Efficient Mean-Field Simulation of Quantum Circuits
Inspired by the Many-Electron Problem

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Classical simulations can provide the exact wave function of quantum circuits (QCs)$^{1-3}$, but are currently limited to $\sim 50$ qubits$^{1,4}$ due to their memory and computational cost, which scale exponentially with qubit number. As quantum hardware advances toward hundreds of interacting qubits$^5$, developing reliable schemes for approximate QC simulations has become a priority. Here we show efficient simulations of QCs with a method inspired by density functional theory (DFT), a widely used approach to study many-electron systems. We demonstrate accurate simulations of various QCs with universal gate sets, reaching up to a billion qubits in size, using only laptop calculations. Our simulations can predict marginal single-qubit probabilities (SQPs) with over 90% accuracy, using memory and computational resources linear in qubit number despite the formal exponential cost of SQPs. We achieve these results by adopting a mean-field description of QCs, and formulating optimal single- and two-qubit gate functionals — analogs of exchange-correlation functionals in DFT$^6$ — to evolve the SQPs without computing the QC wave function. Our findings pave the way for accurate simulations of large QCs and provide a blueprint to adapt electronic structure methods to QC simulations.

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Quantum computers with over 50 qubits have become a reality\(^5\), even though noise and decoherence still limit their reliable operation. This era of noisy intermediate-scale quantum (NISQ) devices promises exciting advances in quantum algorithms with no classical counterpart\(^7,8\). Classical simulations remain essential to understand the physics of these quantum devices, improve their design, and accelerate their progress. An important direction is the development of approximate schemes that are both accurate and computationally efficient, enabling simulations of general QCs with any depth and degree of entanglement, ideally with favorable scaling up to hundreds or thousands of qubits. Work in this area has focused on matrix product states and tensor networks to simulate QCs with specific structures, gate types, degree of entanglement, and noise\(^9–15\), and more recently on simulations of general QCs using neural-network quantum states\(^16\). Despite these notable advances, and because exact simulations of moderate-sized QCs are readily available, progress on approximate QC simulations has remained relatively slow.

Numerical methods have a long history of success for studies of quantum systems\(^17–21\), and thus we ask whether approximate methods from other subfields can be adapted to simulate QCs. There is an intriguing parallel between many-electron and many-qubit systems. In the many-electron problem, which is a grand challenge in condensed matter\(^22,23\), exact solutions are possible only for systems with one electron (the hydrogen atom). Therefore, unlike QC simulations, electronic structure calculations are dominated by approximate methods\(^21,24\), among which density functional theory (DFT) is the main workhorse. Leveraging a mean-field description centered on the electron density, DFT achieves low-polynomial scaling with system size, enabling studies of matter with thousands of interacting electrons\(^24,25\). However, formulating similarly accurate and efficient methods to study QCs with many interacting qubits remains an open challenge. Similar to DFT for molecules and materials, such a method could be game-changing, opening doors for simulations of quantum circuits beyond the NISQ era and upending our current notion of quantum primacy\(^26\).

Here we show a density functional theory for quantum circuits — in short, QC-DFT — able to accurately simulate marginal single-qubit probabilities (SQPs) in QCs with up to a billion qubits (on a laptop), despite the formal exponential cost of SQPs. We present results for various random QCs using two different universal gate sets, and demonstrate the formulation and optimization of QC-DFT gate functionals. We also discuss the scaling of computational cost and SQP distributions with QC size, and show the application of
QC-DFT to a model Hamiltonian. These results demonstrate that even though the exact QC wave function is exponentially complex, marginal probability distributions such as the SQPs can be obtained with an exquisite trade-off of cost and accuracy, opening doors for approximate but reliable simulations of QCs and quantum computers.

The QC wave function for \( N \) qubits can be expanded in the computational basis as

\[
\Psi = \sum_{i_1 i_2 \ldots i_N} c_{i_1 i_2 \ldots i_N} |i_1 i_2 \ldots i_N\rangle = \sum_x c_x |x\rangle
\]

where \( i_n = 0, 1 \) are basis states for a single qubit, \( x \) are binary numbers from 0 to \( 2^{N-1} \), \( c_x \) are state-vector amplitudes, namely expansion coefficients of the QC wave function, and \( |x\rangle = |i_1 i_2 \ldots i_N\rangle \) are \( N \)-qubit states in the computational basis (\( N \)-bit long bitstrings).

For \( N \) qubits, accessing this wave function requires storing and manipulating \( 2^N \) complex numbers, which is out of reach for modern computers for \( N > 50 \). (A laptop can handle \( N \approx 25 \) qubits, and a small computer cluster \( N \approx 30 \) on a single core; parallelization is needed beyond \( N = 30 \).) In a gate-based QC, the wave function evolves at each cycle (or step) via a unitary transformation, and it can be computed exactly with a classical algorithm by applying single- and two-qubit gates as \( 2 \times 2 \) unitary matrices and updating pairs of amplitudes in place\(^1\). From the exact wave function at step \( s \), one can obtain the \( N \)-qubit probability distribution \( \tilde{P}_s(x) = |\langle x | \Psi_s \rangle|^2 \), which can be sampled experimentally by measuring the QC, but is exponentially hard to compute\(^5\).

Here we take a different approach and focus on the evolution of each individual qubit as a result of mean-field interactions with single- and two-qubit gates. We define the single-qubit probability (SQP) for qubit \( n \), with values between 0 and 1, as the probability of measuring qubit \( n \) in the excited state \( |1\rangle \) at step \( s \), regardless of the state of the other qubits:

\[
p_s^{(n)} = \sum_{\{i_q, q \neq n\}} |\langle i_1, i_2, \ldots, i_n=1, \ldots, i_N| \Psi_s \rangle|^2.
\]

The exact SQPs are marginals of the \( N \)-qubit probability distribution \( \tilde{P}_s(x) \), and are also exponentially hard to compute because they require knowledge of the QC wave function. We define the SQP vector at step \( s \), \( \mathbf{p}_s = (p_s^{(1)}, p_s^{(2)}, \ldots, p_s^{(N)})_s \), as the set of SQPs for all qubits in the QC. Note that the SQP vector has \( N \) components, and thus it can be stored with memory resources linear in qubit number \( N \), and that the SQPs can be accessed experimentally by measuring the state of each single qubit rather than that of the entire QC.
We model the evolution of the SQP vector $p_s$ under the effect of single- and two-qubit gates, using an approximate mean-field approach inspired by DFT. In a general QC, single- and two-qubit gates are applied to a set of qubits at each step $s$. As a result, the SQP vector evolves to a new value at step $s + 1$:

$$p_{s+1} = f_G(p_s)$$

where we define the map $f_G$ as the exact gate functional. Here we derive approximate gate functionals that evolve independently the SQPs of qubits acted on by single-qubit gates, and couple qubits acted on by two-qubit gates (here, CZ and CNOT). The rules for evolving the SQP vector $p$ are derived from SQP-dependent gate-qubit interactions, analogs of the density-dependent electron interactions in DFT. Recall that $p$ is the probability of measuring a single qubit in state $|1\rangle$. We define a single-qubit mean-field state consistent with this SQP:

$$|p\pm\rangle = \sqrt{1-p}\,|0\rangle \pm \sqrt{p}\,|1\rangle$$

where we use $\pm$ to take into account two opposite phases between the $|0\rangle$ and $|1\rangle$ states.

For single-qubit gates, we apply the gate $U$ to this mean-field state, and then compute the probability of measuring $|1\rangle$ while taking the phase average over the $\pm$ states. This approach provides explicit rules to update the SQPs at each step:

$$p_{s+1} = \frac{1}{2} \sum_{\pm} |\langle 1|U|p_s\pm\rangle|^2.$$  

This equation defines the local-probability approximation (LPA) gate functional. Using equation (5), we derive the following LPA update rules for common single-qubit gates:

- Pauli X and Y: $p_{s+1} = 1 - p_s$
- Pauli Z, S and T: $p_{s+1} = p_s$
- $H, \sqrt{X}$ and $\sqrt{Y}$: $p_{s+1} = 0.5$.  

These results imply that the Pauli X and Y gates flip the SQP, the Pauli Z, S and T gates leave the SQP unchanged as they act only on the phase, and the Hadamard, Pauli $\sqrt{X}$ and $\sqrt{Y}$ gates set the SQP to 1/2.

For the two-qubit gates considered here, CZ and CNOT, we use our intuition combined with the LPA rules to approximate the SQP evolution. The probability $p^{(c)}$ of the control
qubit is left unchanged, while the probability \( p^{(t)} \) of the target qubit is evolved according to:

\[
\begin{align*}
\text{CZ:} & \quad p^{(t)}_{s+1} = p^{(t)}_s \\
\text{CNOT: if } & \quad p^{(c)} < 0.5, \quad p^{(t)}_{s+1} = p^{(t)}_s \tag{7} \\
\text{if } & \quad p^{(c)} > 0.5, \quad p^{(t)}_{s+1} = 1 - p^{(t)}_s.
\end{align*}
\]

The CZ result follows from the LPA rule for the Pauli Z gate, which leaves the SQP unchanged. The CNOT gate uses a \( p^{(c)} = 0.5 \) threshold for controlling the target qubit, but the case \( p^{(c)} = 0.5 \) is more subtle and needs a separate update rule:

\[
\begin{align*}
\text{CNOT: if } & \quad p^{(c)} = 0.5 \text{ and } p^{(t)} = 0 \text{ or } 1, \quad p^{(t)}_{s+1} = 0.5 \tag{8} \\
\text{if } & \quad p^{(c)} = 0.5 \text{ and } p^{(t)} \neq 0 \text{ or } 1, \quad p^{(t)}_{s+1} = 1 - p^{(t)}_s.
\end{align*}
\]

This choice allows us to address the important case of a Hadamard gate acting on the control qubit of a CNOT gate, as in the Bell-state preparation QC\textsuperscript{27}, a key building block in the random QCs discussed below. In particular, our CNOT and Hadamard update rules give the correct SQPs for all possible two-qubit initial basis states in the Bell-state preparation QC\textsuperscript{27} (see Extended Data Table 1).

We implement these QC-DFT simulations using an in-house code (see Code Availability), and apply them to random and nonrandom QCs ranging from small to large, with up to a billion interacting qubits. For small QCs with less than \( \sim 30 \) qubits, we compare the approximate SQPs with exact values obtained from wave-function (also known as state-vector) QC simulations carried out using the QuEST code\textsuperscript{3} (see Methods). For this comparison, we define the \textit{SQP accuracy} \( A_s \) as the fraction of SQPs predicted correctly by QC-DFT at step \( s \) (equivalently, the SQP error \( 1 - A_s \) is the fraction of qubits with incorrect SQPs).

We first discuss results for random QCs with a universal Clifford+T gate set\textsuperscript{29}, a moderate depth (20 steps), and QC sizes from 20 to 32 qubits. In these QCs, at each step half of the qubits, chosen at random, are acted on by a randomly chosen single-qubit gate in the set, while the other half are acted on by CNOT gates that couple randomly-selected control and target qubits (Fig. 1a). In the exact simulations, the state-vector of the QC is initially set to \( |00\ldots0\rangle_N \) and then evolved according to the gate sequence, while the exact SQPs are computed at each step via equation (2). The exact SQPs, with initial value of \( p = 0 \), evolve nontrivially for 10–15 steps, after which in our random QCs they reach a fully randomized value of \( p = 0.5 \). Our approximate QC-DFT simulations aim to capture this nontrivial SQP
Figure 1. QC-DFT simulations of random quantum circuits using LPA gate functionals. **a,** Random QC using a universal Clifford+T gate set. Each step consists of randomly chosen single-qubit gates applied to half of the qubits and CNOT gates applied to the other half (top). The accuracy of the simulated SQPs at each step is shown for this type of random QCs with different numbers of qubits (bottom). **b,** Random QC with T, $\sqrt{X}$, $\sqrt{Y}$ and CZ gates, taken from Ref.28 but with the H gates removed. Similar to (a), we plot the SQP accuracy for different QC sizes (bottom). Both types of QCs have a depth of 20 steps, with a single step shown in shaded gray. The SQPs are obtained by averaging results from 20 distinct random QC instances in (a) and 10 instances in (b).

dynamics in the first 10–15 steps before randomization occurs.

The results of our QC-DFT simulations for these Clifford+T QCs are shown in Fig. 1a. We find that our approach can predict the SQPs with an accuracy greater than $\sim90\%$ at
all steps. The highest error occurs near steps 5–7, where the qubits become nontrivially correlated, and then decreases to zero when the QC becomes fully randomized, with all SQPs trivially equal to 0.5. Throughout the dynamics, the exact SQP values for most qubits are 0, 0.5, or 1 due to the combined action of the Hadamard and CNOT gates, and thus the main challenge for the approximate simulations is to capture the transitions between these values, as further discussed below. We also simulate Clifford+T QCs with a different structure, which alternates one step where all qubits are acted on by randomly chosen single-qubit gates, and one step where all qubits are acted on by CNOT gates with randomly selected control and target qubits. The results, given in Extended Data Fig. 1, show a similar SQP accuracy of 90% or higher at all steps.

To demonstrate the generality of our approach, we also simulate a different family of random QCs, introduced by Boixo et al.\textsuperscript{28}, which use a T, Pauli $\sqrt{X}$ and $\sqrt{Y}$, and CZ gate set (Fig. 1b). (We removed the Hadamard gate layer from the QCs in Ref.\textsuperscript{28} as it would make the SQPs trivially equal to 0.5 at all steps). The initial conditions are the same as in the Clifford+T circuits discussed above, but the quantum dynamics is richer, with more possible SQP values than in the Clifford+T case due to the combined effects of the T and square-root Pauli gates. Despite this greater complexity, our QC-DFT approach can simulate the dynamics of these QCs with an SQP accuracy greater than 85–90% for sizes ranging from 20 to 30 qubits (Fig. 1b). These results demonstrate that our QC-DFT approach, combined with the LPA rules, can accurately predict the SQPs for a wide range of random QCs without ever computing the exponentially complex QC wave function.

Furthermore, we study whether this accuracy can be improved by fine-tuning the QC-DFT gate functionals, in a spirit similar to improving electronic exchange-correlation functionals in DFT\textsuperscript{25}. Many SQP errors in the LPA simulations derive from applying two consecutive times the same gate to a given qubit — a situation analogous to a strong local interaction in the many-electron problem — or from specific gate sequences acting on a qubit. Because our LPA focuses on local gate-qubit interactions at the current step, it lacks memory effects and cannot accurately describe such multi-gate correlations. To address this problem, we formulate multi-gate approximation (MGA) functionals encoding the effects of gate sequences, and apply them as a correction to the LPA in the first $\sim$10 steps, where multi-gate correlations are important for predicting the SQP dynamics in our random QCs.
We define MGA-\(n\) gate-functionals which treat explicitly single-qubit gate sequences with length \(l \leq n\). Their SQP update rules can be written as

\[
p_{s+1} = |\langle 1 | \prod_{i=s-l}^{s} U_i |0\rangle|^2,
\]

where \(U_i\) is a single-qubit gate acting at step \(i\). This approach captures the effect of sequences of \(l\) gates, from step \(s-l\) to the current step \(s\), and focuses on early multi-gate corrections in the QC by assuming that the gate sequences act on the initial single-qubit state \(|0\rangle\). When using these MGA-\(n\) gate-functionals, the SQPs are evolved at each step using the LPA, but gate-sequences with length up to \(n\) are searched at each step; if a sequence included in the functional is found, then the SQP is updated according to equation (9).

For example, for an MGA functional encoding a sequence of two Hadamard gates \(U_H\), the first gate gives \(p_s = 0.5\) due to the LPA rules, and the second gives \(p_{s+1} = \langle 1 | U_H^2 |0\rangle = 0\).

Similarly, an MGA treating a sequence of two square-root of Pauli X gates gives \(p_s = 0.5\) after the first and \(p_{s+1} = \langle 1 | (\sqrt{\sigma_X})^2 |0\rangle = 1\) after the second \(\sqrt{X}\) gate.

We develop several MGA functionals (see Methods) aimed at improving the SQP accuracy by addressing the shortcomings of the LPA in our random QCs. For the Clifford+T QCs in Fig. 1a, our analysis of the LPA results reveals that two main gate sequences lead to SQP errors: the H−H sequence consisting of two consecutive Hadamard gates applied to the same qubit, which leads to \(p_{s+1} = 0.5\) in the LPA instead of the exact \(p_{s+1} = 0\), and the three-gate sequence H−T−H, which gives \(p_{s+1} = 0.5\) in the LPA instead of the exact result \(p_{s+1} = 0.146447\). Accordingly, we develop a simple MGA-3 functional addressing these two sequences, and apply it to our Clifford+T random QCs. Figure 2a compares the accuracy of this MGA-3 functional with the LPA for the random Clifford+T QCs in Fig. 1a. We apply the multi-gate corrections in the first 7 steps, and find a significant improvement in the SQP accuracy, by roughly 5–8%, during those steps. Beyond step \(\sim 10\), the QC state randomizes and the SQP accuracy becomes nearly identical for the two functionals. We find similar accuracy improvements for Clifford+T random QCs with a different structure, as shown in Extended Data Fig. 2.

For the second family of random QCs discussed above, which employ T, Pauli \(\sqrt{X}\) and \(\sqrt{Y}\), and CZ gates, we develop two types of MGA functionals: MGA-2 addressing only sequences of two consecutive \(\sqrt{X}\) or \(\sqrt{Y}\) Pauli gates, and a systematically improved MGA-6 functional encoding sequences of up to six single- and two-qubit gates. Both of these MGA
Figure 2. Optimized MGA gate functionals. **a,** Accuracy comparison between the LPA and MGA-3 functionals applied to the Clifford+T circuits in Fig. 1a (top). The SQPs at each step are plotted for selected qubits for both functionals and compared with exact results (bottom). **b,** Accuracy comparison between the LPA and two different MGAs, MGA-2 and MGA-6, encoding respectively up to two- and six-gate sequences (top), shown together with the SQPs at each step for selected qubits (bottom). The results in (a) are for QCs with 32 qubits and in (b) for QCs with 20 qubits. The standard deviation of the SQP accuracy is shown for each curve using shaded colors. These results are obtained by averaging over the same number of QCs as in Fig. 1.

functionals lead to accuracy improvements over the LPA, with the MGA-6 further improving over the simpler MGA-2 (Fig. 2b). For both types of random QCs studied here, we analyze the SQP dynamics for selected qubits (bottom panels in Fig. 2) to understand the effects of multi-gate corrections, and find that they span all possible scenarios: the MGA can leave the LPA results unchanged, correct SQP errors in the LPA, fail to correct the LPA errors, or occasionally introduce errors not present in the LPA. When the MGA correction is successful, the SQP accuracy improvement typically lingers for multiple steps, leading to sizable accuracy improvements relative to the LPA. In addition, the multi-gate corrections allow us to capture SQP values different from 0, 0.5 and 1, the only possible values
in the LPA. These results demonstrate a systematic approach for improving QC-DFT gate functionals by explicitly addressing multi-gate correlations.

Figure 3. Computational cost and SQP distribution scaling with quantum circuit size. **a**, Quantum circuit structure used to obtain the computational cost and SQP distribution as a function of QC size. The rules used to generate this type of QC are given in Methods. **b**, Linear scaling of QC-DFT computation time with qubit number. **c**, Invariance of the SQP distribution with respect to QC size for QCs with the same structure, which is given in (**a**). Results are shown for QCs with sizes of 20, 4000, and 10^5 qubits.

The efficiency of our approach allows us to simulate very large QCs. We focus on a family of nonrandom QCs (with Hadamard, Pauli X, Y, Z, and CNOT gates), generated with a set of deterministic rules given in Methods, whose diagram for an example size of 8 qubits is shown in Fig. 3a. Using this class of QCs, with sizes ranging from 20 to 10^9 qubits, we demonstrate that the computational cost of QC-DFT has a linear scaling with number of qubits in the QC (Fig. 3b). We are able to complete the largest calculation, with size one billion qubits, using only a laptop computer for a few hours. Note that both the memory and
computational cost to obtain accurate SQPs scale linearly with QC size and depth in our QC-DFT approach, in clear contrast with the exact SQPs from state-vector simulations\(^3\), for which the memory and computational cost scale exponentially with qubit number.

Our analysis of the nonrandom QCs in Fig. 3a further reveals an intriguing physical result: for QCs with a given structure, the SQP distribution is independent of QC size, and thus is scale-invariant with respect to qubit number, as shown in Fig. 3c for three illustrative QC sizes. (Although the simulations for large \(N\) values cannot be validated against exact results, we have verified that simulations for \(N < 30\) qubits achieve a 90\% SQP accuracy, similar to the other LPA results shown in this work.) This finding shows that the SQP distribution is a fingerprint of the QC uniquely linked to its structure, a result reminiscent of the unique map between the electron density and the material structure in DFT, as proved in the celebrated Hohenberg-Kohn theorems\(^24\). This analysis suggests that the SQPs play a central role in mean-field studies of QCs – similar to the electron density in DFT, which is also a one-body marginal probability – justifying the focus on SQPs in our approach.

We conclude with an application of QC-DFT to obtain the ground-state energy of a simple spin Hamiltonian. Extending the variational quantum eigensolver (VQE)\(^{30,31}\) discussion in Ref.\(^{27}\), we model the \(N\)-qubit Hamiltonian \(H = \bigotimes_{j=1}^{N} \sigma_z^{(j)}\), where \(\sigma_z^{(j)}\) is the Pauli Z gate acting on qubit \(j\), and search the energy minimum starting from the trial wave function \(|\Psi(\theta)\rangle = \prod_{j=1}^{N} R_x(\theta_j) |00\ldots0\rangle_N\), where \(R_x(\theta_j)\) is a rotation through angle \(\theta_j\) around the \(x\)-axis applied to qubit \(j\) (starting from an initial state \(|00\ldots0\rangle_N\)), and \(\theta = (\theta_1, \theta_2, \ldots, \theta_N)\) is the set of rotation angles parametrizing the wave function. For this example Hamiltonian, the energy \(E(\theta)\) can be obtained analytically: the rotation \(R_x(\theta)\) acting on each qubit gives a state \(|\varphi(\theta)\rangle\) written as

\[
R_x(\theta) |0\rangle \equiv |\varphi(\theta)\rangle = \cos(\theta/2) |0\rangle - i \sin(\theta/2) |1\rangle ,
\]

and thus we obtain:

\[
E(\theta) = \langle \Psi(\theta) | H | \Psi(\theta) \rangle = \prod_{j=1}^{N} \langle \varphi(\theta_j) | \sigma_z^{(j)} | \varphi(\theta_j) \rangle = \prod_{j=1}^{N} [\cos^2(\theta_j/2) - \sin^2(\theta_j/2)] = \prod_{j=1}^{N} \cos(\theta_j). \tag{11}
\]

In a state-vector simulation, preparing the trial wave function \(|\Psi(\theta)\rangle\) and computing the associated energy \(E(\theta)\) for any set of angles \(\theta\) requires the application of \(N\) rotations about the \(x\)-axis, with a computational cost growing exponentially with qubit number \(N\).
Therefore, the search for the ground-state energy, for example in a VQE simulation\cite{31}, would require exponential resources. This argument for the computational cost of state preparation and energy calculation holds in general for variational state-vector simulations.

Here we employ QC-DFT as an alternative route for more efficient energy calculations. Using the LPA gate functional, the update rule for the $R_x(\theta)$ rotation is

$$p_{s+1} = \frac{1}{2} \sum_{\pm} \langle 1 | R_x(\theta) | p_s \rangle = p_s \cos^2(\theta/2) + (1 - p_s) \sin^2(\theta/2),$$

which becomes $p_{s+1} = \sin^2(\theta/2)$ for our initial state with $p_s = 0$. Using as trial wave function the resulting mean-field state obtained with equation (4), $|p_{s+1}\rangle = \cos(\theta/2) |0\rangle \pm \sin(\theta/2) |1\rangle$, we write the mean-field energy for a single-qubit Hamiltonian $\sigma_z$ as:

$$\varepsilon_{\text{MF}}(\theta, p_{s+1}) = \langle p_{s+1} | \sigma_z | p_{s+1} \rangle = \cos^2(\theta/2) - \sin^2(\theta/2) = \cos(\theta),$$

where $\varepsilon_{\text{MF}}$ depends explicitly on $p_{s+1}$, the SQP obtained after applying the $R_x(\theta)$ rotation in QC-DFT. This result can be extended to $N$ qubits, by applying rotations $R_x^{(j)}(\theta_j)$ to each qubit $j$ to obtain the $N$-qubit mean-field state $|p_{s+1}\rangle = |p_{s+1}^{(1)}, p_{s+1}^{(2)}, \ldots, p_{s+1}^{(N)}\rangle$, with

$$|p_{s+1}^{(j)}\rangle = \cos(\theta_j/2) |0\rangle_j \pm \sin(\theta_j/2) |1\rangle_j$$

as above. For our Hamiltonian $H = \bigotimes_{j=1}^{N} \sigma_z^{(j)}$, the $N$-qubit mean-field energy $E_{\text{MF}}$ factors into a product of single-qubit mean-field energies, and depends explicitly on the SQPs, $p_{s+1}$, obtained after applying the $x$-axis rotation gates in QC-DFT:

$$E_{\text{MF}}(\theta, p_{s+1}) = \langle p_{s+1} | H | p_{s+1} \rangle = \prod_{j=1}^{N} \varepsilon_{\text{MF}}^{(j)} = \prod_{j=1}^{N} \cos(\theta_j).$$

This mean-field energy is identical to the exact result in equation (11), and it can be obtained in QC-DFT directly from the SQPs, without preparing the trial wave function. Figure 4 shows the energy $E(\theta_1, \theta_2)$ for the two-qubit case computed with QC-DFT on a fine grid of rotation angles $\theta_1$ and $\theta_2$. In this case, since $E(\theta_1, \theta_2) = \cos(\theta_1) \cos(\theta_2)$, the minima are found for $(\theta_1, \theta_2) = (\pi, 0)$ and $(0, \pi)$ (see Fig. 4). For the general case with $N$ qubits, the energy $E(\theta)$ can be computed in QC-DFT using only $O(N)$ memory and computational resources, by applying the $x$-axis rotation gates within the LPA. Conversely, the same calculation has $O(e^N)$ memory and computational cost in state-vector simulations. Although the example examined here has a simple analytic solution, it illustrates the point that QC-DFT can enable exponential speed-ups over state-vector simulations for calculations of ground-state energies.
Figure 4. Energy calculation with QC-DFT. Energy $E(\theta_1, \theta_2)$, color-coded in arbitrary units, for the two-qubit Hamiltonian $H = \sigma_z^{(1)} \sigma_z^{(2)}$ and the trial wave function $\Psi(\theta_1, \theta_2) = R_{x_1}^{(1)}(\theta_1) R_{x_2}^{(2)}(\theta_2) |00\rangle$. The energy is computed with QC-DFT on a fine grid of angles $(\theta_1, \theta_2)$ using equation (14) together with the LPA gate functional for the rotations $R_{x_i}$.

Our formulation of a DFT analog for QC simulations opens several research directions. First, one may use machine learning to improve the QC-DFT gate functionals, as shown recently for exchange-correlation functionals in DFT\textsuperscript{32,33}. The ground truth is readily available from exact calculations on small QCs, and thus in QC-DFT it is straightforward to obtain a training set for supervised learning. Second, extending the QC-DFT formalism to one-qubit density matrices may enable an improved description of gates such as S, T, and Pauli Z, which act on the qubit phase and are currently ignored in our SQP-based approach. Similarly, using two-qubit density matrices may allow capturing qubit correlations beyond the LPA. Third, applying QC-DFT to spin Hamiltonians and quantum algorithms, a point we examined only briefly, is a promising direction that will be explored in future work.

In summary, we demonstrated a density functional theory for quantum circuits, QC-DFT, able to obtain marginals of the full QC probability distribution, the SQPs, with high accuracy and low computational cost. This quantum-circuit analog of DFT is efficient — it can be applied to large systems with up to billions qubits, and orders of magnitude more if the algorithm is parallelized. Our approach paves the way for efficient QC simulations.
inspired by the many-electron problem, laying out an intriguing connection between condensed matter physics and quantum information.

METHODS

Exact QC simulations. The exact QC simulations are carried out using the QuEST code\(^3\). All single- and two-qubit gates are used as provided in the code. We use appropriate rotation operations to implement the square root Pauli gates, and compute the exact SQPs from the state vector. Example input files for QuEST are available in the data sets accompanying this manuscript.

Multi-gate functionals. The MGA-\(n\) functionals are implemented in our QC-DFT code by looking for specific gate sequences in the QC. If a gate sequence encoded in the functional is found within cycle \(s_{\text{max}}\), the SQPs are updated using \(p_{s+1}\) from equation (9). These multi-gate corrections are applied only up to once for each qubit. For the Clifford+T QCs, the MGA-3 functional used in Fig. 2a corrects for the gate sequences H-H (using \(p_{s+1} = 0\)) and H-T-H (\(p_{s+1} = 0.146447\)) up to cycle \(s_{\text{max}} = 7\), including cases where CNOT gates act on the qubit within these sequences. This means that CNOT control and target operations are ignored when looking for these gate sequences – for example, the gate sequence H−CNOT−H acting on a qubit is treated as H−H and corrected. For the QCs in Fig. 2b, the MGA-2 functional corrects for the \(\sqrt{X}−\sqrt{X}\) and \(\sqrt{Y}−\sqrt{Y}\) sequences up to cycle \(s_{\text{max}} = 7\). In this case, the CZ control operations are ignored when looking for gate sequences, while CZ target operations are taken into account. For example, if the gate sequence \(\sqrt{X}−\text{CZ}−\sqrt{X}\) involves the CZ control qubit, it is treated as \(\sqrt{X}−\sqrt{X}\) and the multi-gate correction is applied. If the same sequence is found for the CZ target qubit, the multi-gate correction is not applied.

The MGA-6 functional includes several multi-gate corrections with up to 6-gate sequences, applied up to cycle \(s_{\text{max}}\) between 6 and 10 depending on the sequence. Some sequences take into account CZ gates, while others ignore them. Next we provide the full list of gate-sequences for our MGA-6 functional, using a naming convention for gate sequences where, for a given qubit, the rightmost gate acts at the current step, and the leftmost gate
acts at the earliest step in the sequence; steps where no gates act on the qubit are ignored. This means that sequences are given in the same order as when reading the QC from left to right, ignoring steps with no gates. The CZ gates are explicitly taken into account, in the same way for control and target qubits, unless otherwise stated. With these conventions, the gate sequences treated in our MGA-6 functional are as follows: 2-gate sequences $\sqrt{X} - \sqrt{X}$ and $\sqrt{Y} - \sqrt{Y}$ (both with $p_{s+1} = 1$ and $s_{\text{max}} = 6$); 3-gate sequences $\sqrt{X} - \text{CNOT} - \sqrt{X}$ and $\sqrt{Y} - \text{CNOT} - \sqrt{Y}$ ($p_{s+1} = 1$, $s_{\text{max}} = 6$), $\sqrt{Y} - T - \sqrt{X}$ ($p_{s+1} = 0.14645$, $s_{\text{max}} = 8$, CZ gates ignored) and $\sqrt{Y} - T - \sqrt{Y}$, $\sqrt{X} - T - \sqrt{X}$, and $\sqrt{X} - T - \sqrt{Y}$ ($p_{s+1} = 0.85355$, $s_{\text{max}} = 8$, CZ gates ignored); 4-gate sequences $T - \sqrt{Y} - T - \sqrt{X}$ and $T - \sqrt{X} - T - \sqrt{Y}$ ($p_{s+1} = 0.75$, $s_{\text{max}} = 10$, CZ gates ignored); 5-gate sequences $\text{CNOT} - \sqrt{X} - \text{CNOT} - \sqrt{X}$, $\text{CNOT} - \sqrt{X} - \text{CNOT} - \sqrt{Y}$, $\sqrt{Y} - \text{CNOT} - \sqrt{X} - \sqrt{X}$, and $\sqrt{Y} - \text{CNOT} - \sqrt{Y} - \text{CNOT} - \sqrt{X}$ ($p_{s+1} = 0.5$, $s_{\text{max}} = 10$); 6-gate sequences $\sqrt{Y} - \text{CNOT} - \sqrt{X} - \text{CNOT} - \sqrt{X}$ ($p_{s+1} = 0.14645$, $s_{\text{max}} = 10$), $\sqrt{X} - \text{CNOT} - \sqrt{Y} - \text{CNOT} - \sqrt{Y}$ and $\sqrt{X} - \text{CNOT} - \sqrt{Y} - \text{CNOT} - \sqrt{Y}$ ($p_{s+1} = 0.85355$, $s_{\text{max}} = 10$). These sequences can be found in the MGA-$n$ QC-DFT codes provided in the data sets accompanying this manuscript.

Nonrandom QCs. The nonrandom QCs used for the scaling calculations in Fig. 3 are generated using deterministic rules. For a QC with size $N$ qubits, step 1 consists of alternating $H$ and Pauli $X$ gates; in step 2, a CNOT gate connects each qubit $i < N/2$ (control) to qubit $i + N/2$ (target); step 3 consists of alternating Pauli $Y$ and $Z$ gates; step 4 has CNOT gates every 4 qubits, each with neighboring control and target qubits; step 5 applies $H$ gates every 10 qubits. Only QCs with size $N$ multiple of 4 and 10 have the same structure, and thus give the same SQP distribution as shown above. Codes for generating these QCs and reproducing the calculations in Fig. 3 are provided in the data sets accompanying this manuscript.
DATA AVAILABILITY

The data sets generated and analyzed in this study, as well as the QC-DFT codes, will be made available in the CaltechDATA repository. Additional data and information are available upon reasonable request.

CODE AVAILABILITY

The QuEST code\(^3\) used for the exact QC simulations is an open source software, which can be downloaded at https://quest.qtechtheory.org. The QC drawings were prepared using the Quantikz LaTeX package\(^3\)\(^4\), which can be downloaded at https://ctan.org/pkg/quantikz. The QC-DFT PYTHON code will be made available in the CaltechDATA repository.

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AUTHOR CONTRIBUTIONS

M.B. conceived and designed the research, performed the calculations and analysis, and wrote the manuscript.

COMPETING INTERESTS

The authors declare no competing interests.

ADDITIONAL INFORMATION

Supplementary information The online version contains supplementary information available at [insert URL].

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Extended Data Table 1. LPA functional applied to the Bell-state preparation QC. Exact wave function $\Psi_s$, and the corresponding SQP vector $p_s$, given as a function of step $s$ for the Bell-state preparation two-qubit QC$^{27}$. This QC consists of H applied to qubit 0 (step 1) followed by CNOT with control qubit 0 and target qubit 1 (step 2). As the reader can verify, the LPA rules in equations (5)–(7) give the same SQPs as the exact ones shown in the table, at all steps and for all possible initial states.

| Initial state $\Psi_{s=0}$ | $p_{s=0}$ | $\Psi_{s=1}$ | $p_{s=1}$ | $\Psi_{s=2}$ | $p_{s=2}$ |
|-----------------------------|----------|--------------|----------|--------------|----------|
| $|00\rangle$                | (0,0)    | $\frac{1}{\sqrt{2}} (|00\rangle + |10\rangle)$ | (0.5, 0) | $\frac{1}{\sqrt{2}} (|00\rangle + |11\rangle)$ | (0.5, 0.5) |
| $|01\rangle$                | (0,1)    | $\frac{1}{\sqrt{2}} (|01\rangle + |11\rangle)$ | (0.5, 1) | $\frac{1}{\sqrt{2}} (|01\rangle + |10\rangle)$ | (0.5, 0.5) |
| $|10\rangle$                | (1,0)    | $\frac{1}{\sqrt{2}} (|00\rangle - |10\rangle)$ | (0.5, 0) | $\frac{1}{\sqrt{2}} (|00\rangle - |11\rangle)$ | (0.5, 0.5) |
| $|11\rangle$                | (1,1)    | $\frac{1}{\sqrt{2}} (|01\rangle - |11\rangle)$ | (0.5, 1) | $\frac{1}{\sqrt{2}} (|01\rangle - |10\rangle)$ | (0.5, 0.5) |
Extended Data Figure 1. Additional QC-DFT simulations of Clifford+T random QCs using LPA gate functionals. Random QC using a universal Clifford+T gate set. This type of QC alternates one step where single-qubit gates chosen at random within the set are applied to all qubits, and one step where CNOT gates with randomly chosen control-target pairs are applied to all qubits. This two-step sequence is shaded in gray (top). The accuracy of the simulated SQPs at each step is shown for this type of random QCs, with a depth of 20 steps, for different numbers of qubits (bottom). Each SQP accuracy curve is obtained by averaging results from 20 distinct random QC instances.
Extended Data Figure 2. Additional results for optimized MGA gate functionals. Accuracy comparison for the LPA and MGA-3 functionals applied to the Clifford+T QCs in Extended Data Fig. 1. The main improvements for the MGA-3 over the LPA functional occur between steps 1 and 7, where the multi-gate corrections are applied. These results, shown for QCs with a size of 20 qubits, are obtained by averaging over the same number of QCs as in Extended Data Fig. 1.