Classical algorithms for quantum mean values

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Abstract

We consider the task of estimating the expectation value of an \( n \)-qubit tensor product observable \( O_1 \otimes O_2 \otimes \cdots \otimes O_n \) in the output state of a shallow quantum circuit. This task is a cornerstone of variational quantum algorithms for optimization, machine learning, and the simulation of quantum many-body systems. Here we study its computational complexity for constant-depth quantum circuits and three types of single-qubit observables \( O_j \) which are (a) close to the identity, (b) positive semidefinite, (c) arbitrary. It is shown that the mean value problem admits a classical approximation algorithm with runtime scaling as \( \text{poly}(n) \) and \( 2^{O(\sqrt{n})} \) in cases (a,b) respectively. In case (c) we give a linear-time algorithm for geometrically local circuits on a two-dimensional grid. The mean value is approximated with a small relative error in case (a), while in cases (b,c) we satisfy a less demanding additive error bound. The algorithms are based on (respectively) Barvinok’s polynomial interpolation method, a polynomial approximation for the OR function arising from quantum query complexity, and a Monte Carlo method combined with Matrix Product State techniques. We also prove a technical lemma characterizing a zero-free region for certain polynomials associated with a quantum circuit, which may be of independent interest.

1 Introduction

In this work we consider the computation of expectation values at the output of a shallow quantum circuit. Suppose we are given an \( n \)-qubit quantum circuit \( U \) of depth \( d = \mathcal{O}(1) \) along with \( n \) single-qubit operators \( O_1, \ldots, O_n \). If each operator \( O_j \) is Hermitian then the tensor product \( O \equiv O_1 \otimes O_2 \otimes \cdots \otimes O_n \) is an observable and its mean value with respect to the state \( U|0^n\rangle \) is given by

\[
\mu \equiv \langle 0^n | U^\dagger OU | 0^n \rangle.
\]

The mean value \( \mu \) can be efficiently estimated on a quantum computer by repeatedly preparing the state \( U|0^n\rangle \), measuring each single-qubit observable \( O_j \), and averaging the product of the measured eigenvalues.

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The mean value problem, i.e., estimation of $\mu$, for tensor product observables is a common step of NISQ\(^1\) era quantum algorithms \[1\] since the readout requires only single-qubit operations which tend to be more reliable than two-qubit gates. For example, variational quantum algorithms such as VQE\(^2\) \[2\] or QAOA\(^3\) \[3\] aim at minimizing the expected energy $\langle 0^n|U^\dagger HU|0^n \rangle$, where $H$ is a Hamiltonian and $U$ is a shallow quantum circuit chosen from a suitable variational class. In many interesting cases, such as quantum chemistry simulations \[2, 4–6\], the Hamiltonian $H$ can be written as a linear combination of poly($n$) Pauli operators, and so the expected energy $\langle 0^n|U^\dagger HU|0^n \rangle$ is a sum of poly($n$) mean values $\mu$ of the form Eq. (1). The mean value $\mu$ can also represent an output probability of the quantum circuit, i.e., the probability of observing a particular measurement outcome if we prepare the state $U|0^n \rangle$ and measure some of the qubits in the standard basis. In this case each observable $O_j$ is either a projector $|0 \rangle \langle 0|$, $|1 \rangle \langle 1|$ or the single-qubit identity operator. The estimation of output probabilities is a key step in variational quantum classifiers \[7,8\] where the mean value of the observable $O = |0 \rangle \langle 0| \otimes n$ encodes a single entry of the classifier kernel function. These and other quantum algorithms have prompted the development and demonstration of several error mitigation schemes which target a reliable mean value estimation in the presence of noise \[9–14\].

Given the current enthusiasm for variational quantum algorithms, it is natural to question whether or not they can be more powerful than classical algorithms in some sense. Unfortunately, empirical comparisons are limited by the fact that large scale quantum computers are not yet available. Furthermore, heuristic quantum algorithms are challenging to analyze mathematically and generally do not have performance guarantees. In this paper we investigate the computational power of variational quantum algorithms based on constant-depth circuits by asking whether or not they are “easy” to simulate on a classical computer. *Does the mean value problem require a quantum computer?*

We note that the computational complexity of estimating mean values depends crucially on the type of approximation guarantee requested. One may ask for an approximation $\tilde{\mu}$ which achieves a small *additive error* $\delta$, i.e., $|\tilde{\mu} - \mu| \leq \delta$. Here we assume that the single-qubit observables are normalized in the sense that $\| O_j \| \leq 1$. If $U$ is a polynomial-size circuit, this task is BQP-complete almost by definition. On the other hand, in the case of interest—where $U$ is described by a constant-depth quantum circuit—it captures the power of a restricted model of quantum computation, which consists of repeating a constant-depth quantum computation followed by single-qubit measurements a polynomial number of times and averaging the results. As discussed above, this describes a typical step of variational quantum algorithms.

Alternatively, one may ask for a much more stringent approximation $\tilde{\mu}$ which achieves a small *relative error* $\delta$, i.e., $e^{-\delta} \mu \leq |\tilde{\mu} - \mu| \leq e^{\delta} \mu$. This is clearly at least as difficult as computing an additive error approximation in the case of normalized observables. In fact, this task is $\#P$-hard, and therefore intractable, for a general constant-depth circuit $U$ and $\delta = O(1)\(^4\)$. Thus, a classical algorithm which computes an additive error approximation of $\mu$

\(^1\)Noisy Intermediate Scale Quantum
\(^2\)Variational Quantum Eigensolver
\(^3\)Quantum Approximate Optimization Algorithm
\(^4\)A standard reduction using postselected gate teleportation \[15\] shows that the problem is just as hard as its generalization in which $U$ is given by any circuit of polynomial size, which is $\#P$-hard \[16\].
Table 1: Complexity of the mean value problem

| Quantum circuit $U$   | Observables $O_j$         | Relative error      | Additive error         |
|-----------------------|---------------------------|---------------------|------------------------|
| Polynomial size       | Pos. semidefinite        | #P-hard [16]        | BQP-complete           |
| Constant depth        | Close to $I$              | $P$ [Thm. 1]        | $P$ [Thm. 1]           |
| Constant depth        | Pos. semidefinite        | #P-hard [15,16]     | BQP                    |
| 2D Constant depth     | Hermitian                | #P-hard [15,16]     | BPP [Thm. 5]           |

is simulating an efficient quantum computation, while a classical algorithm which computes a relative error approximation is solving a more challenging problem.

In this paper we consider the complexity of the mean value problem as a function of circuit depth, qubit connectivity, the structure of observables $O_j$, and the type of approximation. We describe classical algorithms for three special cases as detailed below and summarized in Table 1. Our results clarify the circumstances in which variational quantum algorithms may provide a quantum advantage. Some good news is that the mean value problem with super-constant depth quantum circuits remains out of reach for classical computers as far as we know. However, constant-depth circuits on a 2D or 3D grid are not as powerful as may have previously been expected: the corresponding mean value problem can be solved classically in time $O(n)$ and $2^{O(n^{1/3})}$ respectively. We also find that, for general constant-depth circuits without geometric locality, mean value problems with positive semidefinite observables—including e.g., the additive error approximation of output probabilities—can be solved on a classical computer in subexponential time $2^{O(n^{1/2})}$. Our results suggest that achieving a quantum advantage with variational quantum algorithms requires either a super-constant circuit depth (e.g., $d \sim \log n$) or qubit connectivity graphs that cannot be locally embedded in a 2D grid, or observables that cannot be expressed as linear combinations of poly($n$) tensor product operators.

1.1 Summary of results

Algorithm (a): Each $O_j$ is close to the identity Our first result concerns the special case of the mean value problem where each observable $O_j$ is close to the identity operator in the sense that

$$\|O_j - I\| \leq O(2^{-5d}).$$ (2)

Recall that $d = O(1)$ denotes the circuit depth. For observables satisfying Eq. (2) we describe a classical deterministic algorithm that approximates $\mu$ to within a relative error $\delta$. The runtime of the algorithm scales polynomially in the number of qubits $n$ and $\delta^{-1}$. Note
that while we are primarily interested in the case where $O_j$ are Hermitian, our algorithm is not restricted to this case.

The condition Eq. (2) can be satisfied in the case of very noisy measurements. For example, suppose a bit-flip channel $E(\rho) = (1-p)\rho + pX\rho X$ is applied to each qubit immediately before the measurement. Here $p \in [0, 1/2]$ is the error rate. Consider a noisy mean value

$$\mu_p \equiv \langle 0^n | E^{\otimes n}(U) | 0^n \rangle \langle 0^n | U^\dag \rangle | 0^n \rangle.$$

A simple calculation shows that $\mu_p = 2^{-n}\mu$, where $\mu$ is the ideal mean value defined by Eq. (1) with the observables $O_j = I + (1-2p)Z$. Thus our algorithm approximates the noisy mean value $\mu_p$ with a small relative error in the strong noise regime

$$\frac{1}{2} - O(2^{-5d}) \leq p \leq \frac{1}{2}.$$

We envision that observables $O_j$ satisfying Eq. (2) could be measured for verification purposes while executing a variational quantum algorithm. Indeed, a typical step of such an algorithm repeatedly prepares a variational state $U|0^n\rangle$ and measures all qubits in the standard basis. The measurement data collected by the quantum algorithm can be used to approximate the mean value $\mu$ defined in Eq. (1) for any observables $O_j$ diagonal in the standard basis, for example, $O_j = e^{i\theta Z}$. The verification step would compare the mean value $\mu$ inferred from the measurement data and the approximation $\tilde{\mu}$ computed by the classical algorithm. The latter can be computed efficiently whenever $O_j$ obeys Eq. (2), that is, $|\theta| = O(2^{-5d})$. An attractive feature of this method is that the verification step and the algorithm that is being verified access the same measurement data. Thus no additional quantum operations are required.

The algorithm works by classically computing mean values $\mu_S = \langle 0^n | U^\dag \prod_{j \in S} O_j U | 0^n \rangle$ for all subsets of qubits $S$ of size up to $O(\log(\delta^{-1}n))$ satisfying a suitable connectivity property. We show that the number of such subsets is at most $\text{poly}(n)$. Each mean value $\mu_S$ can be computed by restricting the circuit $U$ onto the “lightcone” of $S$. It is shown that the restricted circuit can be simulated classically in time $\text{poly}(n)$. The desired approximation $\tilde{\mu}$ is obtained by combining the mean values $\mu_S$ using the polynomial interpolation lemma due to Barvinok [18]. To this end, we define a degree-$n$ polynomial $f(\epsilon) = \langle 0^n | U^\dag O(\epsilon) U | 0^n \rangle$, where $O(\epsilon)$ is the tensor product of observables $O_j(\epsilon) = I + \epsilon(O_j - I)$. Note that $f(0) = 1$ and $f(1) = \mu$.

Barvinok’s lemma implies that if the polynomial $f(\epsilon)$ is zero-free in a disk $|\epsilon| \leq \beta$ for some constant $\beta > 1$, then $\log f(1) = \log \mu$ can be approximated with an additive error $\delta$ from the Taylor expansion of $\log f(\epsilon)$ at $\epsilon = 0$ truncated at the order $p = O(\log(\delta^{-1}n))$. We show that the coefficients of the Taylor series of $\log f(\epsilon)$ to the $p$-th order are simply related to the mean values $\mu_S$ computed at the first stage of the algorithm. The main technical step in applying Barvinok’s lemma is establishing the zero-freeness condition. For a depth-$d$ quantum circuit composed of two-qubit gates we show that $f(\epsilon)$ is zero-free in a disk of radius $\beta = \epsilon_0/\gamma$, where $\gamma \equiv \max_j \|O_j - I\|$ and $\epsilon_0 = \Omega(2^{-5d})$. We prove this by constructing a probability distribution over $2^n$-bit strings $p_{\epsilon}(z)$ such that $p_{\epsilon}(0^{2n})$ is proportional to $|f(\epsilon)|^2$. The Lovász Local Lemma is then applied to show that the probability $p_{\epsilon}(0^{2n})$ is strictly positive for $|\epsilon| \leq \beta$. This proves $f(\epsilon) \neq 0$ for $|\epsilon| \leq \beta$. The inverse exponential scaling of $\epsilon_0$ with $d$ is shown to be optimal. On the other hand, we show that a random unitary $U$
satisfying the 2-design property typically has a much larger zero-free radius \( \beta = \epsilon_0 / \gamma \), where \( \epsilon_0 \geq 1 - \mathcal{O} \left( \frac{\log(n)}{n} \right) \). This result suggests that the worst-case bound on the applicability region of our algorithm established in Eq. (2) is unlikely to be tight for the vast majority of circuits.

We note that a similar algorithm, also based on Barvinok’s approach, was previously proposed for approximating output probabilities of IQP circuits composed of gates which are sufficiently close to the identity [19].

**Algorithm (b): Each \( O_j \) is positive semidefinite** Our next result is a classical algorithm that approximates the mean value \( \mu \) to within a given additive error \( \delta \), for general constant-depth circuits \( U \) and positive semidefinite tensor product observables. More precisely, we assume that \( \|O_j\| \leq 1 \) and \( O_j \geq 0 \) for all \( j \). The algorithm has runtime exponential in \( \sqrt{n \log(\delta^{-1})} \), with a prefactor logarithmic in \( n \).

Our result also sheds some light on the more general additive error mean value problem for shallow quantum circuits. For more general Hermitian observables \( O_j \) which may not be positive semidefinite, our algorithm outputs an approximation to the absolute value \( |\langle 0^n | U^{\dagger} O U | 0^n \rangle| \) to within an additive error \( \delta \). Thus our algorithm would provide an additive error estimate to the mean value if we only knew the sign! It is an open question whether or not this more general case admits a subexponential classical algorithm.

The algorithm is based on approximating the projector onto the output state \( |\psi\rangle \equiv U|0^n \rangle \) of the quantum circuit by an operator which has a subexponential classical description size. Similar ideas were used in Ref. [20] to establish a certain expansion property of the probability distribution obtained by measuring \( \psi \) in the standard basis. To explain the main idea, let us specialize to the case \( O = |0^n \rangle \langle 0^n | \) in which we aim to estimate an output probability

\[
\mu = |\langle 0^n | \psi \rangle|^2
\]

of a shallow quantum circuit. The output state \( \psi \) of the quantum circuit is the unique state which is orthogonal to each of the commuting projectors \( U|1\rangle \langle 1| U^{\dagger} \) for \( 1 \leq j \leq n \). These operators are simultaneously diagonalized in the basis \( \{|\hat{z}\rangle = U|z\rangle : z \in \{0,1\}^n\} \). The projector \( I - |\psi\rangle \langle \psi | \) has the property that it computes the multivariate OR function in this basis, in the sense that

\[
(I - |\psi\rangle \langle \psi |) |\hat{z}\rangle = \text{OR}(z) |\hat{z}\rangle,
\]

where \( \text{OR}(z) \) is zero iff \( z = 0^n \). Consequently, we obtain an \( \delta \)-approximation \( P \) to the projector \( |\psi\rangle \langle \psi | \) (in the spectral norm) by plugging in an \( \delta \)-approximation of the multivariate OR function on the RHS of Eq. (4). Using an optimal polynomial approximation derived from quantum query complexity [21, 22], one obtains an operator \( P \) which is a sum of \( 2^{\tilde{O}(\sqrt{n \log(\delta^{-1})})} \) terms each acting nontrivially on \( 2^{\tilde{O}(\sqrt{n \log(\delta^{-1})})} \) qubits. The algorithm outputs the estimate \( \tilde{\mu} = \langle 0^n | P | 0^n \rangle \) of the mean value Eq. (3), which can be computed exactly in time \( 2^{\tilde{O}(\sqrt{n \log(\delta^{-1})})} \).

**Algorithm (c): The circuit is geometrically local in 2D or 3D** Our final result is a classical randomized algorithm that approximates the mean value \( \mu \) defined in Eq. (1) to within an additive error \( \delta \) for any single-qubit operators \( O_j \) satisfying \( \|O_j\| \leq 1 \). This
algorithm only applies to constant-depth geometrically local quantum circuits, i.e., circuits with nearest-neighbor gates on a $D$-dimensional grid of qubits. From a practical perspective, the most interesting cases are $D = 2$ and $D = 3$. In the 2D case our algorithm achieves a polynomial runtime $O(n^{\delta-2})$. The scaling with $n$ is optimal since one needs a time linear in $n$ simply to examine each gate in the circuit. However, the $O$ notation hides a very large constant factor that limits practical applications of the algorithm. For comparison, state-of-the-art tensor network simulators [17, 23–25] enable simulation of medium size constant-depth 2D circuits with $n \sim 100$ but have a super-polynomial asymptotic runtime $2^{O(\sqrt{n})}$. In the 3D case our algorithm achieves a sub-exponential runtime $\delta^{-2}2^{O(n^{1/3})}$. We believe that accomplishing the same simulation using the standard tensor network methods [17,26] would require time $2^{O(n^{2/3})}$.

The main idea behind the algorithm is to express the mean value as $\mu = \langle \Psi_0 | W | \Psi_1 \rangle$, where $\Psi_0, \Psi_1$ are Matrix Product States (MPS) of $n$ qubits with bond dimension $O(1)$, and $W$ is a permutation of $n$ qubits. We then approximate $\mu$ using a Monte Carlo algorithm similar to the one proposed by Van den Nest [27]. It is based on the identity

$$\mu = \langle \Psi_0 | W | \Psi_1 \rangle = \sum_{x \in \{0, 1\}^n} \pi(x) F(x),$$

where $\pi(x) = |\langle x | \Psi_0 \rangle|^2$ and $F(x) = \langle x | W | \Psi_1 \rangle \langle x | \Psi_0 \rangle^{-1}$. Using the standard MPS algorithms one can compute the quantity $F(x)$ for any given $x$ in time $O(n)$. Likewise, one can sample $x$ from the probability distribution $\pi(x)$ in time $O(n)$. A simple calculation shows that the variance of a random variable $F(x)$ with $x$ drawn from $\pi(x)$ is at most one. Thus one can approximate $\mu$ by an empirical mean value $\tilde{\mu} = \frac{1}{S} \sum_{i=1}^{S} F(x^i)$, where $x^1, \ldots, x^S$ are independent samples from $\pi(x)$ and $S = O(\delta^{-2})$. The 3D simulation algorithm follows the same idea except that the required MPS bond dimension is $2^{O(n^{1/3})}$.

### 1.2 Open problems

A central open question raised by this work is whether the quantum mean value problem can be solved efficiently on a classical computer in the case of shallow circuits, tensor product observables, and additive approximation error. Alternatively, can we provide some evidence that this task is classically hard? This question directly addresses the computational power of variational quantum algorithms based on shallow circuits.

To shed light on this problem, one may ask whether our algorithms can be improved or generalized. For example, can the subexponential algorithm for positive semi-definite observables be generalized to Hermitian tensor-product observables? Can the additive error mean value problem for 3D shallow circuits be solved in polynomial time on a classical computer? Can the runtime of our algorithms for the 2D and 3D shallow circuits be reproduced using simulators based on tensor network contraction [17]?

Another interesting question is whether large-scale instances of the quantum mean value problem can be solved by hybrid quantum-classical algorithms with limited quantum resources (e.g. small number of qubits). For example, a promising class of hybrid algorithms known as holographic quantum simulators was recently proposed [28,29]. Loosely speaking, such algorithms enable a simulation of 2D lattice models on a 1D quantum computer by
converting one spatial dimension into time. We anticipate that a similar approach can be used to solve \( n \)-qubit instances of the quantum mean value problem with 2D shallow circuits on a quantum computer with only \( O(n^{1/2}) \) qubits. Even though Theorem 5 provides a purely classical linear time algorithm for the problem, its runtime has a very unfavorable scaling with the circuit depth. Hybrid algorithms may potentially remedy this inefficiency.

One may also further probe the complexity of the relative error mean value problem for shallow circuits. While this problem is known to be \#P-hard in the worst case, it is interesting to elucidate broad classes of quantum circuits for which the problem can be solved efficiently. For example, it can be easily shown that the mean value problem admits a polynomial time classical algorithm for Pauli-type observables and quantum circuits that belong to the 3rd level of the Clifford hierarchy [30]. At the same time, approximating output probabilities of such circuits is known to be \#P-hard in the worst case [31].

Random quantum circuits are another possible avenue to explore. For example, it has been conjectured that relative error approximation of output probabilities is \#P-hard for random quantum circuits of sufficiently high depth [32–34]. Does our bound Eq. (56) on the zero-free disk for the polynomial \( f(\epsilon) \) when \( U \) is a random circuit have any bearings on this conjecture? Finally, it may be possible to improve our lower bound \( \epsilon_0 = \Omega(2^{-5d/\gamma} - 1) \) on the zero-free radius for depth-\( d \) circuits, although it cannot be improved beyond \( \Omega(2^{-d}) \) due to the example described in Section 4.

2 Notation

Let \([n] = \{1, 2, \ldots, n\}\). Given a subset of qubits \( S \subseteq [n] \), let \( \mathcal{A}_S \) be an operator algebra that consists of all \( n \)-qubit operators that only act nontrivially on \( S \); also let \( \mathcal{A}_j \equiv \mathcal{A}_{\{j\}} \).

Consider a fixed unitary \( U \).

**Definition 1.** The (forward) lightcone of a qubit \( j \), denoted by \( \mathcal{L}(j) \), is the smallest subset of qubits \( \mathcal{L}(j) \subseteq [n] \) such that \( j \in \mathcal{L}(j) \) and \( U^\dagger \mathcal{A}_j U \subseteq \mathcal{A}_{\mathcal{L}(j)} \). For any subset \( S \subseteq [n] \) we define

\[
\mathcal{L}(S) = \bigcup_{j \in S} \mathcal{L}(j).
\]

We also define the backward lightcone \( \mathcal{L}^{-}(S) \) by replacing \( U \) with \( U^\dagger \) in the above.

Therefore, for any \( S \subset [n] \), the unitary \( U \) maps any operator acting on \( S \) to an operator supported on \( \mathcal{L}(S) \), and the circuit \( U^\dagger \) maps any operator supported on \( S \) to an operator supported on \( \mathcal{L}^{-}(S) \).

The forward and backward lightcones have the following symmetry.

**Proposition 1.** Let \( j, k \in [n] \). Then \( j \in \mathcal{L}(k) \) if and only if \( k \in \mathcal{L}^{-}(j) \).

**Proof.** The statement is clearly true if \( j = k \), so consider the case \( j \neq k \). Below we show that \( k \notin \mathcal{L}^{-}(j) \) implies \( j \notin \mathcal{L}(k) \), which establishes the “only if” direction. The “if” direction then follows as it is the same statement with \( U \) replaced by \( U^\dagger \).

So suppose \( k \notin \mathcal{L}^{-}(j) \). Equivalently, any operator in \( \mathcal{A}_k \) commutes with any operator in \( U \mathcal{A}_j U^\dagger \). Equivalently, any operator in \( U^\dagger \mathcal{A}_k U \) commutes with any operator in \( \mathcal{A}_j \), which is the statement that \( j \notin \mathcal{L}(k) \). \( \square \)
It will also be convenient to define iterated lightcones.

**Definition 2.** Given a unitary \( U \), define iterated forward and backward lightcones of \( S \subseteq [n] \)

\[
\mathcal{L}(S, 1) = \mathcal{L}(S) \\
\mathcal{L}(S, 2) = \mathcal{L}^-(\mathcal{L}(S)) \\
\mathcal{L}(S, 3) = \mathcal{L}(\mathcal{L}^-(\mathcal{L}(S))) \\
\vdots
\]

\[
\mathcal{L}_-(S, 1) = \mathcal{L}_-(S) \\
\mathcal{L}_-(S, 2) = \mathcal{L}(\mathcal{L}_-(S)) \\
\mathcal{L}_-(S, 3) = \mathcal{L}(\mathcal{L}_-(\mathcal{L}_-(S))) \\
\vdots
\]

We also define the maximum iterated lightcone sizes

**Definition 3.** For each positive integer \( c \) define

\[
\ell_c = \max\{ \max_{1 \leq j \leq n} |\mathcal{L}(j, c)|, \max_{1 \leq j \leq n} |\mathcal{L}^-(j, c)| \}
\]

The quantities \( \ell_c \) quantify the growth of the lightcone under repeated applications of \( U \) or \( U^\dagger \). Clearly we have the upper bound

\[
\ell_c \leq (\ell_1)^c. \tag{5}
\]

Indeed, if \( U \) is a depth-\( d \) circuit composed of two-qubit gates then

\[
\ell_c \leq 2^{cd} \quad c \geq 1, \quad \text{(lightcone growth, depth-\( d \) circuit)} \tag{6}
\]

In some cases Eq. (5) is a poor upper bound. For example, if all gates are restricted to be nearest-neighbor two-qubit gates on a \( D \)-dimensional grid then we have

\[
\ell_c \leq (2cd)^D \quad c \geq 1, \quad \text{(lightcone growth, \( D \)-dimensions)} \tag{7}
\]

For our purposes the most important distinguishing feature of constant depth circuits is that \( \ell_c = \mathcal{O}(1) \) for any constant \( c \).

### 3 Simulation by polynomial interpolation

Let us define the polynomial

\[
f(\epsilon) = \langle 0^n | U^\dagger O(\epsilon) U | 0^n \rangle \tag{8}
\]

where \( \epsilon \in \mathbb{C} \) and \( O(\epsilon) \equiv \bigotimes_{j=1}^n O_j(\epsilon) \) and

\[
O_j(\epsilon) = I + \epsilon (O_j - I).
\]

Clearly, \( f(0) = 1 \) and \( f(1) = \mu \) is the quantity we wish to approximate. Our main result is the following theorem.
Theorem 1. There exists a deterministic classical algorithm that takes as inputs a quantum circuit \( U \) acting on \( n \) qubits, an error tolerance \( \delta > 0 \), and a product operator \( O = \bigotimes_{j=1}^{n} O_j \) such that
\[
\|O_j - I\| \leq \frac{1}{60\beta \cdot \ell_1 \cdot \ell_4}
\]
for all \( j \), where \( \beta > 1 \) is an absolute constant. The algorithm outputs a complex number \( \tilde{\mu} \) that approximates \( \mu = \langle 0^n | U^\dagger O U | 0^n \rangle \) with a multiplicative error \( \delta \), that is
\[
|\log \mu - \log \tilde{\mu}| \leq \delta.
\]
\( (10) \)
The running time of the algorithm is \((n\delta^{-1})^\mathcal{O}(\ell_1)\).

For constant-depth circuits \( d = \mathcal{O}(1) \) we have \( \ell_1, \ell_4 = \mathcal{O}(1) \) and we obtain the claimed efficient algorithm to compute \( \mu \). For a general depth-\( d \) circuit composed of two-qubit gates \( U \) or a geometrically local circuit in \( D \)-dimensions we may plug in Eq. (6) or Eq. (7) respectively to see how the runtime and the condition Eq. (9) depend on depth \( d \).

To prove Theorem 1, we use a zero-free region lemma and Barvinok’s interpolation lemma.

Lemma 1. (Zero-free region) Let \( U \) be a quantum circuit, \( O = \bigotimes_{j=1}^{n} O_j \) be a product operator, and let \( \gamma = \max_j \|O_j - I\| \). The polynomial \( f(\epsilon) \) is zero-free on the disk \( |\epsilon| \leq \epsilon_0 \), where
\[
\epsilon_0 = \frac{1}{60\gamma \cdot \ell_1 \cdot \ell_4}.
\]
(11)
The proof of Lemma 1 is deferred to Section 4. By choosing \( \gamma \) small enough as stated in the main theorem, we are guaranteed that \( f(\epsilon) \neq 0 \) on a disk of radius \( |\epsilon| \leq \epsilon_0 = \beta \). Using Barvinok’s lemma (lemma 2) we can interpolate between \( f(0) \) and \( f(1) \).

Below we shall write \( g^{(m)}(\epsilon) \equiv g^{(m)}(0) \) for the \( m \)-th derivative of a function \( g(\epsilon) \) evaluated at \( \epsilon = 0 \). Let us agree that \( g^{(0)} = g(0) \).

Lemma 2. (Barvinok’s interpolation lemma \([18, 35]\)) Let \( f(\epsilon) \) be a polynomial of degree \( n \) and suppose \( f(\epsilon) \neq 0 \) for all \( |\epsilon| < \beta \), where \( \beta > 1 \) is a real number. Let us choose a branch of
\[
g(\epsilon) = \ln f(\epsilon) \quad \text{for } |\epsilon| \leq 1
\]
and consider the its Taylor polynomial
\[
T_p(\epsilon) = g^{(0)} + \sum_{k=1}^{p} \frac{\epsilon^k}{k!} g^{(k)}.
\]
Then
\[
|g(\epsilon) - T_p(\epsilon)| \leq \frac{n\beta^{-p}}{(p+1)(\beta - 1)} \quad \text{for all } |\epsilon| \leq 1.
\]
Assuming that \( \beta > 1 \) is fixed a priori (below we use \( \beta = 2 \)) and setting
\[
\tilde{\mu} = \exp[T_p(1)]
\]
one can achieve the bound Eq. (10) by choosing

\[ p = \mathcal{O}(\ln n\delta^{-1}), \]

where \( \mathcal{O} \) depends only on \( \beta \).

To complete the proof of Theorem 1, in the remainder of this section we show that \( \hat{\mu} \) can be computed using runtime \( (n\delta^{-1})^\mathcal{O}(\epsilon) \). As was shown by Barvinok [18], the derivatives of \( g(\epsilon) \) can be obtained from those of \( f(\epsilon) \) by solving a simple linear system. Indeed, start with the identity \( f'(\epsilon) = f(\epsilon)g'(\epsilon) \). Taking the derivatives using the Leibniz rule and setting \( \epsilon = 0 \) one gets

\[ f^{(m)} = \sum_{j=0}^{m-1} \binom{m-1}{j} f^{(j)} g^{(m-j)}, \quad m = 1, \ldots, p. \quad (12) \]

This is a triangular linear system that determines \( g^{(1)}, \ldots, g^{(p)} \) in terms of \( f^{(1)}, \ldots, f^{(p)} \)

\[
\begin{align*}
    g^{(1)} &= f^{(1)} \quad (13) \\
    g^{(2)} &= f^{(2)} - f^{(1)} g^{(1)} \quad (14) \\
    g^{(3)} &= f^{(3)} - f^{(2)} g^{(1)} - 2 f^{(1)} g^{(2)} \quad (15)
\end{align*}
\]

and so on. Here we noted that \( f^{(0)} = f(0) = 1 \).

It remains to calculate the derivatives \( f^{(1)}, \ldots, f^{(p)} \). To do so, it is convenient to first define \( \epsilon = (\epsilon_1, \ldots, \epsilon_n) \in \mathbb{C}^n \) and consider the multivariate version of Eq. (8) and then evaluate the results at \( \epsilon = (\epsilon, \epsilon, \ldots, \epsilon) \). To this end let

\[ f(\epsilon) = \langle 0^n | U^\dagger O(\epsilon) U | 0^n \rangle, \quad (16) \]

where \( O(\epsilon) = \bigotimes_{j=1}^n O_j(\epsilon_j) \) and

\[ O_j(\epsilon_j) = I + \epsilon_j (O_j - I). \]

A monomial is defined by \( M(\epsilon) = \alpha \prod_{j=1}^n \epsilon_j^{m_j} \), where \( \alpha \neq 0 \) is a complex coefficient and all \( m_j \geq 0 \) are integers. We say \( M(\epsilon) \) is supported on the set \( S \subseteq [n] \) if and only if \( m_j > 0 \) for all \( j \in S \) and \( m_j = 0 \) for all \( j \not\in S \). The degree of \( M(\epsilon) \) is defined by \( \sum_{j=1}^n m_j \). Let \( T_p(\epsilon) \) be the Taylor series for \( g(\epsilon) = \ln f(\epsilon) \) at \( \epsilon = 0^n \) truncated at the order \( p = \log_2 (n\delta^{-1}) \). By definition, the series \( T_p(\epsilon) \) is a sum of monomials with degree at most \( p \).

**Definition 4.** Consider a subset \( S \subseteq [n] \). Define \( g_S(\epsilon) \) as the sum of all monomials in \( T_p(\epsilon) \) that are supported on \( S \), evaluated at the point \( \epsilon = (\epsilon, \ldots, \epsilon) \). Define \( h_S(\epsilon) \) as the sum of all monomials in \( T_p(\epsilon) \) that are supported on some subset of \( S \), evaluated at the point \( \epsilon = (\epsilon, \ldots, \epsilon) \).

Below we use the convention \( g_\emptyset(\epsilon) = 0 \) and \( h_\emptyset(\epsilon) = 0 \). By definition, \( g_S(\epsilon) \) and \( h_S(\epsilon) \) are polynomials of degree at most \( p \). Let us discuss some basic properties of \( g_S(\epsilon) \) and \( h_S(\epsilon) \). First, since the support of a monomial is uniquely defined and \( g_S(\epsilon) \) gets contributions from monomials of degree at least \( |S| \), we have

\[
T_p(\epsilon) = \sum_{S \subseteq [n] : 1 \leq |S| \leq p} g_S(\epsilon). \quad (17)
\]

Thus the task of computing \( T_p(\epsilon) \) reduces to computing \( g_S(\epsilon) \) for all subsets \( S \) of size at most \( p \). First, we claim \( g_S(\epsilon) \) can be computed in terms of \( h_S(\epsilon) \) as follows.
Proposition 2 (Inclusion-Exclusion).

\[ g_S(\epsilon) = \sum_{T \subseteq S} (-1)^{|S \setminus T|} h_T(\epsilon) \]  
for any subset \( S \subseteq [n] \).

Proof. Indeed, let us prove Eq. (18) by induction in \( |S| \). The base case is \( |S| = 1 \). Then \( g_S(\epsilon) = h_S(\epsilon) \) by definition. Suppose we have already proved Eq. (18) for all subsets \( S \) of size \( |S| \leq m \). Let \( S \) be a subset of size \( m + 1 \). Then by definition,

\[ g_S(\epsilon) = h_S(\epsilon) - \sum_{T \subset S} g_T(\epsilon), \]  
where the sum runs over all proper subsets of \( S \). Since \( |T| \leq m \), we use the induction hypothesis to express \( g_T(\epsilon) \) in terms of \( h_R(\epsilon) \) with \( R \subseteq T \). It gives

\[ g_S(\epsilon) = h_S(\epsilon) - \sum_{T \subset S} \sum_{R \subseteq T} (-1)^{|T \setminus R|} h_R(\epsilon). \]  
Changing the summation order one gets

\[ g_S(\epsilon) = h_S(\epsilon) - \sum_{R \subseteq S} h_R(\epsilon) \sum_{T \subseteq S} (-1)^{|T \setminus R|}. \]  
Let us add and subtract the term \( (-1)^{|T \setminus R|} \) with \( T = S \). We get

\[ g_S(\epsilon) = h_S(\epsilon) - \sum_{R \subseteq S} h_R(\epsilon) \left[ -(-1)^{|S \setminus R|} + \sum_{R \subseteq T \subseteq S} (-1)^{|T \setminus R|} \right]. \]  
Using the well-known identity

\[ \sum_{T : R \subseteq T \subseteq S} (-1)^{|T \setminus R|} = \begin{cases} 1 & \text{if } R = S, \\ 0 & \text{otherwise} \end{cases} \]  
one arrives at

\[ g_S(\epsilon) = h_S(\epsilon) - h_S(\epsilon) + \sum_{R \subseteq S} h_R(\epsilon)(-1)^{|S \setminus R|} = \sum_{R \subseteq S} h_R(\epsilon)(-1)^{|S \setminus R|}. \]  
This proves the induction hypothesis.

Next we claim that \( h_S(\epsilon) \) can be computed for any given subset \( S \) in time \( 2^{O(\ell_1|S|)} \). Indeed, define a polynomial

\[ \mu_S(\epsilon) \equiv \langle 0^n | U^\dagger \prod_{j \in S} O_j(\epsilon) U | 0^n \rangle. \]  
Let \( T_{p,S}(\epsilon) \) be the Taylor expansion of \( \ln \mu_S(\epsilon) \) at \( \epsilon = 0 \) truncated at the \( p \)-th order. Note that

\[ h_S(\epsilon) = T_{p,S}(\epsilon). \]
Indeed, both polynomials are obtained from $g(\epsilon)$ by retaining monomials of degree at most $p$ supported on some subset of $S$ and then setting $\epsilon = (\epsilon, \ldots, \epsilon)$. We claim that the polynomial $\mu_S(\epsilon)$ can be computed in time roughly $2^{O(\ell_1|S|)}$. Indeed, one can first restrict the circuit $U$ by removing any gate which acts outside of $\mathcal{L}(S)$. The latter contains at most $\ell_1|S|$ qubits. The restricted circuit can be simulated by the brute-force method in time $2^{O(\ell_1|S|)}$. Once the polynomial $\mu_S(\epsilon)$ is computed, one can solve the triangular linear system expressing $T_{p,S}(\epsilon)$ in terms of the first $p$ coefficients of $\mu_S(\epsilon)$ using Barvinok’s method [18].

Finally, we claim that $g_S(\epsilon) = 0$ unless $S$ has a certain connectivity property.

**Definition 5.** A subset $S \subseteq [n]$ is said to be $\mathcal{L}$-connected if any partition $S = S_1S_2$ into disjoint non-empty subsets $S_1, S_2$ satisfies $\mathcal{L}(S_1) \cap \mathcal{L}(S_2) \neq \emptyset$.

**Lemma 3.** $g_S(\epsilon) = 0$ unless $S$ is $\mathcal{L}$-connected.

**Lemma 4.** The number of $\mathcal{L}$-connected subsets $S \subseteq [n]$ of size $p$ is at most $n(3\ell_2)^{p-1}$.

Combining Lemmas 3 and Eq. (17), we infer that computing $T_p(\epsilon)$ amounts to computing $g_S(\epsilon)$ for each $\mathcal{L}$-connected subset $S$ of size at most $p$. By Lemma 4, the number of such subsets is at most

$$n \sum_{q=1}^{p} (3\ell_2)^{q-1} = n \frac{(3\ell_2)^p - 1}{3\ell_2 - 1} \leq \frac{n(3\ell_2)^{p-1}}{1 - 1/(3\ell_2)} = \frac{3n}{2} (3\ell_2)^{p-1}.$$  \hspace{1cm} (27)

From Proposition 2 one infers that computing $g_S(\epsilon)$ for a given subset $S$ of size $|S| \leq p$ amounts to computing $h_T(\epsilon)$ for all $T \subseteq S$. The number of subsets $T \subseteq S$ is $2^{|S|} \leq 2^p$. As shown above, one can compute $h_T(\epsilon)$ for any given subset $T$ in time roughly $2^{O(\ell_1|T|)} \leq 2^{O(\ell_1p)}$. Thus the overall runtime required to compute $T_p(\epsilon)$ scales as

$$\frac{3n}{2} (3\ell_2)^{p-1} \cdot 2^p \cdot 2^{O(\ell_1p)} \leq n(3\ell_2)^{p-1}2^{O(\ell_1p)} = (n\delta^{-1})^{O(\ell_1)},$$

where in the first inequality we used Eq. (5).

**Proof of Lemma 3.** Suppose $S$ is not $\mathcal{L}$-connected. Choose a partition $S = S_1S_2$ such that $S_1, S_2$ are disjoint non-empty subsets and $\mathcal{L}(S_1) \cap \mathcal{L}(S_2) = \emptyset$. Define a multi-variate polynomial

$$\mu_S(\epsilon) = \langle 0^n | U^\dagger \prod_{j \in S} O_j(\epsilon_j) U | 0^n \rangle.$$  \hspace{1cm} (28)

Since the lightcones of $S_1$ and $S_2$ do not overlap, $\mu_S(\epsilon)$ is a product of some polynomial depending on $\{\epsilon_j : j \in S_1\}$ and some polynomial depending on $\{\epsilon_j : j \in S_2\}$. By definition, $g_S(\epsilon)$ is obtained from the Taylor series of $\ln \mu_S(\epsilon)$ at $\epsilon = 0^p$ by retaining all monomials of degree $1, 2, \ldots, p$ supported on $S$ and setting $\epsilon = (\epsilon, \ldots, \epsilon)$. However, since $\ln \mu_S(\epsilon)$ is a sum of some function depending on $\{\epsilon_j : j \in S_1\}$ and some function depending on $\{\epsilon_j : j \in S_2\}$, the Taylor series of $\ln \mu_S(\epsilon)$ contains no monomials supported on $S$. Thus $g_S(\epsilon) = 0$, as claimed. \hfill \Box
Proof of Lemma 4. Define a graph $G$ with the set of vertices $[n]$ such that vertices $i, j$ are connected by an edge iff
\[ \mathcal{L}(i) \cap \mathcal{L}(j) \neq \emptyset. \]
Using Proposition 1 we see that this condition implies $j \in \mathcal{L}_{\perp}(\mathcal{L}(i)) = \mathcal{L}(i, 2)$. Therefore the graph $G$ has maximum vertex degree at most $\ell_2$. By definition, a subset $S$ is $\mathcal{L}$-connected iff $S$ is a connected subset of vertices in $G$. The number of connected subsets $S \subseteq [n]$ of size $p$ that contain a given vertex $j$ is at most $(e\ell_2)^{p-1}$, where $e = \exp(1)$, see Lemma 5 in [36]. Thus the total number of connected subsets of size $p$ is at most $n(3\ell_2)^{p-1}$. 

\section{Zero-free region}

In this section we study the zero-free radius of the polynomial $f(\epsilon)$ defined in Eq. (8). In Section 4.1 we prove Lemma 1, which establishes an $n$-independent lower bound on the zero-free radius of the polynomial $f(\epsilon)$ for constant-depth circuits. In particular, for a depth-$d$ circuit composed of two-qubit gates, the radius Eq. (11) is at least
\[ \epsilon_0 = \Omega(\gamma^{-1/2^{-5d}}), \]
where we used Eq. (6). A simple example shows that this bound is tight up to constant factors in the exponential. In particular, it is easy to see that for each $d \geq 1$, the $2^d$-qubit GHZ state
\[ |\text{GHZ}_{2^d}\rangle = \frac{1}{\sqrt{2}} (|0\rangle^{\otimes 2^d} + |1\rangle^{\otimes 2^d}) \]
can be prepared by a depth-$d$ circuit composed of two-qubit gates. We may choose each operator
\[ O_j = I + Z_j \]
so that $\gamma = \max_j \|O_j - I\| = 1$, $O_j(\epsilon) = I + \epsilon Z_j$, and
\[ f(\epsilon) = \frac{1}{2} \left( (1 + \epsilon)^{2^d} + (1 - \epsilon)^{2^d} \right), \]
which has zero free radius $O(2^{-d})$, as can be seen by verifying that $f$ has a root at $\epsilon = (-1 + e^{i\pi/2^d})(1 + e^{i\pi/2^d})^{-1}$.

While this example shows that there exist depth-$d$ circuits with zero-free radius exponentially small in $d$, we expect that such circuits are non-generic. To support this claim, in Section 4.2 we consider the zero-free radius for the polynomial $f(\epsilon)$ with operators given by Eq. (30) and unitary $U$ drawn at random from any ensemble which forms a unitary 2-design. In this case we show that with high probability the zero-free radius of $f$ is very close to 1.

\subsection{Proof of Lemma 1}

The proof is based on the Lovász Local Lemma [37].
Theorem 2 (Lovász Local Lemma). Suppose $E_1, E_2, \ldots, E_m$ are events in a probability space, that each event $E_j$ is independent of all but at most $K$ of the others, and that $\Pr[E_j] \leq p$ for all $j$. If $p \cdot \exp(1) \cdot K < 1$ then

$$\Pr[\bigcap_j \overline{E_j}] > 0. \quad (31)$$

Here $\overline{E_j}$ is the negation of event $E_j$, so Eq. (31) is the probability that none of the events $E_1, E_2, \ldots, E_m$ occur. We will also use the following simple fact:

Lemma 5. For each $j = 1, \ldots, n$ and $\epsilon \in \mathbb{C}$, there is a 2-qubit unitary $B_j(\epsilon)$ such that

$$\frac{1}{\|O_j(\epsilon)\|} O_j(\epsilon) = (I \otimes \langle 0|) B_j(\epsilon) (I \otimes |0\rangle) \quad (32)$$

and

$$\| (I \otimes \langle 1|) B_j(\epsilon) (I \otimes |0\rangle) \| \leq 2\sqrt{\gamma |\epsilon|} \quad (33)$$

Proof. Let $j$ and $\epsilon$ be given and define $A = ||O_j(\epsilon)||^{-1}O_j(\epsilon)$. We may write $A = U'M$ where $U'$ is unitary and $M = (A^\dagger A)^{1/2}$ (polar decomposition of $A$). Note that $\|M\| = \|A\| = 1$. Now let

$$B = (U' \otimes I) \left( M \otimes Z + (I - M^2)^{1/2} \otimes X \right),$$

where $Z$ and $X$ are single-qubit Pauli matrices. One can easily check that $B$ is unitary. Moreover

$$(I \otimes \langle 0|) B (I \otimes |0\rangle) = U'M = A,$$

and

$$\| (I \otimes \langle 1|) B (I \otimes |0\rangle) \| = \|I - A^\dagger A\|^{1/2} \leq (\|I - A\| + \|A - A^\dagger A\|)^{1/2} \leq (2\|I - A\|)^{1/2}, \quad (36)$$

where we used the triangle inequality along with the facts that $\|A\| = 1$ and $\|I - A^\dagger\| = \|I - A\|$. Now using the fact that

$$\|O_j(\epsilon)\| \leq 1 + |\epsilon|\|O_j - I\| \leq 1 + \gamma |\epsilon|,$$

along with the triangle inequality, we get

$$\|I - A\| \leq \|(1 + \gamma |\epsilon|)^{-1} (O_j(\epsilon) - I)\| + \|(1 + \gamma |\epsilon|)^{-1} I - I\| \leq \left( \frac{2\gamma |\epsilon|}{1 + \gamma |\epsilon|} \right) \leq 2\gamma |\epsilon|. \quad (37)$$

Plugging into Eq. (36), we arrive at Eq. (33).
Proof of Lemma 1. For each \( j \in [n] \) consider the 2-qubit unitary \( B_j(\epsilon) \) described by Lemma 5. Note that Eq. (32) implies (cf. Eq. (37))

\[
\| (I \otimes \langle 0 |) (B_j(\epsilon) - I) (I \otimes | 0 \rangle) \| \leq 2\gamma|\epsilon|,
\]

(38)

Now for each \( j \in [n] \) let us adjoin an ancilla qubit labeled \( n + j \) so that \( B_j(\epsilon) \) acts nontrivially on qubits \( j \) and \( n + j \), out of \( 2n \) qubits in total. Define \( V_j(\epsilon) = (U^\dagger \otimes I)B_j(\epsilon)(U \otimes I) \) and let \( S_j \subseteq [2n] \) be the qubits which it acts on nontrivially. In particular,

\[
S_i \subseteq \mathcal{L}(i) \cup \{ n + i \} \quad \quad 1 \leq i \leq n,
\]

(39)

where \( \mathcal{L}(i) \) and all lightcones discussed below are with respect to the \( n \)-qubit unitary \( U \). For future reference we also note that the unitaries \( \{ V_j(\epsilon) \} \) are commuting, i.e.,

\[
[V_j(\epsilon), V_r(\epsilon)] = 0 \quad 1 \leq j \leq r \leq n.
\]

(40)

and that

\[
\{ i : j \in S_i \} \subseteq \begin{cases} \mathcal{L}_+(j) & \text{if} \quad 1 \leq j \leq n \\ j - n & \text{if} \quad n + 1 \leq j \leq 2n. \end{cases}
\]

(41)

Indeed, from Eq. (39) and Proposition 1 we see that \( j \in S_i \) only if either \( j = n + i \), or the backward lightcone of \( j \) contains \( i \).

Define \( V(\epsilon) = \prod_j V_j(\epsilon) \). Then (using Eq. (32))

\[
f(\epsilon) = \left( \prod_{j=1}^n \| O_j(\epsilon) \| \right) \langle 0^{2n}|V(\epsilon)|0^{2n} \rangle.
\]

(42)

Consider the probability distribution over \( 2n \)-bit strings defined by

\[
p_\epsilon(z) = |\langle z|V(\epsilon)|0^{2n} \rangle|^2.
\]

To prove the lemma it suffices to show that for all \( \epsilon \) satisfying \( |\epsilon| \leq \epsilon_0 \), where \( \epsilon_0 \) is given by Eq. (11), we have

\[
p_\epsilon(0^{2n}) > 0.
\]

Indeed, using Eq. (42) we see that this implies \( |f(\epsilon)| > 0 \), since for each \( j \) we have

\[
\| O_j(\epsilon) \| \geq 1 - \gamma\epsilon_0 > 0
\]

whenever \( |\epsilon| \leq \epsilon_0 \).

To this end, let us fix some \( \epsilon \) satisfying \( |\epsilon| \leq \epsilon_0 \). Define events \( E_j \) for \( j = 1, 2, \ldots, 2n \) such that \( E_j \) is the event that \( z_j = 1 \) with respect to the probability distribution \( p_\epsilon \). Then

\[
\Pr [E_j] = \langle 0^{2n}|V^+(\epsilon)|1 \rangle \langle 1_j|V(\epsilon)|0^{2n} \rangle = \langle 0^{2n}|Q_j|0^{2n} \rangle
\]

where

\[
Q_j = \prod_{i,j \in S_i} V_i^+(\epsilon) |1 \rangle \langle 1 | \prod_{i,j \in S_i} V_i(\epsilon)
\]

(43)

(44)
Here we used the fact that a gate $V_j^\dagger(\epsilon)$ such that $j \notin S_i$ has no support on qubit $j$ and thus commutes with both $|1\rangle \langle 1|_j$ (as well as all other unitaries $V_i^\dagger(\epsilon)$, cf. Eq. (40)). All such gates appearing on the left can then be commuted through and cancel with their corresponding term $V_i(\epsilon)$ on the right.

The events $E_j$ and $E_k$ are independent whenever the corresponding operators $Q_j$ and $Q_k$ have disjoint support. Now for $1 \leq j \leq n$ let $\bar{j} = j$ and for $n + 1 \leq j \leq 2n$ let $\bar{j} = n - j$. The support of $Q_j$ satisfies

\[
\text{Support}(Q_j) \subseteq \mathcal{L}(\mathcal{L}_-(\bar{j})) \cup \{n + \mathcal{L}_-(\bar{j})\} \quad 1 \leq j \leq 2n, 
\]

where we have defined $\{n + \mathcal{L}_-(\bar{j})\} = \{n + r : r \in \mathcal{L}_-(\bar{j})\}$.

Using Eq. (45) we see that $Q_j$ and $Q_k$ have disjoint support unless

\[
\mathcal{L}(\mathcal{L}_-(\bar{j})) \cap \mathcal{L}(\mathcal{L}_-(\bar{k})) \neq \emptyset.
\]

Using Proposition 1 we see that the condition Eq. (46) implies

\[
\bar{k} \in \mathcal{L}_-(\bar{j}, 4).
\]

Therefore each event $E_j$ is independent of all but at most $K$ others, where

\[
K = 2 \max_{1 \leq i \leq n} |\mathcal{L}_-(i, 4)| \leq 2\ell_4
\]

We shall now upper bound the probability of each event $E_j$. First consider the case $j = n + r$ for some $1 \leq r \leq n$. In this case

\[
\Pr[E_{n+r}] = \langle 0^{2n}| V_i^\dagger(\epsilon)|1\rangle \langle 1|_{n+r} V_i(\epsilon)|0^{2n}\rangle \leq 4\gamma|\epsilon| \quad 1 \leq r \leq n, 
\]

where we used Eq. (33). Next suppose $j \in \{1, 2, \ldots, n\}$. In this case we have

\[
\Pr[E_j] = \langle 0^{2n}| \prod_{i \in \mathcal{L}_-(j)} V_i^\dagger(\epsilon)|1\rangle \langle 1|_{j} \prod_{i \in \mathcal{L}_-(j)} V_i(\epsilon)|0^{2n}\rangle = \alpha_j + \beta_j, 
\]

where

\[
\alpha_j = \langle 0^{2n}| \prod_{i \in \mathcal{L}_-(j)} V_i^\dagger(\epsilon) \langle 1|_{j} \otimes |00\ldots0\rangle \langle 00\ldots0|_{n+j} V_i(\epsilon)|0^{2n}\rangle 
\]

and

\[
\beta_j = \langle 0^{2n}| \prod_{i \in \mathcal{L}_-(j)} V_i^\dagger(\epsilon) \langle 1|_{j} \otimes (I - |00\ldots0\rangle \langle 00\ldots0|_{n+j}) V_i(\epsilon)|0^{2n}\rangle. 
\]

To upper bound $\alpha_j$, observe that each operator $I \otimes \langle 0| V_i(\epsilon) I \otimes |0\rangle$ appearing in Eq. (50) can be approximated by the identity. In particular, Eq. (38) gives

\[
\|I \otimes \langle 0|_{n+i} (V_i(\epsilon) - I) I \otimes |0\rangle_{n+i}\| \leq 2\gamma|\epsilon|. 
\]

Eq. (52) implies that the right-hand-side of Eq. (50) is close to zero (indeed, if all operators $V_i(\epsilon)$ in Eq. (50) were replaced by the identity then it would evaluate to zero). More precisely,
we may combine Eqs. (50, 52) and recursively use the triangle inequality to replace each gate $V_{k}(\epsilon)$ on the right by $I$. The errors add linearly, and we arrive at

$$\alpha_{j} \leq 2\gamma|\epsilon||L_{\leftarrow}(j)|.$$  \hspace{1cm} (53)

To upper bound $\beta_{j}$, we expand

$$I - |00\ldots0\rangle\langle00\ldots0|_{\mathcal{L}_{\leftarrow}(j)} = \sum_{z \in \{0,1\}^{n}|_{\mathcal{L}_{\leftarrow}(j)} \atop z \neq 00\ldots0} |z\rangle\langle z|$$

in Eq. (51) and use Eqs. (32, 33) to obtain

$$\beta_{j} \leq \sum_{z \in \{0,1\}^{n}|_{\mathcal{L}_{\leftarrow}(j)} \atop z \neq 00\ldots0} (2\sqrt{\gamma|\epsilon|})^{2|z|} = (1 + 4\gamma|\epsilon|)^{|\mathcal{L}_{\leftarrow}(j)|} - 1 \leq e^{4\gamma|\epsilon||\mathcal{L}_{\leftarrow}(j)|} - 1 \leq 8\gamma|\epsilon||\mathcal{L}_{\leftarrow}(j)|.$$  \hspace{1cm} (54)

where in the last line we used the facts that $e^{x} - 1 \leq 2x$ for $x \leq 1$ and $|\epsilon| \leq \epsilon_{0} \leq (4\gamma|\mathcal{L}_{\leftarrow}(j)|)^{-1}$.

Putting together Eqs. (53, 54, 49, 48) we have the upper bound

$$\Pr[E_{j}] \leq 10\gamma|\epsilon|\ell_{1}$$ \hspace{1cm} (55)

for all $1 \leq j \leq 2n$.

Now from Eqs. (55, 47) we see that the Lovász local lemma guarantees $p_{\epsilon}(0^{2n}) > 0$ as long as

$$10\gamma|\epsilon|\ell_{1} \cdot \exp(1) \cdot 2\ell_{4} < 1$$

Upper bounding $\exp(1) \leq 3$ and rearranging, we arrive at Eq. (11).

## 4.2 Zero-free region for random unitaries

In this section for convenience we specialize to the case $O(\epsilon) = \prod_{j=1}^{n} O_{j}(\epsilon)$ where

$$O_{j}(\epsilon) = I + \epsilon Z_{j}.$$  

As in previous sections, we consider the polynomial $f(\epsilon) = \langle 0^{n}|U^{\dagger}O(\epsilon)U|0^{n}\rangle$.

**Theorem 3.** Suppose $U$ is drawn from a unitary 2-design and let $\alpha \in \{1, 2, \ldots, \}$ be given. Then, with probability at least $1 - n^{-\alpha}$, $f(\epsilon)$ is zero-free in a closed disk

$$\epsilon \leq R(n) \quad \text{where} \quad R(n) = 1 - \mathcal{O}(\log(n)/n).$$  \hspace{1cm} (56)

Here the constant implied by the big-$\mathcal{O}$ notation depends on $\alpha$. Below we shall use the notation $Z(s) = \prod_{j=1}^{n} Z_{j}^{s_{j}}$ and $X(s) = \prod_{j=1}^{n} X_{j}^{s_{j}}$ where $s \in \{0,1\}^{n}$ and $X_{j}, Z_{j}$ are Pauli operators acting on qubit $j$. We will use the following properties of unitary 2-designs.
Lemma 6. Suppose $U$ is drawn from a unitary 2-design. Then
\[
\mathbb{E}_U[\langle 0^{2n} | U^\dagger \otimes U^\dagger (Z(r) \otimes Z(s)) U \otimes U | 0^{2n} \rangle] = \begin{cases} 
0 & , r \neq s \\
2^{-n} \left( \frac{4^n - 2^n}{4^n - 1} \right) & , r = s \neq 0^n . \\
1 & , r = s = 0^n 
\end{cases}
\]

Proof. Since $U$ is drawn from a unitary 2-design, we may WLOG evaluate the expectation value over the Haar measure.

First consider the case $r \neq s$ and assume WLOG that $r \neq 0^n$. Then we may choose an $X$-type Pauli $X(q)$ such that
\[
\{X(q), Z(r)\} = 0 \quad \text{and} \quad [X(q), Z(s)] = 0.
\]
Then using the invariance of the Haar measure we have
\[
\mathbb{E}_U[\langle 0^{2n} | U^\dagger \otimes U^\dagger (Z(r) \otimes Z(s)) U \otimes U | 0^{2n} \rangle] = \frac{1}{4^n - 1} \mathbb{E}_U[\sum_{Q \in \mathcal{P}_n \setminus I} \langle 0^{2n} | U^\dagger \otimes U^\dagger (Q \otimes Q) U \otimes U | 0^{2n} \rangle] - \frac{1}{4^n - 1}
\]
which completes the proof of the second case. In the above we used the fact that $X \otimes X + Y \otimes Y + Z \otimes Z = 2SWAP - I$ where $SWAP$ is the two-qubit unitary which permutes the qubits. The third case $r = s = 0^n$ is trivial.

Proof of Theorem 3. We may write
\[
f(\epsilon) = \sum_{k=0}^{n} c_k \epsilon^k
\]
where
\[
c_k = \sum_{s \in \{0,1\}^n : |s| = k} \langle 0^n | U^\dagger Z(s) U | 0^n \rangle.
\]
Note that \( c_0 = 1 \). A simple computation using Lemma 6 gives
\[
\mathbb{E}_U [ |c_k|^2 ] \leq \frac{1}{2^n} \binom{n}{k} \quad 1 \leq k \leq n. \tag{60}
\]
Now suppose \( |\epsilon| \leq R \leq 1 \). Then
\[
|f(\epsilon) - 1| = |\sum_{k=1}^{n} c_k \epsilon^k| \leq \sum_{k=1}^{n/3} |c_k| R^k \leq \sum_{k=1}^{n/3} |c_k| + \sum_{k=n/3}^{n} |c_k| R^k.
\]
Applying Cauchy-Schwarz to each of the two terms on the RHS gives
\[
|f(\epsilon) - 1| \leq \sqrt{n/3 \left( \sum_{k=1}^{n/3} |c_k|^2 \right)^{1/2} + \left( \sum_{k=n/3}^{n} |c_k|^2 \right)^{1/2}} \frac{R^{n/3}}{\sqrt{1 - R^2}}. \tag{61}
\]
Using Eq. (60) we get
\[
\mathbb{E}_U \left[ \sum_{k=1}^{n/3} |c_k|^2 \right] \leq \frac{1}{2^n} \sum_{k=1}^{n/3} \binom{n}{k} \leq 2^{H(1/3)-1} n \leq 2^{-0.08n},
\]
where \( H(\cdot) \) is the binary entropy function. Using Markov’s inequality, we have that with probability at least \( 1 - (1/2)n^{-\alpha} \) over the choice of \( U \),
\[
\sum_{k=1}^{n/3} |c_k|^2 \leq \frac{2n^\alpha}{2^{0.08n}}. \tag{62}
\]
Likewise we have
\[
\mathbb{E}_U \left[ \sum_{k=1}^{n} |c_k|^2 \right] \leq 1
\]
and with probability at least \( 1 - (1/2)n^{-\alpha} \) over the choice of \( U \),
\[
\sum_{k=1}^{n} |c_k|^2 \leq 2n^\alpha \tag{63}
\]
By a union bound we have that with probability at least \( 1 - n^{-\alpha} \) both Eq. (62) and Eq. (63) hold. To complete the proof we show that if both of these events occur then the claimed bound on the zero-free radius of \( f \) holds. Indeed, plugging Eqs. (62,63) into Eq. (61) gives
\[
|f(\epsilon) - 1| \leq \left( \frac{2n^{\alpha+1}}{3} \right)^{1/2} 2^{-0.04n} + \sqrt{2n^\alpha \frac{R^{n/3}}{\sqrt{1 - R^2}}}. \tag{64}
\]
Now for all sufficiently large \( n \) we may choose \( R(n) = 1 - \mathcal{O}(\log(n)/n) \) to make the RHS at most \( 1/2 \). This establishes that \(|f(\epsilon)| \geq 1/2 \) for all \( |\epsilon| \leq R(n) \) and therefore that \( f \) is zero-free in this disk.
5 Additive approximation for general shallow circuits

In this section we give a subexponential classical algorithm for estimating the absolute value $|\langle 0^n | U^\dagger O U | 0^n \rangle|$ of the mean to a given additive error, for a tensor product observable $O = O_1 \otimes O_2 \ldots \otimes O_n$. In the case where each observable $O_j$ is positive semidefinite this provides a subexponential algorithm for the mean value problem.

**Theorem 4.** Let $U$ be an $n$-qubit, depth-$d$ quantum circuit and suppose that $\|O_j\| = 1$ for all $j \in [n]$. There exists a classical algorithm which, given $\delta \in (0, 1/2)$, computes an estimate $E \in \mathbb{R}$ such that

$$|E - |\langle 0^n | U^\dagger O U | 0^n \rangle|| \leq \delta.$$ 

The runtime of the algorithm is upper bounded as $2^{\tilde{O}(4^d \sqrt{n \log(\delta^{-1})})}$.

Theorem 4 is obtained as a straightforward corollary of the following algorithm for additively approximating output probabilities of constant-depth circuits.

**Lemma 7.** Let $V$ be an $n$-qubit, depth-$d$ quantum circuit. There exists a classical algorithm which, given $\delta \in (0, 1/2)$, computes an estimate $q \in \mathbb{R}$ such that

$$|q - |\langle 0^n | V | 0^n \rangle|^2| \leq \delta.$$ 

The runtime of the algorithm is upper bounded as $2^{\tilde{O}(2^d \sqrt{n \log(\delta^{-1})})}$.

Let us now see how Theorem 4 follows from Lemma 7. Suppose we are given $\delta$ and $U$. From Lemma 5, for each $j = 1, 2, \ldots, n$ we may efficiently compute a two qubit unitary $B_j$ such that

$$(I \otimes \langle 0 |)(I \otimes | 0 \rangle) B_j (I \otimes | 0 \rangle) = O_j$$

where we used the theorem’s assumption that $\|O_j\| = 1$. Now consider a $2n$ qubit system where for each $j$ we adjoin an ancilla qubit $n + j$ and the unitary $B_j$ acts between these two qubits. Define $B = \bigotimes_{j=1}^n B_j$. We may then use the algorithm from Lemma 7 with $V = (U^\dagger \otimes I) B (U \otimes I)$, $n' = 2n$, $d' = 2d + 1$, and $\delta' = 0.5\delta^2$ to obtain an estimate $q$ such that

$$|q - |\langle 0^{2n} | (U^\dagger \otimes I) B (U \otimes I) | 0^{2n} \rangle|^2| \leq 0.5\delta^2.$$ 

or equivalently

$$|q - |\langle 0^n | U^\dagger O U | 0^n \rangle|^2| \leq 0.5\delta^2. \quad (66)$$

Now if $q < 0.5\delta^2$ then the above implies that $|\langle 0^n | U^\dagger O U | 0^n \rangle| < \delta$ and in this case we simply output $E = 0$ as our $\delta$-error estimate. On the other hand if $q > 0.5\delta^2$ then we output $E = \sqrt{q}$ as our estimate; using Eq. (66) we get

$$|\sqrt{q} - |\langle 0^n | U^\dagger O U | 0^n \rangle|| \leq \frac{0.5\delta^2}{\sqrt{q} + |\langle 0^n | U^\dagger O U | 0^n \rangle|} \leq \frac{0.5\delta^2}{\sqrt{q}} < \frac{\delta}{\sqrt{2}}.$$ 

Lemma 7 is a simple consequence of the following well-known fact [21, 22].
Lemma 8 ([21]). Let \( \delta \in (0,1/2) \) be given. There exists a univariate polynomial \( g : \mathbb{R} \to \mathbb{R} \) of degree
\[
L = \mathcal{O} \left( \sqrt{n \log(\delta^{-1})} \right)
\] (67)
such that
\[
g(0) = 1 \quad \text{and} \quad |g(c)| \leq \delta \quad \text{for each} \quad c = 1, 2, \ldots, n.
\] (68)
The coefficients of the polynomial can be computed in time polynomial in \( n \).

We shall now review how the polynomial claimed in the Lemma is obtained in a standard way from a quantum query algorithm, see Refs. [21, 22, 38] for more details. In particular, consider the problem of computing the OR of an \( n \)-bit string \( x = x_1 x_2 \ldots x_n \), given quantum query access to \( x \). It is known that this function can be computed with error probability at most \( \delta \) using a number of queries \( T = \mathcal{O}(\sqrt{n \log(\delta^{-1})}) \) [21]. The probability that the quantum algorithm outputs 0 is a multilinear polynomial \( p(x_1, x_2, \ldots, x_n) \) in the input bits \( x_1, x_2, \ldots, x_n \) of degree at most \( 2T \) [38]. The algorithm has the feature that \( p \) depends only on the Hamming weight \( w = \sum_{i=1}^{n} x_i \) of the string \( x \), and therefore we may write
\[
p(x_1, x_2, \ldots, x_n) = g(w)
\]
where \( g : \mathbb{R} \to \mathbb{R} \) is a univariate degree \( 2T \) polynomial. The algorithm succeeds with probability 1 if \( x = 00 \ldots 0 \) and errs with probability at most \( \delta \) in all other cases. Therefore \( g(0) = 1 \) and \( |g(w)| \leq \delta \) for all \( w = 1, 2, \ldots, n \). Note that in order to compute the coefficients of \( g \) it suffices to evaluate it at \( 2T \leq n \) points \( w \in \{0, 1, 2, \ldots, n\} \).

The remarkable small-error \( \sqrt{\log(\delta^{-1})} \) dependence [21, 39]—which can also be achieved for polynomials computing symmetric functions other than OR [22]—is related to the fact that we only care about the values of the polynomial \( g \) at integer values of \( c \). A weaker error bound scaling as \( \mathcal{O}(\log(\delta^{-1})) \) can be obtained more directly using a Chebyshev polynomial [40] (or alternatively, via a suboptimal quantum algorithm which reduces error by parallel repetition). A more direct refinement of the Chebyshev polynomial approach is used in Ref. [39] but leads to a slightly loose bound which matches Eq. (67) up to factors polylogarithmic in \( n \).

Proof of Theorem 7. Let us define
\[
H = \sum_{j=1}^{n} U|1\rangle\langle 1|_j U^\dagger,
\]
where \( |1\rangle\langle 1|_j \) acts nontrivially only on the \( j \)th qubit. Note that the eigenvalues of \( H \) are the integers between 0 and \( n \), and that the state
\[
|\psi\rangle = U|0^n\rangle
\]
is the unique state satisfying \( H|\psi\rangle = 0 \). Let \( \delta \) be given and consider the polynomial of degree \( L = L(\delta) \) described by Lemma 8. Using Eq. (68) and the spectrum of \( H \) we see that
\[
\|g(H) - |\psi\rangle\langle \psi|\| \leq \delta,
\]
and therefore
\[ \left| \langle 0^n | U | 0^n \rangle - \langle 0^n | g(H) | 0^n \rangle \right| \leq \delta. \]
To prove the theorem it remains to show that \( \langle 0^n | g(H) | 0^n \rangle \) can be computed exactly using the claimed runtime. Note that for any positive integer \( r \) we may express
\[ \langle 0^n | H^r | 0^n \rangle = \langle 0^n | U \left( \sum_{j=1}^{n} |1\rangle \langle 1|_j \right)^r U^\dagger | 0^n \rangle \]
The right hand side is a sum of at most \( n^r \) terms of the form
\[ \langle 0^n | U | 11 \ldots 1 \rangle \langle 11 \ldots 1 | S U^\dagger | 0^n \rangle \] (69)
where \( S \subset [n] \) satisfies \( |S| \leq r \). Since \( U \) has depth \( d \), the operator
\[ U | 11 \ldots 1 \rangle \langle 11 \ldots 1 | S U^\dagger \]
acts nontrivially on at most \( 2^d |S| \) qubits. Therefore each term Eq. (69) can be computed exactly using a runtime \( 2^{O(2^d r)} \), and \( \langle 0^n | H^r | 0^n \rangle \) can be computed with runtime \( n^r 2^{O(2^d r)} \).
Since \( g(H) \) is a polynomial of degree \( L \) with efficiently computable coefficients, we may compute \( \langle 0^n | g(H) | 0^n \rangle \) using runtime
\[ \text{poly}(n) + Ln^L 2^{O(2^d L)} = 2^{O(2^d \sqrt{n \log(\delta^{-1})})}, \]
where the first term on the LHS is the time used to compute the coefficients of the polynomial, and the second term is the time used to compute \( \langle 0^n | H^r | 0^n \rangle \) for \( 1 \leq r \leq L \).

6 Additive approximation for 2D and 3D circuits

In this section we consider tensor product observables \( O = O_1 \otimes O_2 \otimes \cdots \otimes O_n \), where \( O_j \) are arbitrary hermitian single-qubit operators satisfying
\[ ||O_j|| \leq 1. \] (70)
As before, our goal is to estimate the mean value \( \mu = \langle 0^n | U^\dagger OU | 0^n \rangle \). We prove the following.

**Theorem 5.** Consider a 2D grid of \( n \) qubits. Suppose \( U \) is a depth-\( d \) quantum circuit composed of nearest-neighbor two-qubit gates. There exists a probabilistic classical algorithm that computes an approximation \( \bar{\mu} \) satisfying \( |\bar{\mu} - \mu| \leq \delta \) with probability at least \( 2/3 \). The algorithm has runtime scaling as \( n \delta^{-2} 2^{O(d^2)} \).

**Proof.** Define operators
\[ Q_j = U^\dagger (O_j \otimes I_{\text{else}}) U. \] (71)
Here \( I_{\text{else}} \) applies the identity operator to all qubits in \([n] \setminus \{j\} \). Obviously, the operators \( Q_1, \ldots, Q_n \) pairwise commute. Furthermore, \( Q_j \) acts nontrivially only within a lightcone of radius \( d \) centered at the \( j \)-th qubit. We show an example of such lightcone for \( d = 2 \) in Fig. 1. It will be convenient to coarse-grain the lattice into super-sites with local Hilbert
space of dimension $D = 2^{4d^2}$. Each super-site represents a block of qubits of size $2d \times 2d$. An example for $d = 2$ is shown in Fig. 1.

Let $\Lambda$ be the coarse-grained lattice. It has linear size $L \times L$, where

$$L \approx \frac{\sqrt{n}}{2d}.$$ 

We shall label sites $u \in \Lambda$ by pairs of integers $(i, j)$, where $1 \leq i, j \leq L$. Let us agree that $i$ and $j$ label rows and columns of $\Lambda$ respectively. Define a plaquette $p(i, j)$ as a $2 \times 2$ cell of $\Lambda$ spanning super-sites $(i, j)$, $(i + 1, j)$, $(i, j + 1)$, and $(i + 1, j + 1)$. Let $Q_{i,j}$ be the product of all operators $Q_s$ whose support is fully contained in the plaquette $p(i, j)$. If the support of $Q_s$ is contained in more than one plaquette, assign $Q_s$ to one of them to avoid duplication. Then

$$Q_1Q_2\cdots Q_n = \prod_{1 \leq i,j \leq L-1} Q_{i,j}.$$ 

(72)

Here we noted that all $Q$’s pairwise commute, so the order does not matter. This yields

$$\mu = \langle \Psi_0 | \Psi_1 \rangle \text{ where } |\Psi_b\rangle = \prod_{(i,j) : j = b \pmod{2}} Q_{i,j} |0^n\rangle.$$ 

(73)

The product ranges over $1 \leq i, j \leq L - 1$ to ensure that all plaquettes $p(i, j)$ are fully inside the lattice. We claim that for each $b \in \{0, 1\}$ there exists a linear order on the set of $n$ qubits such that the state $\Psi_b$ is Matrix Product State (MPS) with a small bond dimension that depends only on the circuit depth $d$. Below we prove the claim for the state $\Psi_1$ (exactly the same arguments apply to $\Psi_0$).

Let $C_1, C_2, \ldots, C_L$ be the consecutive columns of $\Lambda$. Assume for simplicity that $L = 2K$ is an even integer. A direct inspection shows that none of the plaquettes $p(i, j)$ with odd coordinate $j$ crosses the boundary between vertical strips

$$A_\alpha = C_{2\alpha-1}C_{2\alpha}, \quad \alpha = 1, 2, \ldots, K.$$ 

Figure 1: **Left**: qubits live at sites of the 2D square lattice. The lightcone of a single qubit generated by a depth-2 circuit is highlighted in red. **Right**: the coarse-grained lattice $\Lambda$. Each $4 \times 4$ block of sites becomes a super-site of the coarse-grained lattice. A plaquette is a $2 \times 2$ cell spanning four adjacent super-sites. The support of any operator $Q_j$ is covered by a single plaquette.
The strips $A_{\alpha}$ are shown in Fig. 2 for $K = 3$. For example, all plaquettes $p(i, 1)$ are fully contained in the strip $A_1$, plaquettes $p(i, 3)$ are fully contained in $A_2$ etc. Thus $\Psi_1$ is a tensor product of $K$ single-strip states associated with $A_1, \ldots, A_K$, 

$$|\Psi_1\rangle = |\Psi_1(A_1)\rangle \otimes |\Psi_1(A_2)\rangle \otimes \cdots \otimes |\Psi_1(A_K)\rangle,$$

where

$$|\Psi_1(A_{\alpha})\rangle = \prod_{(i,j) : p(i,j) \subseteq A_{\alpha}} Q_{i,j} |0\rangle_{A_{\alpha}}.$$

We claim that each single-strip state $\Psi_1(A_{\alpha})$ is an MPS with bond dimension $\chi \leq D^3$. Recall that $D$ is the local Hilbert space dimension of each super-site.

Indeed, consider a fixed strip $A_{\alpha}$ and choose a snake-like linear order such that $A_{\alpha} = \{1, 2, \ldots, 2L\}$, see Fig. 2. Consider any bipartite cut $A_{\alpha} = A'_{\alpha}A''_{\alpha}$, where $A'_{\alpha}$ and $A''_{\alpha}$ are consecutive blocks of super-sites. A direct inspection shows that there are at most two plaquettes $p(i,j)$ that are contained in the strip $A_{\alpha}$ and cross the chosen cut, see Fig. 3. Furthermore, the corresponding plaquette operators $Q_{i,j}$ act nontrivially on at most three super-sites located next to the cut, see Fig. 3. Thus the Schmidt rank of $\Psi_1(A_{\alpha})$ across the chosen cut is at most $\chi = D^3$. Accordingly, $\Psi_1(A_{\alpha})$ is an MPS with bound dimension $\chi$. The same applies to the full state $\Psi_1$ since the latter is a tensor product of the states $\Psi_1(A_{\alpha})$. By the symmetry, the same arguments apply to the state $\Psi_0$. It should be emphasized that the linear orders in the MPS representation of $\Psi_0$ and $\Psi_1$ are not the same. Thus, the desired mean value can be written as

$$\mu = \langle \Psi_0 | W | \Psi_1 \rangle,$$

where $W$ is a permutation of $n$ qubits that accounts for the difference between linear orders used by $\Psi_0$ and $\Psi_1$. The MPS description of the states $\Psi_b$ can be computed starting from the circuit $U$ and the list of observables $O_j$ using the well-known algorithms [41–43]. It takes time $n \cdot \text{poly}(\chi) = n2^{O(d^2)}$.

Let $\gamma_b = ||\Psi_b||$, where $b = 0, 1$. Note that $\gamma_b \leq 1$ since we assumed $||O_j|| \leq 1$ for all $j$ and $U$ is a unitary operator. Furthermore, one can compute $\gamma_b$ in time $O(n\chi^3)$ using the standard MPS algorithms [44]. Define normalized states $|\Phi_b\rangle = \gamma_b^{-1} |\Psi_b\rangle$. Then

$$\mu = \gamma_0 \gamma_1 \langle \Phi_0 | W | \Phi_1 \rangle.$$

Figure 2: Coarse-grained lattice of size $L = 5$ and the snake-like linear order that define Matrix Product States $\Psi_1(A_1), \Psi_1(A_2), \Psi_1(A_3)$. 

![Figure 2](image-url)
Figure 3: Examples of a bipartite cut of the chain $A_\alpha$ and plaquettes crossing the cut. For each cut there are at most two plaquette operators $Q_{i,j}$ capable of creating entanglement across the cut. The state $\Psi_1(A_\alpha)$ is obtained from the all-zero basis state by applying all plaquette operators $Q_{i,j}$ contained in $A_\alpha$. The above shows that $\Psi_1(A_\alpha)$ is a Matrix Product State with a small bond dimension, $\chi \leq D^3$.

Define a probability distribution
\[ \pi(x) = |\langle x|\Phi_0\rangle|^2, \quad x \in [D]^L \]
and a function
\[ F(x) = \gamma_0 \gamma_1 \langle x|W|\Phi_1\rangle / \langle x|\Phi_0\rangle \]
which is well-defined whenever $\pi(x) > 0$. Then $\mu$ coincides with the mean value of $F(x)$ over the distribution $\pi(x)$,
\[ \mu = \sum_x \pi(x) F(x). \quad (76) \]

The random variable $F(x)$ has the variance
\[ \text{Var}(F) \leq \sum_x \pi(x) |F(x)|^2 = (\gamma_0 \gamma_1)^2 \sum_x |\langle x|\Phi_1\rangle|^2 = (\gamma_0 \gamma_1)^2 \leq 1. \quad (77) \]

Define an empirical mean value $\tilde{\mu} = S^{-1} \sum_{i=1}^S F(x^i)$, where $x^1, \ldots, x^S \in [D]^L$ are independent samples from the distribution $\pi(x)$ and the number of samples is $S = 3\delta^{-2}$. By Chebyshev inequality, $|\tilde{\mu} - \mu| \leq \delta$ with probability at least $2/3$. It remains to notice that any amplitude $\langle x|\Phi_b\rangle$ can be computed using the standard MPS algorithms [44] in time $O(n \chi^3)$. Accordingly, one can compute $F(x)$ for any given string $x$ in time $O(n \chi^3)$. The probability distribution $\pi(x) = |\langle x|\Phi_0\rangle|^2$ can be sampled in time $n \cdot \text{poly}(\chi)$ using the algorithm of Ref. [43], see Theorem 1 thereof. To summarize, the overall cost of approximating $\mu$ is $n\delta^{-2}\text{poly}(\chi) = n\delta^{-2}2^{O(d^2)}$. □

Suppose now that $U$ is a geometrically local depth-$d$ quantum circuit on a three-dimensional grid of $n$ qubits of linear size $n^{1/3}$. Define the coarse-grained lattice $\Lambda$ as a two-dimensional grid, see Fig. 1, where each super-site represents a block of qubits of size $2d \times 2d \times n^{1/3}$. The lattice $\Lambda$ has size $L \times L$ with $L \approx n^{1/3}/2d$. Now each super-site has the local Hilbert space
of dimension $D = 2^{4d^2 n^{1/3}}$. Repeating exactly the same arguments as above one gets a representation $\mu = \langle \Psi_0 | W | \Psi_1 \rangle$, where $\Psi_b$ are MPSs with bond dimension $\chi \leq D^3 = 2^{O(d^2 n^{1/3})}$ and $W$ is a permutation of $n$ qubits. Thus one can estimate $\mu$ within an additive error $\delta$ in time $n^{\delta^{-2}} \text{poly}(\chi) = \delta^{-2} 2^{O(d^2 n^{1/3})}$.

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