UniversalQCompiler

Raban Iten, 1,† Oliver Reardon-Smith, 2 Luca Mondada, 1
Ethan Redmond, 1 Ravjot Singh Kohli, 2 and Roger Colbeck 2,†
1 Institute for Theoretical Physics, ETH Zürich, 8093 Zürich, Switzerland
2 Department of Mathematics, University of York, YO10 5DD, UK
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We introduce an open source software package UniversalQCompiler written in Mathematica that allows the decomposition of arbitrary quantum operations into a sequence of single-qubit rotations (with arbitrary rotation angles) and controlled-NOT (C-NOT) gates. Together with the existing package QI, this allows quantum information protocols to be analysed and then compiled to quantum circuits. Our decompositions are based on Phys. Rev. A 93, 032318 (2016), and hence, for generic operations, they are near optimal in terms of the number of gates required. UniversalQCompiler allows the compilation of any isometry (in particular, it can be used for unitaries and state preparation), quantum channel or positive-operator valued measure (POVM), although the run time becomes prohibitive for large numbers of qubits. The resulting circuits can be displayed graphically within Mathematica or exported to \LaTeX. We also provide functionality to translate the circuits to OpenQASM, the quantum assembly language used, for instance, by the IBM Q Experience.

I. INTRODUCTION

A universal quantum computer should be able to perform arbitrary computations on a quantum system. It is common to break down a given computation into a sequence of elementary gates, each of which can be implemented with low cost on an experimental architecture. However, given an abstract representation of the desired computation, such as a unitary matrix, it is in general difficult and time consuming to find a low-cost circuit implementing it. Here, we introduce an open source Mathematica package, [UniversalQCompiler], that allows for automation of the compiling process on a small number of qubits. The package requires an existing Mathematica package QI, which can easily handle common computations in quantum information theory, such as partial traces over various qubits or the Schmidt decomposition. Since the code is provided for Mathematica, our packages are well adapted for analytic calculations and can be used alongside the library of mathematical tools provided by Mathematica. Together, these constitute a powerful set of tools for analysing protocols in quantum information theory and then compiling the computations into circuits that can finally be run on an experimental architecture, such as IBM Q Experience (see Figure 1 for an overview). UniversalQCompiler focuses on the compilation process, and performs a few basic simplifications on the resulting quantum circuit. Hence, one might want to put the gate sequences obtained from UniversalQCompiler into either a source-to-source compiler or a transpiler (see for example [1,3]) in order to optimize the gate count of the circuits further or to map them to a different hardware, which may have restrictions on the qubit-connectivity [4–8].

The package UniversalQCompiler provides code for all the decompositions described in [9], which are near optimal in the required number of gates for generic computations in the quantum circuit model (in fact, the achieved C-NOT counts differ by a constant factor of about two from a theoretical lower bound given in [9]). Note that our decompositions may not lead to optimal gate counts for computations of a special form lying in a set of measure zero (see [9] for the details), as for example for a unitary that corresponds to the circuit performed for Shor’s algorithm [10]. Hence, to optimize the gate counts when decomposing operations of certain special forms, such as diagonal gates, multi-controlled single-qubit gates and uniformly-controlled gates, we provide separate commands. In addition, we provide methods for analyzing, simplifying and manipulating gate sequences. Outputs are given in a bespoke gate list format, and can be exported as graphics, or to \LaTeX using the format of Q-circuit [11].

UniversalQCompiler is intended to be an academic software library that focuses on simplicity and adaptability of the code and it was not our focus to optimize the (classical) run time of the decomposition methods (the theoretical decompositions mainly focused on minimizing the C-NOT count). A detailed documentation as well as an example notebook are published together with our code and should help the user to get started quickly. The aim of this paper is to give an overview over the package UniversalQCompiler and to provide some theoretical background about the decomposition methods that it uses. A separate manual is provided with the package that provides more details.

We work with the universal gate library consisting of arbitrary single-qubit rotations and C-NOT gates (we also explain how to convert gate sequences from this univer-

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* Electronic address: itenr@ethz.ch
† Electronic address: roger.colbeck@york.ac.uk
1 See our webpage for a reference to the github repository and the documentation: http://www-users.york.ac.uk/~rc973/UniversalQCompiler.html
2 https://github.com/rogercolbeck/QI
FIG. 1: Overview over the use of UniversalQCompiler. The Mathematica package QI can be used to do common computations in quantum information and manipulate quantum operations, such as unitary matrices. Given an abstract representation of a quantum computation, UniversalQCompiler takes it as an input and outputs a quantum circuit implementing the computation. Thereby, we distinguish the following classes of operations: isometries (including unitaries and state preparation as special cases), quantum channels and POVMs. The picture depicts example-circuits for each class of operations on two qubits. The circuit could then be further optimized and prepared for a specific quantum hardware architecture by an (external) transpiler. To simplify interfacing with a transpiler or a circuit optimizer (for instance the PyZX quantum circuit optimizer \[3\]), we provide a python script (based on ProjectQ \[12, 13\]) to translate the Mathematica outputs to the quantum assembly language OpenQASM.

In Section II, we define the elementary gates we are working with, i.e., the single-qubit rotations and the C-NOT gate.

In Section III we describe how to use UniversalQCompiler to decompose arbitrary isometries from \(m\) to \(n \geq m\) qubits describing the most general evolution that a closed quantum system can undergo. Mathematically, an isometry from \(m\) to \(n\) qubits is an inner-product preserving transformation that maps from a Hilbert space of dimension \(2^m\) to one of dimension \(2^n\). Physically, such an isometry can be thought of as the introduction of \(n - m\) ancilla qubits in a fixed state (conventionally \(|0\rangle\)) followed by a general \(n\)-qubit unitary on the \(m\) input qubits and ancilla qubits. Unitaries and state preparation on \(n\) qubits are two important special cases of isometries from \(m\) to \(n\) qubits, where \(m = n\) and \(m = 0\), respectively.

In Section IV we consider the decomposition of quantum channels from \(m\) to \(n\) qubits (no longer restricting to \(m \leq n\)). A quantum channel describes the most general evolution an open quantum system (i.e., a quantum system that may interact with its environment) can undergo. Mathematically, a quantum channel is a completely positive trace-preserving map from the space of density operators on \(m\) qubits to the space of density operators on \(n\) qubits. UniversalQCompiler takes a mathematical description of such a quantum channel (which can be supplied in Kraus representation or as a Choi state) and returns a gate sequence that implements the channel (in general after tracing out some qubits at the end of the circuit). The decomposition is nearly optimal for generic channels working in the quantum circuit model \[9\]. However, working in more general models would allow further reductions in the number of gates \[14\]. We plan to implement code for the decompositions described in \[14\] in the future. For an overview of possible applications of implementing channels, see \[15\].

In Section V we describe how to implement arbitrary POVMs on \(m\) qubits describing the most general measurements that can be performed on a quantum system. Similarly to the case of channels, working in generalized models can reduce the gate count further \[14\], and we plan to implement these in a future version. See also \[16\] for an application of UniversalQCompiler for synthesis of POVMs.

In Section VI we describe some simple rules that can be used to simplify circuits and that are implemented within UniversalQCompiler.

Finally, in Section VII we explain how to automatically translate our circuits to the open quantum assembly language (OpenQASM) \[17\], which allows our package to interface with other quantum software packages.

II. UNIVERSAL GATE LIBRARY

Our gate library consists of arbitrary single-qubit rotations and C-NOT gates. This set of gates is known to
be universal [18], i.e., any quantum computation can be decomposed into a sequence of gates in this set. We use the following convention for rotation gates

\[
R_x(\theta) = \begin{pmatrix} \cos(\theta/2) & i \sin(\theta/2) \\ i \sin(\theta/2) & \cos(\theta/2) \end{pmatrix},
\]

(1)

\[
R_y(\theta) = \begin{pmatrix} \cos(\theta/2) & -i \sin(\theta/2) \\ i \sin(\theta/2) & \cos(\theta/2) \end{pmatrix},
\]

(2)

\[
R_z(\theta) = \begin{pmatrix} e^{i\theta/2} & 0 \\ 0 & e^{-i\theta/2} \end{pmatrix}.
\]

(3)

Note that in [19], we used the convention \(R_x'(\theta) = R_x(-\theta)\), \(R_y'(\theta) = R_y(-\theta)\) and \(R_z'(\theta) = R_z(-\theta)\). In addition, we use the following two-qubit gate

\[
\text{C-NOT} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}.
\]

(4)

In Appendix [A] we explain how to convert gate sequences from this universal set to the one that comprises single-qubit rotations and Mølmer-Sørensen gates without increasing the number of two-qubit gates.

Note that, when displaying circuits, we use \[\begin{array}{c}
\end{array}\] to represent measurement in the computational basis where the classical outcome is retained, and \[\begin{array}{c}
\end{array}\] to represent the qubit being traced out (equivalent to measuring and forgetting the outcome).

### III. COMPILEON OF ISOMETRIES

UniversalQCompiler provides three different decompositions for generic isometries from \(m\) to \(n\) qubits given as a \(2^n \times 2^m\) complex matrix \(V\) satisfying \(V^\dagger V = \mathbb{I}\) (and an additional decomposition that only works for \(m = 0\), i.e., for state preparation). For an overview of the gate counts and the running time complexity of the different methods, see Table I. For a comparison with a theoretical lower bound on the number of C-NOT gates, see Table I in [9]. In the following, first we give some information about the different decomposition schemes. Then we explain the methods DecIsometry and DecIsometryGeneric, which choose the optimal decomposition scheme automatically. An example of an output circuit created by DecIsometry is given in Figure 2.

#### A. Column-by-column decomposition

The column-by-column decomposition (method: ColumnByColumnDec) was introduced in [9] and achieves near optimal C-NOT counts for generic isometries from \(m\) to \(n\) qubits. As the name suggests, the isometry is decomposed in a column-wise fashion (see [9] for the details). This decomposition achieves the lowest known C-NOT counts for generic isometries with \(1 \leq m \leq n - 2\). For isometries of a special form, it may also achieve lower C-NOT counts for \(m = 0, n - 1, n\) (after running the simplifications described in Section VI and removing gates that implement the identity during the decomposition). In particular, it usually performs well for isometries with many zeros, since the number of gates to decompose the columns is reduced in such cases.

The column-by-column decomposition requires \(2^{m+n}\) C-NOTs to leading order for the decomposition of an isometry from \(m\) to \(n\) qubits. Its classical time complexity is \(O(n2^{2m+n})\) (see Appendix [B]), which scales significantly better in \(m\) than the other decomposition methods for isometries. Note also that it is straightforward to parallelize parts of the column-by-column decomposition, which may help to lower the run time significantly for practical implementations (but we have not done so in the version 0.1 of our package).

#### B. Quantum Shannon Decomposition (QSD)

The Quantum Shannon Decomposition (method: QSD) was introduced for unitaries in [21] and adapted to isometries in [9]. It achieves lower C-NOT counts than the column-by-column decomposition for generic isometries from \(m\) to \(n\) qubits with \(m = n - 1\) or \(m = n\),

| Method | C-NOT count for a generic \(m\) to \(n\) isometry | Classical run time | References |
|--------|-----------------------------------------------|-------------------|------------|
| CCD\(^a\) | \(2^{m+n} - \frac{1}{2} 2^n + \mathcal{O}(n^2) 2^m\) | \(\mathcal{O}(n2^{2m+n})\) | [9] |
| QSD\(^b\) | \(\frac{23}{14} (4^n + 2 \cdot 4^n) + \mathcal{O}(m)\) | \(\mathcal{O}(2^n)\) | [21],[9] |
| Knill | \(\frac{23}{14} (2^{m+n} + 2^n) + \mathcal{O}(n^2) 2^m\) if \(n\) is even | \(\mathcal{O}(2^n)\) | [22],[9] |
| | \(\frac{115}{96} (2^{m+n} + 2^n) + \mathcal{O}(n^2) 2^m\) if \(n\) is odd | \(\mathcal{O}(2^n)\) | [22],[9] |
| SP\(^c\) | \(\frac{23}{14} 2^n\) [here \(m = 0\)] | \(\mathcal{O}(2^{3n})\) | [23],[9] |

### TABLE I: Overview of the asymptotic number of C-NOT gates and the classical run time required to decompose \(m\) to \(n\) isometries using different decomposition schemes. Abbreviations used: \(^a\)Column-by-column decomposition of an isometry; \(^b\)Decomposition of an isometry using the Quantum Shannon Decomposition; \(^c\)State preparation.
FIG. 2: Circuit for a randomly chosen isometry from one to three qubits. The two ancilla qubits are always initialized in the state $|0\rangle$, where an arbitrary state $|\psi\rangle$ is provided as an input on the least significant qubit. The output of the computation is read out from all three qubits at the end of the circuit. The circuit was produced by running $st\leftarrow\text{DecIsometry}[\text{PickRandomIsometry}[2,8]]$ in Mathematica and then calling \texttt{LaTeXQ Circuit}[st] to export the circuit to \texttt{ETEX}. To save space we do not depict the angles here, but these are found by our code and can be output if desired.

whereas the QSD is not well adapted to the case $m \ll n$. Its classical time complexity is independent of $m$ and given by $O(2^{3n})$ (see Appendix B.2).

C. Knill’s decomposition

Knill’s decomposition scheme (method: \texttt{KnillDec}) described in [9] and based on [23, 24] expands an isometry $V$ to a unitary $U$ maximizing the number of eigenvalues of $U$ that are equal to one. The unitary $U$ can then be decomposed into a circuit (described in [9, 22]) that requires $c\cdot(k+1)^2 + kO(n^2)$ C-NOT gates for a unitary on $n$ qubits with $k$ eigenvalues that are not equal to one, where $c = 23/24$ if $n$ is even and $c = 115/96$ if $n$ is odd. For a generic isometry $V$ from $m$ to $n$ qubits, the unitary extension, $U$, can be chosen to have $2^m$ eigenvalues that are not equal to one and hence requires $c\cdot(2^{n+m} + 2^n) + 2mO(n^2)$ C-NOT gates to leading order. However, for isometries of a special form for which the unitary extensions has fewer than $2^m$ eigenvalues that are not equal to one, Knill’s decomposition may achieve lower C-NOT counts than the others (for an example, see the notebook “Examples.nb” that is provided together with the package). The classical time complexity of the decomposition is independent of $m$ to leading order and given by $O(2^{3n})$ (see Appendix B.3).

D. State preparation

For the special case of state preparation on $n$ qubits (i.e., for an isometry from 0 to $n$ qubits), the best known decomposition scheme is based on the Schmidt decomposition of the quantum state [23] (method: \texttt{StatePreparation}). The scheme was slightly improved for state preparation for an odd number of qubits in [9] leading to a C-NOT count of $23/24\cdot2^n$ for state preparation on $n$ qubits. This is lower than the number of C-NOTs required to decompose an $n$-qubit state with uniformly controlled gates [24], which is $2^n$ to leading order\(^3\). However, the classical time complexity is $O(2^{7n/8})$ (see Appendix B.4 for the details), which is worse than the complexity $O(n2^n)$ for state preparation using uniformly controlled gates.

Remark (States with low Schmidt rank). The Schmidt rank of a bipartite quantum state $\psi_{AB}$ is given by the minimal number of Schmidt coefficients required for its Schmidt decomposition. States with a small Schmidt rank correspond to weakly entangled quantum systems, and occur naturally in the study of the grounds states of certain types of Hamiltonian (see, e.g., [23]). In the future, we plan to adapt the decomposition for state preparation introduced in [23] to states with low Schmidt ranks (where the splitting of the sub-systems has to be specified). We expect this adaptation to lower the C-NOT count significantly for such states. Moreover, in the related task of approximate state preparation, one could lower the gate count by setting small Schmidt coefficients equal to zero.

E. Choosing the optimal decomposition

The method \texttt{DecIsometry}[V] decomposes the isometry V into a sequence of single-qubit rotations and C-NOT gates by running all three decompositions (and in the case $m = 0$ also the one for state preparation), simplifying the gate sequences using the methods described in Section VI, and choosing the output gate sequence that achieves the lowest C-NOT count. To decompose a random isometry V (of high dimensions), we suggest to use \texttt{DecIsometryGeneric}[V], which chooses the decomposition method that achieves the lowest C-NOT count for a generic isometry with the same dimensions as V and hence has a shorter running time compared to \texttt{DecIsometry}[V] (since it runs only one decomposition).

\(^3\) By default, the decomposition based on uniformly controlled gates [24] is used for the decomposition of the first column in the method \texttt{ColumnByColumnDec}. The option \texttt{FirstColumn \to \texttt{StatePreparation}} allows use of the scheme based on the Schmidt decomposition [23] for its decomposition.
As sub-routines, we use optimal decompositions of two-qubit gates [19] (method: DecUnitary2Qubits) and optimal state preparation on three qubits [20] (method: StatePrep3Qubits).

IV. COMPILATION OF QUANTUM CHANNELS

In the following, we consider the implementation of quantum channels in the quantum circuit model (method: DecChannelInQCM). For the decomposition of channels, it is most convenient to work with the Kraus representation of the channel. Every quantum channel $\mathcal{E}$ from $m$ to $n$ qubits with Kraus rank $K$ can be represented by Kraus operators $A_i$, which are complex matrices of dimension $2^m \times 2^n$ such that $\sum_{i=1}^{K} A_i A_i^\dagger = I$ and $\mathcal{E}(\rho) = \sum_{i=1}^{K} A_i \rho A_i^\dagger$ for all density operators $\rho$ of dimension $2^m$. To change the Kraus representation to a Choi state [20] or vice versa, we provide the methods KrausToChoi and ChoiToKraus, respectively.

An arbitrary channel from $m$ to $n$ qubits (given as a list of Kraus operators) can be provided as an input to DecChannelInQCM, which returns a gate sequence (with some trace-out operations at the end) that implements the channel (see Figure 3 for an example). The decomposition uses Stinespring’s theorem [27] stating that a channel of Kraus rank $K = 2^k$ can be represented by an isometry from $m$ to $n+k$ qubits. Then, the channel can be implemented by using one of the decomposition schemes for isometries and tracing out the ancillas at the end of the circuit. The C-NOT count for a channel from $m$ to $n$ qubits of Kraus rank $2^k$ is therefore $2^{m+n+k}$ to leading order. This is nearly optimal for the decomposition of generic channels in the quantum circuit model [9].

Note also that all channels from $m$ to $n$ qubits have a Kraus representation with at most $2^{m+n}$ elements. The command MinimizeKrausRank is provided to do the reduction to the minimal number of Kraus operators (which may be lower than $2^{m+n}$ for channels of a special form).

V. COMPILATION OF POVMs

Positive-operator valued measures (POVMs) describe the most general measurements that can be performed on quantum systems. In the following, we consider the implementation of POVMs on $m$ qubits in the quantum circuit model (method: DecPOVMInQCM). Every POVM $\mathcal{M}$ on $m$ qubits with $L$ possible measurement outcomes can be represented by $L$ operators $0 \leq E_i \leq 1$ satisfying $\sum_{i=1}^{L} E_i = I$. The probability of getting the $i$th outcome when performing the POVM on an $m$ qubit state $\rho$ is then given by $\text{tr}[E_i \rho]$.

To demonstrate the use of DecPOVMInQCM, we consider state discrimination (see for example [28] for a review). Suppose a state is chosen from a known set of (not necessarily pure) density operators $\{\phi_i\}_i$, where $\phi_i$ is chosen with probability $p_i$. The goal is to correctly guess which state was chosen, by performing a measurement on the given state. In general, the optimal strategy for such a task is to perform a (non-projective) POVM. Since it is (in general) difficult to find the optimal POVM, a “pretty good” choice was introduced in [29, 30]. Using DecPOVMInQCM we can find a quantum circuit to implement these POVM elements. Running this circuit on some quantum hardware would then give us a (classical) output that corresponds to a pretty good guess of which state was given to us. As a concrete example, we take $\phi_1 = |0\rangle\langle 0|$, $\phi_2 = |1\rangle\langle 1|$ and $\phi_3 = |+\rangle\langle +|$, where $|+\rangle := 1/\sqrt{2}(|0\rangle + |1\rangle)$, assuming that each state is chosen with the same probability $p_i = 1/3$. The pretty good measurement has POVM elements $M_i = p_i \phi_i^{-1/2} \phi_i \phi_i^{-1/2}$, where $\phi = \sum_i p_i \phi_i$. Using DecPOVMInQCM gives a quantum circuit with two ancilla qubits (see Figure 4). The outcomes can be interpreted as follows: $(x, y) = (0, 0)$ corresponds to a guess that the chosen state was $\phi_1$, $(x, y) = (0, 1)$ corresponds to a guess of $\phi_2$ and $(x, y) = (1, 0)$ corresponds to a guess of $\phi_3$. Note that $(x, y) = (1, 1)$ has probability zero.

VI. SIMPLIFICATIONS OF GATE SEQUENCES

Given a sequence of single-qubit rotations and C-NOT gates, it may be possible to find a shorter gate sequence...
that implements the same operation. We provide the method `SimplifyGateList`, which uses some simple rules to reduce the gate count. The number of single-qubit gates is reduced by merging single-qubit rotations in cases where more than two occur consecutively on the same qubit. The merged single-qubit unitary can then be decomposed using the following well-known Lemma [31].

**Lemma 1 (ZYZ decomposition)** For every unitary operation $U$ acting on a single qubit, there exist real numbers $\alpha, \beta, \gamma$ and $\delta$ such that

$$U = e^{i\alpha} R_z(\beta) R_y(\gamma) R_z(\delta). \quad (5)$$

By symmetry, Lemma 1 holds for any two orthogonal rotation axes. We decompose the merged unitary using the ZYZ decomposition if the previous C-NOT gate controls on the considered qubit, and we decompose it using the XYX decomposition otherwise. Since the $R_z$ gates commute with the control of C-NOT gates and $R_x$ gates with the target, one of the rotation gates can be commuted to the left of the C-NOT, as summarized in the following circuit equivalence.

We do this procedure starting from the end of the circuit and we also cancel C-NOT gates where we have two in a row (or with commuting C-NOT gates in-between) with the same control and target. The resulting circuit contains at most four single-qubit rotations after each C-NOT gate. Note that to do the simplifications we have to traverse only once through the circuit, hence the classical run time of this procedure is linear in the number of gates of the circuit.

For example, the following circuit (for arbitrary rotation angles)

gets simplified to the following (by only traversing the circuit once).

![Circuit Diagram](image)

FIG. 4: Circuit for a POVM on one qubit implementing the pretty good measurement for distinguishing the states $\phi_1 = |0\rangle|0\rangle$, $\phi_2 = |1\rangle|1\rangle$ and $\phi_3 = \pm |+\rangle\langle+| \ (\text{the rotation angles are not depicted for simplicity}). The POVM elements are given by $M_1 = 1/4 \cdot \{\{1, 1\}, \{1, 1\}\}$, $M_2 = 1/8 \cdot \{(3 + 2\sqrt{2}, -1), \{-1, 3 - 2\sqrt{2}\}\}$ and $M_3 = 1/8 \cdot \{(3 - 2\sqrt{2}, -1), \{-1, 3 + 2\sqrt{2}\}\}$. The probability to measure $|i\rangle$ (with $i \in \{1, 2, 3\}$) on the two ancilla qubits for a given state $\rho$ on the third qubit is given by $\text{tr} M_i \rho$. The circuit was produced by running $\text{st}=$DecPOVMInQCM$\{M_1, M_2, M_3\}$ in Mathematica and then $\text{LaTeXQCircuit}[st]$ to export the circuit to TeX. Again, the rotation angles are not depicted for simplicity.

**VIII. FUTURE WORK**

In a future version we plan to implement code for the decompositions of quantum channels and POVMs in more general models than the quantum circuit model that allow for measurements in between the gate sequence and to classical control on the measurement results [14]. This will significantly reduce the C-NOT count for channels and POVMs. We also plan to introduce functionality to decompose more general measurements where the post-measurement state is important.

Currently, we do not provide code for the transformation from the gate library consisting of C-NOT and single-qubit gates to the one consisting of XX and single-qubit gates. If one would like to run a circuit on trapped ions, the transpiler should perform the conversion.

A remaining open question is how to use these decompositions as a starting point for circuit optimization. As a straightforward application, one could do peephole optimization, by taking a large circuit and extracting parts of it that act on, e.g., three qubits, and resynthesize the unitary corresponding to the circuit. If this leads...
to a shorter circuit, this could then replace the original. Alternatively, one could build up sets of increasingly complicated templates \( \mathbb{I} \), i.e., circuits that implement the identity operator, using our universal decomposition schemes. Indeed, choosing a (parametrized) circuit, writing it as a unitary and synthesizing a new circuit for it, directly leads to a (parametrized) template. These templates could then be used to simplify parts of larger circuits.

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Appendix A: Transforming our gate library to one that is well adapted for trapped ions

The common universal gate set used for trapped ions consists of single-qubit gates \( R(\theta, \phi) \) and the Mølmer-Sørensen gate \( \text{XX}(\phi) \) (see for example \([32]\)) defined as follows.

\[
R(\theta, \phi) = \begin{bmatrix} \cos(\theta/2) & -i \exp(-i\phi) \sin(\theta/2) \\ -i \exp(i\phi) \sin(\theta/2) & \cos(\theta/2) \end{bmatrix}, \quad \text{XX}(\phi) = \begin{bmatrix} \cos(\phi) & 0 & 0 & -i \sin(\phi) \\ 0 & \cos(\phi) & -i \sin(\phi) & 0 \\ 0 & -i \sin(\phi) & \cos(\phi) & 0 \\ -i \sin(\phi) & 0 & 0 & \cos(\phi) \end{bmatrix}.
\]

In particular, we have \( R_x(\theta) = R(-\theta, 0) \) and \( R_y(\theta) = R(-\theta, \pi/2) \). Having a circuit consisting of C-NOT gates, one can use the following identity to replace each C-NOT gates with a single XX gate and single qubit gates \([35]\). Note that this transformation does not increase the two-qubit gate count.

\[
\begin{array}{c}
R_y(-\pi/2) \\
\text{XX}(-\pi/2) \\
R_x(\pi/2) \\
R_y(\pi/2)
\end{array} = 
\begin{array}{c}
R_x(\pi/2) \\
\text{XX}(\pi/2) \\
R_y(-\pi/2) \\
R_x(-\pi/2)
\end{array}
\]

In the following, we show how to merge the single-qubit gates in a circuit containing XX and single-qubit rotations, such that the resulting circuit contains at most one \( R(\theta, \phi) \) gate after each XX gate, and additionally a possible \( R_x \) gate on each of the qubits at the beginning of the circuit. To do so, we use that the XX gate commutes with the \( R_x \) gate (on both qubits) \([35]\) together with the following decomposition.

\[\text{Lemma 2 (R-R_x decomposition)}\] Given a \( 2 \times 2 \) unitary matrix, \( U \), there exist reals \( \alpha, \theta, \phi, \) and \( \delta \) such that

\[U = e^{i\alpha} R(\theta, \phi) R_x(\delta).\] (A1)

\[\text{Proof.}\] From (the generalized) Lemma \([1]\) it follows that there exist reals \( \alpha, \beta, \gamma, \delta \), such that

\[U = e^{i\alpha} R_x(\beta) R_y(\gamma) R_x(\delta).\] (A2)

The circuit equivalence (12) in \([35]\) implies that there exists reals \( \theta, \phi \) such that \( R(\theta, \phi) R_x(\beta) R_y(\gamma) R_x(\delta) = \mathbb{I} \), or, equivalently, \( R_x(\beta) R_y(\gamma) = R(\theta, \phi) R_x(-\beta) \). It follows that

\[U = e^{i\alpha} R_x(\beta) R_y(\gamma) R_x(\delta) = e^{i\alpha} R(\theta, \phi) R_x(-\beta) R_x(\delta) = e^{i\alpha} R(\theta, \phi) R_x(\delta),\] (A3)

where \( \delta := \tilde{\delta} - \beta \).

This leads to the circuit equivalence

\[\text{XX}(\phi) U = R_x \]

which we can apply recursively starting at the end of the circuit as follows. We first merge all the single-qubit rotations into single-qubit unitaries before applying the above circuit equivalence at the last XX gate appearing in the circuit and merge the \( R_x \) gates into the proceeding single-qubit unitary. We then apply the circuit equivalence to the second to last XX gate in the circuit, and so on. The single-qubit unitaries that remain at the end can be written in terms of \( R \)-gates.

Appendix B: Classical time complexity for the decomposition of isometries

In this section we give some details about how to find the classical time complexity for the different decomposition schemes for isometries. Note that these complexities refer to numerical cases (not analytic calculations).

1. Classical complexity for the column-by-column decomposition

To leading order, we only have to consider the decomposition and simulation (i.e., the application to quantum states) of the uniformly controlled gates. The decomposition scheme for a uniformly controlled single-qubit gate with \( k \) controls introduced in \([24]\) has time complexity \( \mathcal{O}(k2^{k}) \), and computing the updated state after its application to an \( n \)-qubit state has time complexity \( \mathcal{O}(2^{n}) \) (one has to update all the entries of the state vector in general). Hence, to update all \( 2^{\alpha} \) columns of an isometry
from $m$ to $n$ qubits has time complexity $\mathcal{O}(2^{m+n})$.\footnote{Decomposing the $t^{th}$ column with the column-by-column decomposition, the columns $1, \ldots, t-1$ are in the states $e^{i\phi_{0}} |0\rangle, \ldots, e^{i\phi_{t-2}} |t-2\rangle$ for some real phases $\phi_{0}, \ldots, \phi_{t-2}$, and hence the application of uniformly controlled gates on these columns has constant time complexity. We ignore this here, since it does not change the overall time complexity of the column-by-column decomposition.} Note that it is straightforward to parallelize the application of a uniformly controlled gate to the different columns of an isometry (and also the application to a single-column), which can speed up practical implementations significantly (but we do not take this into account here for the complexity measure). The complexity of decomposing one column is

$$\sum_{k=0}^{n-1} \mathcal{O}(k2^k + 2^{m+n}) = \mathcal{O}(n2^{m+n})$$

Hence, the complexity to decompose all of the $2^m$ columns is $\mathcal{O}(n2^{2m+n})$.

2. Classical complexity for the Quantum Shannon Decomposition

The Quantum Shannon Decomposition of an isometry from $m$ to $n$ qubits is based on the Cosine-Sine-Decomposition of an unitary expansion of the isometry $[9, 21]$. Since the unitary expansion is a matrix of dimension $2^n \times 2^n$, the time complexity to perform the Cosine-Sine-Decomposition of it is $\mathcal{O}(2^{3n})$ [34].

3. Classical Complexity for Knill’s decomposition

Knill’s decomposition of an isometry from $m$ to $n$ qubits requires running several subroutines from linear algebra to find the unitary $U$ from Lemma [5] and its eigenvalue decomposition, which is required for the decomposition (see [9, 22] and Appendix C for the details). The most time consuming operations are:

- Finding an orthonormal basis of the null space of $V^\dagger - I_{2^n \times 2^n}$ of dimension $2^m \times 2^n$ in the proof of Lemma [5]
- Multiplying the matrices $W$ and $W''$ of dimension $(2^n - 2^m) \times (2^n - 2^m)$ in the proof of Lemma [4]
- Finding the eigenvalues and eigenvectors of a $2^n \times 2^n$ unitary matrix with eigenvalues that differ from 1.

All of these operations can be implemented with time complexity $\mathcal{O}(2^{3n})$.

The time complexity of the remaining part of Knill’s decomposition is dominated by the decomposition of the state preparation operations, which are denoted by $V_t$ in Lemma [3]. By Appendix B 4 state preparation (using the decomposition scheme introduced in [23]) has time complexity $\mathcal{O}(2^{3n/2})$. For Knill’s decomposition, we have to perform this decomposition $2m+1$ times, and hence the “decomposition-phase” of Knill’s scheme has time complexity $\mathcal{O}(2^{m+n+3n/2})$.

We conclude that the whole decomposition has time complexity $\mathcal{O}(2^{3n} + 2^{m+3n/2}) = \mathcal{O}(2^{3n})$ (since $m \leq n$).

4. Classical complexity for state preparation

The method introduce in [23] requires calculating the Schmidt decomposition of the given state on $n$ qubits as well as decomposing two unitaries on each half of the qubits. To calculate the Schmidt decomposition, one performs the singular value decomposition on a matrix of dimension $2^{n/2} \times 2^{n/2}$, which has complexity $\mathcal{O}(2^{3n/2})$ [34]. Decomposing the unitaries can also be done with complexity $\mathcal{O}(2^{n/2})$ (see Appendix B 2). We conclude that state preparation as done in [23] has classical time complexity $\mathcal{O}(2^{3n/2})$.

Appendix C: Theoretical details required for the implementation of Knill’s decomposition

In this appendix, we give some details about Knill’s decomposition introduced in [22] that are required for its implementation. To help keep track of dimensions, throughout this section we will use $\{|i\rangle_D\}_{i=0}^{D-1}$ to denote an orthonormal basis for $\mathbb{C}^D$ for any $D \in \mathbb{N}$.

Lemma 3 Let $U$ be an $N \times N$ unitary matrix with eigendecomposition $U = \mathbb{I} + \sum_{i=0}^{t-1} |v_i\rangle\langle v_i|$, with $\{|v_i\rangle\}$ orthonormal, $e^{i\theta_i} \neq 1$ and $t \geq 1$ (i.e., $U$ has $t$ eigenvalues that differ from 1). Then $U = \prod_{i=1}^{N} V_i P_i V_i^\dagger$, where $V_i$ is any unitary that takes $|0\rangle$ to $|v_i\rangle$ and $P_i = \mathbb{I} + (e^{i\theta_i} - 1)|0\rangle\langle 0|$.

Proof. Write $V_t = |v_t\rangle|0\rangle + R_t$, where $R_t = \sum_{j=1}^{t-1} |r_j\rangle\langle j|$ so that $R_t |0\rangle = 0$. In order that $V_t$ is unitary, we require $R_t R_t^\dagger = \mathbb{I} - |v_t\rangle\langle v_t|$. Then,

$$V_t P_t V_t^\dagger = (|v_t\rangle\langle 0| + R_t)(\mathbb{I} + (e^{i\theta_t} - 1)|0\rangle\langle 0|)(|0\rangle\langle v_t| + R_t^\dagger) = e^{i\theta_t}|v_t\rangle\langle v_t| + R_t R_t^\dagger = \mathbb{I} + (e^{i\theta_t} - 1)|v_t\rangle\langle v_t|.$$ 

The product is hence $U$. \hfill \blacksquare

We now show (along the lines of [22]) that any $N \times M$ isometry can be extended to a unitary with at most $M$ eigenvalues that differ from 1.

Lemma 4 Let $X$ and $Y$ be $N \times M$ matrices such that $X^\dagger X = Y^\dagger Y$. Then there exists an $N \times N$ unitary $U$ such that $UX = Y$.
Proof. Let $M \leq N$, and $Y = WSV$ be the SVD of $Y$, with $\Sigma = \sum_{i=1}^{N} \sigma_{i} |i\rangle_N \langle i|_M$ where $\{\sigma_{i}\}$ are non-negative real numbers. Note that $W$ is $N \times N$, $V$ is $M \times M$ and $\Sigma$ is $N \times M$.

We have $Y^{\dagger}Y = V^{\dagger} \Sigma \Sigma^{\dagger} V$. Thus $V^{\dagger}XV^{\dagger} = \Sigma^{\dagger} \Sigma$ for some (non-normalized) vectors $\{v_{i}\}_{i=1}^{M}$, $v_{i} \in \mathbb{C}^{N}$. Then $V^{\dagger}XV^{\dagger} = \sum_{i,j} (v_{i}|v_{j})_{M} |i\rangle_{M} \langle j|_{M}$, hence $(v_{i}|v_{j})_{M} = \sigma_{i} \delta_{ij}$. We hence define the $N \times N$ matrix $W = \sum_{i,j \neq q} \sigma_{i}^{q} |i\rangle_{N} \langle j|_{N}$, so that $W^{\dagger}XV^{\dagger} = \Sigma$. Note that $W^{\dagger}W^{\dagger} = \sum_{i,j \neq q} \sigma_{i}^{q} |i\rangle_{N} \langle i|_{N}$. and that $W^{\dagger}$ can be extended to a unitary $W^{\dagger}$ without affecting its action on $XV^{\dagger}$. Then, if we take $W = WW^{\dagger}$, we have $UX = WW^{\dagger}X = WSVV^{\dagger} = Y$. The case $M > N$ can be treated similarly.

Lemma 5 Let $N$ and $M \leq N$ be positive integers and $V$ be an $N \times M$ matrix satisfying $V^{\dagger}V = \mathbb{I}_{M}$, i.e., $V$ is an isometry. There exists an $N \times N$ unitary matrix $U$ such that $U|\langle N\rangle_{N} = V|\langle M\rangle_{M}$ for $i = \{0, \ldots, M-1\}$, and which has at least $N-M$ eigenvalues equal to 1.

Proof. First note that $V$ can be written in terms of its columns $|v_{i}\rangle \in \mathbb{C}^{N}$ via $V = \sum_{i=0}^{M-1} |v_{i}\rangle_{M}$, $v_{i} \in \mathbb{C}^{N}$ numbered from $i = M$ to $N-1$. Since $\{\{v_{i}\}\}_{i=0}^{N-1}$ is an orthonormal basis for $\mathbb{C}^{N}$, the matrix $\sum_{i=0}^{N-1} |v_{i}\rangle_{N} \langle v_{i}|_{N} =: \hat{U}$ is then a unitary satisfying $\hat{U}|\langle N\rangle_{N} = V|\langle M\rangle_{M}$ for $i = \{0, \ldots, M-1\}$. We need to show that it is always possible to choose the set $\{\{v_{i}\}\}_{i=0}^{N-1}$ such that $U$ has at least $N-M$ eigenvalues equal to 1. Note that this is equivalent to $U^{\dagger}$ having at least $N-M$ eigenvalues equal to 1.

Let us write $U^{\dagger} = \begin{pmatrix} W^{\dagger} \\ W \end{pmatrix}$, where $W$ is $(N-M) \times N$ so that for any $N \times K$ matrix $X$ for some positive integer $K$, $U^{\dagger}X = \begin{pmatrix} W^{\dagger}X \\ WX \end{pmatrix}$. Note that, by unitarity, $V^{\dagger} + W^{\dagger}W = \mathbb{I}_{N}$.

$V^{\dagger}-I_{M,N}$ has dimension $M \times N$ and hence its nullspace dimension is at least $N-M$ (here $I_{M,N}$ denotes the $M \times N$ matrix $I_{M,N} = \sum_{i=0}^{M-1} |i\rangle_{M} \langle i|_{N}$). Let us take $|f_{i}\rangle \in \mathbb{C}^{N}$ to be an orthonormal basis for this nullspace for $i \in \{0, \ldots, q-1\}$ so that $V^{\dagger}|f_{i}\rangle = |f_{i}\rangle$ for $i \in \{0, \ldots, q-1\}$.

Consider now the $N \times (N-M)$ matrix $X = \sum_{i=0}^{q-1} |f_{i}\rangle\langle f_{i}|_{N-M}$, and divide it into $X_{1}$ and $X_{2}$, where $X_{1}$ comprises the first $M$ rows, and $X_{2}$ the remaining $N-M$ rows (e.g., $X_{1} = \sum_{i=0}^{M-1} |i\rangle_{N} \langle x_{i}|$). By construction, $V^{\dagger}X = I_{M,N}X = X_{1}$ and hence $X_{1}^{\dagger}X_{1} = X^{\dagger}V^{\dagger}VX$. Furthermore, $X_{2}^{\dagger}X_{2} = X_{1}^{\dagger}X_{1} = X_{2}^{\dagger}X_{2} = X_{2}^{\dagger}X_{2}$. Since there is unitary freedom in $W$, it follows from Lemma 3 that it can be chosen such that $WX = X_{2}$. With this choice, $U^{\dagger}X = X$, and hence the $N-M$ columns of $X$ are eigenvectors of $U^{\dagger}$ with eigenvalue 1.

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