limit to $\mathbb{G} = \mathbb{O}(d^n)$ for both open and closed boundary conditions; and (ii) The local gates are sampled from the orthogonal group $G^l_{j,j'} = \mathbb{O}(d^2)$ if j, j' are not equal to one, and $G^l_{j,j'} = \mathbb{SP}(d^2/2)$ if j or j' are equal to one, for in these cases one can prove that for large L the distribution converges to $\mathbb{G} = \mathbb{SP}(d^n/2)$ [27]. We note that in these two cases we were unable to analytically compute the spectral gap. However, in our manuscript we propose a technique to numerically compute these gaps via Density Matrix Renormalization Group (DMRG) for up to $n = 70$ qubits. The results of the unitary cases align exactly with the theoretical prediction. Then, calculations show that the spectral gap of a single layer from the orthogonal group is greater than that of the unitary and even passes the unitary limit of 16/25 at around 26 qubits. The limit of the orthogonal group, does not seem to be much higher than that of the unitary as the spectral gap at 70 qubits is around .6460. As for the symplectic group, the spectral gap seems to be larger than both that of the unitary and orthogonal group for open and closed boundary conditions (surpassing the unitary limit of 16/25 at $n = 24$, and being equal to .6461 at $n = 70$). With open boundaries, the gap of orthogonal and symplectic appear to converge, whereas with closed there is a notable difference, as the gap for symplectic unitaries is larger. Finally, we can verify that in the orthogonal and symplectic cases, the open and closed boundary spectral gaps are not related by a square root as in the unitary case.

Conclusions and Impact: The study of random quantum circuits is central in quantum information and computation. While there exists several works in the literature which provide bounds to the spectral gaps of locally random quantum circuits, our work is the first one which—to our knowledge—provides an explicit formula for $\lambda^{(n)}_{max}$. Our hope is that the tools and techniques developed here can be used as blueprints to either exactly compute, or better approximate, spectral gaps in other scenarios and for more general groups.

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