Quantum information [1] replaces bits with two-level quantum-mechanical systems (qubits) \( \mathcal{H} = \mathbb{C}|0\oplus|1\). The state space of \( n \) qubits is \( \mathcal{H}^\otimes n \); pure states are superpositions of bit-strings \( |\psi\rangle = \sum b_1 b_2 \cdots b_n |b_1 b_2 \cdots b_n\rangle \). Traditionally, a quantum computation consists of a closed-system (unitary) evolution \( |\psi\rangle \rightarrow |u|\psi\rangle \), followed by a measurement to obtain classical information. Although no more than \( n \) bits of classical information can be extracted from an \( n \)-qubit system, quantum computers can nevertheless outperform their classical counterparts when solving certain discrete problems [2, 3]. Famously, a successful large-scale implementation of Shor’s integer factorization [4] could compromise contemporary cryptography algorithms.

Quantum circuits [5] provide a simple framework for discussing quantum computation. A quantum circuit describes a computation as a discrete sequence of unitary evolutions (gates), which often involve only a small subset of the available qubits. Indeed, as multi-qubit couplings can be difficult to control, quantum algorithms are generally given as a sequence of two-qubit operations. To allow error correction, the set of permissible two-qubit gates is restricted to a particularly simple type of coupling called controlled-not (CNOT). Fortunately, circuits containing only CNOT gates and one-qubit unitaries can be constructed, given the target evolution [6, 7].

Quantum logic synthesis seeks algorithms for creating small quantum circuits. Published results typically rely on matrix factorizations [8] and Lie group decompositions [9, 10]. A universal circuit whose parameters may be tuned to implement any \( n \)-qubit unitary requires at least \( (4^n - 3n - 1)/4 \) CNOTs [11]. When \( n = 2 \), this lower bound of three is matched by explicit constructions [11–13]. For generic \( n \)-qubit operators, there is a lower bound of 14 CNOTs and a special-purpose construction requiring 40 CNOTs [14]. Most notably, a recent Letter [15] asymptotically matches the lower bound with an algorithm that produces a sharp asymptotic in \( n \)-qubits, requiring \( 8.7 \times 4^n \) CNOTs versus older constructions requiring roughly \( 50 \times n^2 \times 4^n \) [7]. A recent manuscript [16] lowers the count to \( 4^n - 2^n+1 \). Yet all current \( n \)-qubit techniques [7, 8, 15–17] remain a factor of four away from the lower bound. Moreover, all \( n \)-qubit techniques perform poorly on small operators, e.g. producing circuits with at least eight CNOT gates in the case of two qubits.

In this Letter, we derive a new universal quantum circuit, containing \( (1/2) \times 4^n - 3 \times 2^{n+1} + 1 \) CNOTs for an arbitrary \( n \)-qubit operator. This represents an improvement by a factor of two over the best known results for both the 3-qubit and \( n \)-qubit case, and is a factor of two away from the lower bound [11] of \( (4^n - 3n - 1)/4 \). Efficient quantum circuits are useful for quantum state preparation [18, 19]; ours carry \( |0\rangle \rightarrow |u|\psi\rangle \) using \( 2^{n+1} - 2n - 2 \) CNOT gates.

We provide a brief outline of the circuit synthesis argument before treating details. We introduce the quantum multiplexor \( a \oplus b \), which enacts the \( n - 1 \) qubit unitary evolution \( a \) or \( b \) on the least significant qubits as the top line carries \( |0\rangle \) or \( |1\rangle \). This allows the Cosine-Sine Decomposition (CSD) of numerical matrix analysis to be restated as follows: any \( n \)-qubit operator can be decomposed into two quantum multiplexors and a so-called uniformly controlled rotation. As uniformly controlled rotations are known to admit small circuits, we implement the quantum multiplexor with one uniformly controlled rotation and two \((n - 1)\)-qubit unitary operators and induct.

Traditionally, the CSD [21, 22] is used to find [27] the following decomposition of an even-dimensional unitary matrix \( u \) into smaller unitaries \( a, a', b, b' \) and real diagonal matrices \( c, s \) such that \( s^2 + c^2 = 1 \).

\[
\begin{pmatrix}
  a & b \\
  b & a \\
\end{pmatrix}
\begin{pmatrix}
  c & -s \\
  s & c \\
\end{pmatrix}
\begin{pmatrix}
  a' & 0 \\
  0 & b' \\
\end{pmatrix}
\]

We note that the central piece is just \( \exp(i\sigma_z \arccos c) \). On the other hand, the side factors \( (a \oplus b) \) and \((a' \oplus b')\) are quantum multiplexors. We assert that there exist unitary \( v, w \) and unitary diagonal \( d \) satisfying

\[
\begin{pmatrix}
  a & b \\
  b & a \\
\end{pmatrix}
\begin{pmatrix}
  v & 0 \\
  0 & v \\
\end{pmatrix}
\begin{pmatrix}
  d & 0 \\
  0 & d \\
\end{pmatrix}
\begin{pmatrix}
  w & 0 \\
  0 & w \\
\end{pmatrix}
\]

To find them, define \( d \) and \( v \) by diagonalizing \( ab^\dagger = vd^2v^\dagger \). Then \( w = dv^\dagger b \). As \( d \oplus d^\dagger \) is \( e^{i\sigma_z \arccos d} \), we obtain the following matrix decomposition.

**NQ Decomposition:** For any \( 2k \times 2k \) unitary matrix, \( u \), there exist \( k \times k \) unitaries \( v_1, v_2, v_3, v_4 \), and \( k \times k \) Hermitian diagonals \( \delta_1, \delta_2, \delta_3 \), such that

\[
u = (I_2 \otimes v_1)e^{i\sigma_z \otimes \delta_1}(I_2 \otimes v_2)e^{i\sigma_z \otimes \delta_2}(I_2 \otimes v_3)e^{i\sigma_z \otimes \delta_3}(I_2 \otimes v_4)\]
This is closely related to the Khaneja Glaser decomposition (KGD) [9, 25]. We note that the three terms \(\exp(i\sigma \otimes \delta)\) are just uniformly controlled rotations [16], as they apply the rotation \(i\sigma \otimes \delta\) to \(\sigma\)'s qubit if \(\delta\)'s qubits — the controls — are in the state \(|j\rangle\). If \(\delta\) acts on \(k\) qubits, then \(\exp(i\sigma \otimes \delta)\) can be implemented with \(2k\) CNOTs, as may be seen from Fig. 1. Earlier accounts [16, 20] provide a different algorithm for implementing \(\sigma\)'s wire and square controls on \(d\)'s wires, as these gates apply a different \(\sigma\)-rotation to the target line for each value of the control bits. To derive the above decomposition, write \(\delta = \delta_1 \otimes I_2 + \delta_2 \otimes \sigma_z\). Recalling the well-known two-qubit circuit identity \(C_1^2 (\sigma_\sigma \otimes \sigma_z) C_2^2 = I_2 \otimes I_2\), we can rewrite \(\sigma \otimes \delta = \sigma \otimes \delta_1 \otimes I_2 + \delta_1 (\sigma_\sigma \otimes \sigma_z) C_1^2\). Exponentiating, we obtain a circuit like that depicted in the center of the above figure. Finally, we note that some CNOT gates can be cancelled when applying this decomposition recursively.

As illustrated in Figure 2, we now have a recursive algorithm for implementing \(n\)-qubit operators. Let \(c_j\) be the number of CNOT gates needed to implement a \(j\)-qubit operator. Then \(c_j \leq 4c_{j-1} + 3 \times 2^{j-1}\). In particular, if there is some method of implementing \(\ell\)-qubit operators using no more than \(c_\ell\) CNOT gates, then we obtain the following inequality for \(c_n\).

\[
c_n \leq 4n - (c_2 + 3 \times 2^{n-1}) - 3 \times 2^{n-1}
\]

If we apply the decomposition until only one-qubit operators remain, then \(c_n \leq (3/4) \times 4^n - 3 \times 2^{n-1}\) CNOT gates. This is already an improvement over the best previously published algorithm [16]. If we instead terminate the recursion with two-qubit operators, we can use the 3-CNOT circuit decompositions of two-qubit operators [11–13] to obtain a total CNOT-count of \((9/16) \times 4^n - 3 \times 2^{n-1}\).

To obtain our advertised CNOT count of \((4^n - 3 \times 2^{n-2} + 2)/2\), one final optimization is necessary. Having halted the recursion, we note that \(4^{n-2}\) two-qubit operators remain to be implemented. The two-qubit operators are all on the same lines, but are separated by the controls of uniformly controlled rotations. As diagonal operators can pass through controls, we note that for any two-qubit operator \(\psi\), there is a diagonal two-qubit operator \(d\) so that \(vd\) and \(dv\) may be implemented using two CNOTs ([23], Prop. III.3.) Thus we may ensure that the final two-qubit operator in the circuit can be implemented using two CNOT gates by extracting the requisite diagonal and absorbing it into the previous two-qubit operator. We now repeat the process, this time with the second-to-last and third-to-last operators, and continue on towards the beginning of the circuit. In this manner, we save one CNOT in the implementation of every two-qubit gate but the first, obtaining the count above. The count for \(n = 3\) is worth noting separately. For this small number of qubits, the 21 CNOT circuit is the best known at present (cf. [14]).

We describe a simple but efficient technique for state preparation — that is, to transform \(|0\rangle\) into a given \(n\)-qubit state \(|\phi\rangle\). Consider first the case of real states — that is, suppose that \(|\phi\rangle \in \mathbb{R}\) for computational basis vectors \(|j\rangle\). Partition the vector representing \(|\phi\rangle\) into 2-element blocks, and consider each as a vector in \(\mathbb{R}^2\). Let the \(j\)-th have length \(\lambda_j\) and form an angle of \(\theta_j\) with the \(x\)-axis. Taking \(|\phi\rangle = \sum \lambda_j |j\rangle\) and \(\delta = \sum \theta_j |j\rangle \langle j|\), we see that \(\exp(i\delta \otimes \sigma_z) |\phi\rangle |0\rangle = |\phi\rangle\). The recursive technique suggested by this equation yields a circuit with \(2^n - 2\) CNOTs. To adjust the relative phase between components of \(\phi\), we apply a diagonal operator, \(d\). These can be decomposed into circuits by a technique very similar to that just described. Following [20], we partition the matrix of \(d\) into \(2 \times 2\) blocks along the diagonal. Define \(\lambda_j\) to be the average phase in the \(j\)-th block, and \(\theta_j\) to be the relative phase between its entries. Taking \(d' = \exp(i \sum \alpha_j |j\rangle \langle j|)\) and \(\delta = \sum \theta_j |j\rangle \langle j|\), we see that \(d = (d' \otimes I) \exp(i \delta \otimes \sigma_z)\). Again, we recursively obtain a CNOT-count of \(2^n - 2\). Finally, we note that combining these circuits allows some cancelations lowering the total count to \(2^{n+1} - 2n - 2\). This is a factor of four from the current lower bound [24].

Most of the CNOT gates used in our decomposition act on nearest neighbors. Clearly this is the case for the CNOT gates generated to implement the two-qubit operators that appear in the terminal case of the recursion. Moreover, in Fig. 1 it can be observed that only \(2^{n-k}\) CNOT gates of length \(k\) (where the length of a local CNOT is 1) will appear in the circuit implementing a uniformly controlled rotation with \(n\) control bits. We show in Fig. 3 how to decompose a length \(k\) CNOT into \(4k - 4\) length 1 CNOTs. It follows that \(9 \times 2^{n-1} - 8\)
nearest-neighbor CNOTs suffice to implement the uniformly controlled rotation \( \exp(i \sigma \otimes \delta) \), where \( \delta \) is an \((n - 1)\)-qubit diagonal Hermitian operator. Therefore requiring that only nearest-neighbor CNOT gates appear in the circuit decomposition introduces only a factor of nine into the leading term of our CNOT count.

Our approach to quantum circuit synthesis emphasizes simplicity; a well-pronounced top-down structure, and practical computation via the CSD. The universal circuit reported in this work achieves the best known controlled-not counts, both in practice and asymptotically. Although the CNOT count of 21 achieved by this circuit in three qubits is currently best practice (cf. [14]), any new specialty techniques for constructing universal three- and four-qubit circuits may be incorporated easily to improve the \( n \)-qubit universal circuit. The NQ algorithm for instantiating the universal circuit relies on standard matrix decompositions and a novel decomposition of quantum multiplexors. As a result, the circuit has only half as many controlled-not’s as there are real degrees of freedom in the unitary operator input. Due to a theoretical lower bound [11], this count cannot be improved by more than a factor of two. Additionally, we demonstrate an asymptotically optimal controlled-not count on the one-dimensional (spin chain) architecture where all CNOT gates necessarily act on nearest-neighbor qubits. When mapping the new universal circuit into this setting, the number of CNOTs increases by less than one order of magnitude. This result suggests that appropriate quantum circuit synthesis allows to dramatically decrease communication between qubits in array-based architectures without requiring asymptotically heavier computation. In the special case of Shor’s algorithm, additional corroborating evidence can be found in [26].

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Matlab’s GSVD function performs the CSD. The source code can be found by typing which gsvd at the Matlab prompt.