Criteria for exact qudit universality

Gavin K. Brennen, ^{1,*} Dianne P. O'Leary, ^{2,3,†} and Stephen S. Bullock ^{3,‡} ¹National Institute of Standards and Technology, Atomic Physics Division, Gaithersburg, Maryland 20899-8420, USA ²University of Maryland, Department of Computer Science, Collge Park, Maryland 20742, USA ³National Institute of Standards and Technology, Mathematical and Computational Sciences Division, Gaithersburg, Maryland 20899-8910, USA (Received 1 September 2004; revised manuscript received 21 December 2004; published 16 May 2005)

We describe criteria for implementation of quantum computation in qudits. A qudit is a d-dimensional system whose Hilbert space is spanned by states $|0\rangle, |1\rangle, ..., |d-1\rangle$. An important earlier work [A. Muthukrishnan and C.R. Stroud, Jr., Phys. Rev. A **62**, 052309 (2000)] describes how to exactly simulate an arbitrary unitary on multiple qudits using a 2d-1 parameter family of single qudit and two qudit gates. That technique is based on the spectral decomposition of unitaries. Here we generalize this argument to show that exact universality follows given a discrete set of single qudit Hamiltonians and one two-qudit Hamiltonian. The technique is related to the QR-matrix decomposition of numerical linear algebra. We consider a generic physical system in which the single qudit Hamiltonians are a small collection of $H^x_{jk} = \hbar \Omega(|k\rangle\langle j| + |j\rangle\langle k|)$ and $H^y_{jk} = \hbar \Omega(i|k\rangle\langle j| - i|j\rangle\langle k|)$. A coupling graph results taking nodes 0, ..., d-1 and edges $j \leftrightarrow k$ iff H^x_{jk} are allowed Hamiltonians. One qudit exact universality follows iff this graph is connected, and complete universality results if the two-qudit Hamiltonian $H = \hbar \Omega |d-1,d-1\rangle\langle d-1,d-1|$ is also allowed. We discuss implementation in the eight dimensional ground electronic states of 87 Rb and construct an optimal gate sequence using Raman laser pulses.

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I. INTRODUCTION

An important theoretic construct used in the field of quantum information is the qubit. Its utility follows from the simple but significant recognition that all two-dimensional subspaces, regardless of the underlying physical system, can be regarded as informationally equivalent. This has made it possible to discuss quantum computation in terms of single qubit and two qubit gates without the need to analyze the specific interactions that realize operations within a physical system or between subsystems. An important issue in this regard is that a necessary condition for efficient quantum computation is the existence of an underlying tensor product structure on the Hilbert space \mathcal{H} . If all computation were performed on a single $d=\dim(\mathcal{H})$ level system then some physical resource such as space or energy would grow with the dimension of the system [1]. In contrast, the analogous resources grow poly-logarithmically with the dimension when the system is composed of many subsystems. By this argument, a computation performed on qubits (d=2) is in some sense the most compact foliation of Hilbert space.

Nevertheless, there are compelling reasons to consider computation on qudits with d>2. First, most candidate systems for a quantum computer encode the qubit in a subspace of a larger accessible Hilbert space. Examples of systems with multiple states that can be coherently controlled include charge-position states in quantum dots [2], rotational and vibrational states of a molecule [3], harmonic oscillator states

*Electronic address: gavin.brennen@nist.gov

[4], and ground electronic states of alkali atoms [5]. Using higher dimensional subspaces already endowed in these systems may be more efficient in terms of the number of interacting gates needed during a computation. This is critical for error control because interactions between qudits tend to open channels for interactions with the decohering environment. By contrast, in many physical systems, single qudit control is a well-developed technology that can be done with high precision. Second, there is some evidence that the error thresholds for fault tolerant computation improve when the encoding is done with qudits where d > 2 and prime [6].

Previous work has established conditions for simulating unitaries on many qudits. Vlasov [7] shows that any unitary $U \in U(d^n)$ can be simulated with arbitrary precision using two specific noncommuting single qudit Hamiltonians complemented by a two qudit interaction Hamiltonian. Brylinski and Brylinski [8] prove the necessary and sufficient criteria for exact qudit universality. Exact universality means that any unitary and, by unitary extension to a larger Hilbert space, any quantum process, can be simulated with zero error. The result is that arbitrary single qudit gates complemented by one entangling two qudit gate is needed. Neither of these methods is constructive. Muthukrishnan and Stroud [9] give a constructive procedure for an exact simulation of an arbitrary unitary on n qudits using single qudit and two qudit gates. Their approach uses the spectral decomposition of unitaries and involves a gate library consisting of a family of continuous parameter gates.

Here we describe an approach that uses the QR decompositions on unitaries to achieve exact universal computation on qudits. The analysis is done at the Hamiltonian level, i.e., we describe a minimal set of Hamiltonians needed to perform computation on qudits. Our primary motivation is to

[†]Electronic address: oleary@cs.umd.edu

[‡]Electronic address: stephen.bullock@nist.gov

find a construction which requires a small number of control resources and the fewest number of control pulses. By small we mean that using a sequence of control pulses with k free parameters each, the number of control pulses times k should be close to the number of parameters in the unitary group U(d), namely, d^2 . Our construction has the advantage that the single qudit gates are generated by a fixed set of Hamiltonians that couple pairs of states in the single qudit logical basis. The gates perform rotations, parametrized by two angles, about orthogonal axes within the associated twodimensional subspace. For the example of two states coupled by a electromagnetic field, the two angles correspond to the pulse area and the mixing angle of the in phase and in quadrature components of the driving field. Additionally, our decomposition requires only a single one parameter twoqudit gate: the controlled-phase gate. This gate is generated by a two-qudit Hamiltonian H_{int} that generates a phase on a single product state of two qudits. Such interactions can be engineered in many atom optical systems.

In this paper, the general results are developed with close contact to the example of computation in the d=8 qudit encoded in the ground hyperfine states of ⁸⁷Rb. In Sec. II we describe the construction of single qudit unitaries using the QR decomposition. We introduce a coupling graph to describe how states are connected to each other by physical Hamiltonians. The set of rotation planes may be incomplete, i.e., each state may not be connected to every other state. However, provided the graph is connected, an efficient decomposition can be found. Multiqudit computation is addressed in Sec. III. Using a construction of a singlycontrolled Householder gate demonstrated in the Appendix, we show that $O(d^4)$ elementary single- and two-qudit gates from our library suffice to generate arbitrary two qudit unitaries. This construction completes the requirements for exact universality. We conclude with a summary of the results in Sec. IV.

II. ONE-QUDIT UNITARIES

We show how to construct an arbitrary single qudit unitary with exact precision. The idea relies on applying control fields that couple only two basis states at a time. Using the fields to generate an arbitrary unitary on a two-dimensional subspace of the qudit, one can then use a sequence of such operations on different pairs of states to construct a unitary on the entire *d*-dimensional space. We show that this can be done efficiently, meaning in as few gates as possible, provided there exists a pathway between any two states via pairwise couplings.

Recall that any determinant one unitary operator on a two-dimensional Hilbert space can be described by a Bloch sphere rotation. In the subspace \mathcal{H}_{jk} spanned by the orthonormal basis $\{|j\rangle,|k\rangle\}$ such a rotation is written $U_{jk}(\gamma,\theta,\phi)=e^{-i\vec{\gamma}\cdot\hat{\lambda}_{jk}}$, where the vector $\vec{\gamma}=\gamma(\sin(\theta)\times\cos(\phi),\sin(\theta)\sin(\phi),\cos(\theta))$ is parametrized by its length $|\vec{\gamma}|=\gamma$ and its polar coordinates (θ,ϕ) on the Bloch sphere. The chosen basis for the subalgebra is both unitary and Hermitian and its components along the axes of the Bloch sphere

 $\operatorname{are} \{\lambda_{jk}^{z} = |j\rangle\langle j| - |k\rangle\langle k|, \lambda_{jk}^{y} = -i|j\rangle\langle k| + i|k\rangle\langle j|, \lambda_{jk}^{x} = |j\rangle\langle k| + |k\rangle\langle j|\}.$

Any such unitary can be generated by only two members of the subalgebra. This follows by the Euler decomposition of SU(2) into a product of three rotations about two orthogonal axes on the Bloch sphere. In this paper we focus on the set of Hamiltonians

$$H_{ik}^{x} = \hbar \Omega \lambda_{ik}^{x}, \quad H_{ik}^{y} = \hbar \Omega \lambda_{ik}^{y}. \tag{1}$$

For convenience of notation, we assume the strength of each coupling is equal to Ω and allow the time duration t that each Hamiltonian is left on to be a free parameter. In some cases, the two Hamiltonians in Eq. (1) can be turned on simultaneously. By adjusting the relative strengths of the couplings, one can then realize any rotation about an axis on the equator of the Bloch sphere $(\theta = \pi/2)$. For brevity, we write such rotations as $U_{jk}(\gamma, \phi) = e^{-i[\cos(\phi)H^x_{jk}-\sin(\phi)H^y_{jk}]\gamma/(\hbar\Omega)}$, where it is understood that if the couplings H^x_{jk} , H^x_{jk} cannot be turned on together then $U_{j,k}(\gamma, \phi)$ requires three elementary gates. The matrix form of the unitary $U_{j,k}(\gamma, \phi)$ in the logical basis is

$$U_{j,k}(\gamma,\phi) = \begin{pmatrix} I_j & & & & \\ & I_j & & & \\ & & \cos(\gamma) & & -ie^{i\phi}\sin(\gamma) & \\ & & I_{k-j-1} & & \\ & & -ie^{-i\phi}\sin(\gamma) & & \cos(\gamma) & \\ & & & I_{d-k-1} \end{pmatrix},$$
(2)

where I_r denotes the r-dimensional identity operator and we assumed j < k. In linear algebra applications these operations are named "Givens rotations." They define a coordinate axis rotation in the plane spanned by the vectors $\{|j\rangle, |k\rangle\}$ and are a tool used to zero elements of a matrix.

Realization of an arbitrary unitary evolution $V \in U(d^n)$ follows in two steps. The first corresponds to a QR decomposition $\lceil 10,11 \rceil$ of the matrix U.

Using the allowed set of Hamiltonians, we may realize matrices of Givens rotations physically. Generically, the QR decomposition writes an invertible G=UT, where $U=G_1G_2\cdots G_l$ is a product of Givens rotations and hence unitary and T is upper triangular. Note that if G=V is unitary, then so likewise is $T=U^{\dagger}G$, whence T is in this case a diagonal matrix which applies relative phases to computational basis states.

Using techniques for realizing diagonal computations [12], a sequence of Hamiltonians realizing T is constructed.

We illustrate the idea using a Givens rotation in the QR reduction of a unitary $V \in U(d)$ as above. We may choose U a Givens rotation so as to zero the matrix element $[UV]_{d-1,0}$ (where the indices run $0,1,\ldots,d-1$). An appropriate choice is $U_{d-2,d-1}(\gamma,\phi)$ where the angles γ , ϕ are chosen to satisfy

tan
$$\gamma = |[V]_{d-1,0}/[V]_{d-2,0}|,$$

$$\phi = \pi/2 + \arg([V]_{d-2,0}) - \arg([V]_{d-1,0}). \tag{3}$$

Then letting $[V]'_{**}$ denote a changed entry, we obtain

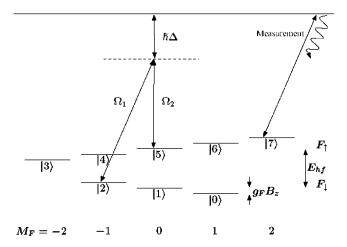


FIG. 1. A single d=8 qudit encoded in the ground-state hyperfine levels of ^{87}Rb . A pair of lasers can couple states in different hyperfine manifolds according to the selection rule $\Delta M_F=0,\pm 1$. Projective measurements of population in state $|7\rangle$ are made by observing resonant fluorescence on a cycling transition to the excited state. Any pair of states can be coupled by swapping neighbors together pairwise and similarly any state can be measured by swapping to $|7\rangle$.

$$U_{d-2,d-1}V = \begin{pmatrix} [V]_{0,0} & [V]_{0,1} & \cdots & [V]_{0,d-1} \\ \vdots & \ddots & & \vdots \\ [V]'_{d-2,0} & [V]'_{d-2,1} & \cdots & [V]'_{d-2,d-1} \\ 0 & [V]'_{d-1,1} & \cdots & [V]'_{d-1,d-1} \end{pmatrix}. \tag{4}$$

In the next step, one chooses a unitary $U_{d-3,d-1}$ to zero the matrix element $[U_{d-2,d-1}V]_{d-2,0}$. Continuing in this way, the product $\prod_{i=2}^{d} U_{d-i,d-1}$ zeros all the elements below the upper left diagonal entry. By unitarity, this sequence also zeros all but the diagonal element in the top row. Iterating the sequence over all columns to zero elements below the diagonal then brings the unitary V to diagonal form. The maximum number of Givens rotations needed is d(d-1)/2. The residual diagonal unitary T has d parameters. As each Givens rotation has two parameters the total number of free parameters in the algorithm is $\dim[U(d)]=d^2$. We note that the above choice of Givens rotations assumes that one can physically couple any two logical basis states. In fact this particular sequence is not necessary. One can achieve a QR reduction using d(d-1)/2 Givens rotations with a restricted set of couplings. This is proven in Sec. II C.

A. Example: One-qudit Unitaries in 87Rb

Generically, control over a quantum system involves a tradeoff in the number of resources used and the complexity of the control algorithm. In the language of single qudit computation, the goal is to realize an arbitrary unitary on the qudit with as few gates and control fields as possible. We analyze this complexity for the example of controlling ground electronic states of a single atom. Specifically, we describe the coupling graph alluded to in the introduction in this case before defining it in general.

Consider the atomic species ⁸⁷Rb per Fig. 1. There are

two ground state hyperfine manifolds with total spin $F_{\downarrow}=1$ and $F_{\uparrow}=2$ split in energy by the hyperfine interaction E_{hf} . Each manifold consists of 2F+1 degenerate magnetic sublevels M_F for a total of eight distinguishable states. The degeneracy can be lifted by applying a longitudinal magnetic field B_z . For small fields, the resultant Zeeman interaction is linear in the magnetic quantum number: $H_B=g_FB_zM_F$, where the Lande g factors satisfy $g_{F_{\downarrow}}=-g_{F_{\uparrow}}$ [13].

Control fields that act on ground-state hyperfine levels can couple to either the nuclear spin or to the electronic spin. These two mechnisms are distinguished by the strength of the coupling with respect to the hyperfine interaction. We consider coupling that is weak relative to E_{hf} using a pair of laser beams on Raman resonance between two sublevels at a time. The effective atom-laser Hamiltonian H_{AL} in the subspace \mathcal{H}_{jk} is then

$$H_{ALjk} = \cos(\phi)H_{jk}^{x} - \sin(\phi)H_{jk}^{y}, \tag{5}$$

where $\Omega = |\Omega_1 \Omega_2|/\Delta$ is the product of the individual laser Rabi frequencies divided by the detuning Δ from the excited state, and $\phi = \phi_1 - \phi_2$ is the relative phase of the two beams. A Raman coupling will also introduce ac stark shifts on all the basis states. Generally, in the subspace $\{|j\rangle, |k\rangle\}$ this will introduce an effective $H_{j,k}^z$ coupling term. However, if the laser Rabi frequencies are chosen such that $|\Omega_1| = |\Omega_2|$, then $H_{j,k}^z = 0$. Therefore, the Raman coupling between the two states does indeed generate the Givens rotation $U_{j,k}$ up to diagonal phases accumulated on the other basis states. Such phases can then be accounted for in the subsequent step of the QR algorithm.

In order to selectively couple two states only it is necessary that their energy difference be unique. In the linear Zeeman regime, this can only be accommodated when the two levels reside in different hyperfine manifolds. The allowed couplings are constrained by angular momentum selection rules which dictate the change in magnetic spin quantum number during a single pulse sequence. It will be important to minimize spontaneous emission during the pulse sequence by choosing a large detuning Δ of each laser from the excited states. For a detuning much greater than the excited state hyperfine structure, but less than than the fine structure splitting, the angular momentum selection rules dictate ΔM_F $=0,\pm1$. Using two-laser pulses of the appropriate frequency and polarization, the states $|F_{\perp}, M_F\rangle$ and $|F_{\uparrow}, M_F + \Delta M_F\rangle$, where $\Delta M_F = 0, \pm 1$ can then be coupled together. This is shown schematically in Fig. 1 where states $|2\rangle$ and $|5\rangle$ are coupled by a σ_{+} – π polarized laser pair. As a further resource constraint, we assume that one laser coupled to the F_{\uparrow} manifold has fixed π polarization so that the transition $|F_{\perp},0\rangle \leftrightarrow |F_{\uparrow},0\rangle$ is disallowed.

At this point we pause to comment on the resources necessary for single qudit compution using Raman pulses. For a fixed Zeeman splitting, it will be necessary to have lasers tuned to Raman resonance for eight allowed couplings. This may be achievable using two phase locked lasers that are frequency modulated appropriately. Another recourse is to change the magnetic field strength for each pairwise state coupling so that only one laser pair with a fixed frequency difference is necessary. The phase shifts accumulated on the

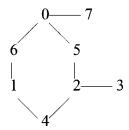


FIG. 2. This is the coupling graph for the coupled hyperfine states of ⁸⁷Rb (see Fig. 1.) As it is connected, the collection of atom-laser couplings allows for universal one-qudit computation.

basis states during the change in Zeeman interaction can be accounted for in the gate sequence.

We wish to show that the above set of atom-laser Hamiltonians suffices to construct an arbitrary unitary evolution of eight dimensional state space $\mathcal{H}_1 = \mathbb{C}[0] \oplus \cdots \oplus \mathbb{C}[7]$. Take $V \in U(8)$ as the target one-qudit evolution. The goal then is to decompose V into a sequence of evolutions by these atom laser Hamiltonians

$$V = \exp(-iH_{AL}^1 t_1/\hbar) \cdots \exp(-iH_{AL}^l t_l/\hbar). \tag{6}$$

Additionally, we prefer *efficient* decompositions, i.e., we wish to use as few laser pulses (as small an l) as possible. This is sometimes not possible, depending on which states $|j\rangle$, $|k\rangle$ are coupled by an H_{AL} . In order to classify when the QR step is possible, we introduce the notion of a "coupling graph," by example.

⁸⁷Rb coupling graph. The ⁸⁷Rb coupling graph has vertices labelled by 0,1,...,7. In addition, consulting Fig. 1, we also allow in the following edges, corresponding to the atomlaser coupled hyperfine states:

$$\{(0,5),(0,6),(0,7),(1,4),(1,6),(2,3),(2,4),(2,5)\}.$$
 (7)

In particular, the edges encode the selection rule for the hyperfine states. The graph is reproduced in Fig. 2. We note for future use that it is connected. Provided the states $|j\rangle$, $|k\rangle$ are coupled, we may produce any determinant-one unitary evolution of \mathcal{H}_{ik} .

Now note that since the coupling graph is connected, we may in fact sequentially construct a Givens rotation on any \mathcal{H}_{jk} . Indeed, even if $|j\rangle$ and $|k\rangle$ are not paired, there exists a sequence $|j_0\rangle=|j\rangle,|j_1\rangle,|j_2\rangle,\dots,|j_l\rangle=|k\rangle$ such that each consecutive pair admits atom-laser Hamiltonians. Moreover, taking $\phi=\pi/2$, $\theta=\pi/2$ in Eq. (2) shows that we may use these pairings to swap states up to relative phase. Hence, since we may physically construct some sequence of Hamiltonians for any Givens rotation, we see that the first step of the QR decomposition is possible.

This leaves open the question of efficiency. For example, one might hope that in a graph as highly connected as that for 87 Rb few or no swaps might be required. This is indeed possible as we now show. It is convenient to reorder the unitary in a logical basis labeled $\{7,0,6,5,3,2,4,1\}$. By successive Givens rotations, one may bring a unitary V to diagonal form column by column where the sequence is chosen so as to not void zeroes created in earlier steps. Each of the columns can be reduced to a single unimodular entry on the

diagonal by a sequence of Givens rotations $U_{j,k}$ acting on the two-dimensional subspace \mathcal{H}_{jk} . The complete sequence is as follows: Column 7 reduction: $U_{4,1}U_{2,4}U_{2,3}U_{5,2}U_{0,5}U_{0,6}U_{7,0}$, column 0 reduction: $U_{4,1}U_{2,4}U_{2,3}U_{5,2}U_{0,5}U_{0,6}$, column 6 reduction: $U_{2,5}U_{2,3}U_{4,2}U_{1,4}U_{6,1}$, column 5 reduction: $U_{4,1}U_{2,4}U_{2,3}U_{5,2}$, column 3 reduction: $U_{4,1}U_{2,4}U_{3,2}$, column 2 reduction: $U_{4,1}U_{2,4}U_{3,4}$, column 4 reduction: $U_{4,1}U_{4,1}U_{4,1}U_{4,1}$

Note that in general, constructing U_{jk} requires 2d(j,k)-1 basic Hamiltonians, where d(j,k) is the distance between j and k in the graph corresponding to the pairing relation. For qudit computation in ${}^{87}\text{Rb}$ using Raman pulses, the graph is sufficiently connected so that the distance is never greater than one in the QR decomposition above. There are a total of $8\times7/2=28$ gates in the reduction to diagonal form. Each gate $U_{j,k}\in SU(2)$ has two parameters so this gives 56 parameters. An arbitrary $u\in SU(d)$ requires d^2-1 parameters so the additional seven parameters correspond to seven relative phases left on the diagonal.

B. Relative phases

The goal of this section is to show that should the Hamiltonian graph be connected and $T = \sum_{j=0}^{d-1} \mathrm{e}^{i\varphi_j} |j\rangle\langle j|$ be a diagonal element of U(d), then we may realize T with the allowed Hamiltonians H^x_{jk} , H^y_{jk} . In fact, we only need to construct T up to a global phase so we can provide the construction for the unitary $T' \in SU(d)$, $T' = \sum_{j=0}^{d-1} \mathrm{e}^{i\phi_j} |j\rangle\langle j|$, where $\phi_{d-1} = -\sum_{j=0}^{d-2} \phi j$. We first note that although it is not explicitly an allowed Hamiltonian, we may for any (j,k) edge within the coupling graph simulate the effect of $H^z_{jk} = \hbar \Omega \lambda^z_{jk}$. Indeed, for any fixed angle γ we have

$$e^{-iH_{jk}^2\gamma'(\hbar\Omega)} = U_{j,k}(-\pi/4,\pi/2)U_{j,k}(-\gamma,0)U_{j,k}(\pi/4,\pi/2).$$
(8)

The goal then is to find an efficient sequence of z rotations that simulates T':

$$\prod_{l=0}^{d-2} \exp(-iH_{j_lk_l}^z t_l/\hbar) = T'.$$
 (9)

Given that the coupling graph is connected, choose a subset S of d-1 edges $\lambda_{jk}^z = |j\rangle\langle j| - |k\rangle\langle k|$ that leave the graph connected. We can represent the elements of S as vectors in a d-dimensional real vector space spanned by the orthonormal vectors $\{e_j\}$, i.e., $\lambda_{jk}^z = e_j - e_k$. We then construct a $(d-1) \times d$ matrix M out of the row vectors in S: $M = \{\lambda_{0k_0}^z, \lambda_{1k_1}^z, \dots, \lambda_{d-2k_{d-2}}^z\}$. The appropriate timings t_j in Eq. (9) necessary to simulate T' are given by solutions to the matrix equation $M^T \vec{\theta} = \vec{\phi}$, where $\vec{\theta} = -\Omega(t_0, \dots, t_{d-2})$ and $\vec{\phi} = (\phi_0, \dots, \phi_{d-2}, \phi_{d-1})^T$. Straightforward Gaussian elimination shows that the dimension of the row space of M is d-1, thus there is a unique solution to the vector $\vec{\theta}$.

The result is that any diagonal unitary can be simulated up to a global phase using $3 \times (d-1)$ gates from the gate library. This sequence can be reduced by a factor of three if z rotations can be implemented directly without conjugation. Further, all the Hamiltonians H_{ik}^z are diagonal and hence com-

mute, so z rotations that act on disjoint subspaces can be implemented in parallel using additional control resources.

C. One-qudit universality for generic coupling graphs

We found that for computation in the ground electronic states of ⁸⁷Rb, a single qudit unitary could be brought to diagonal form using the fewest possible Givens rotations. This is not peculiar to that system but is in fact possible for any system with a connected coupling graph [14].

Lemma II.1. Given a d-node coupling graph \mathcal{G} of allowed Givens rotations, then any $U \in SU(d)$ can be brought to diagonal form using d(d-1)/2 allowed rotations if and only if \mathcal{G} is connected.

Proof. Suppose \mathcal{G} is connected. Form any spanning tree for it, and renumber the nodes so that the path from node d (the root of the tree) to any node *j* passes through no node numbered lower than i; such a numbering can be constructed by successively deleting leaf nodes and numbering in order of deletion. (For ⁸⁷Rb, we formed the tree by breaking the edge between nodes 6 and 1 and used the logical basis ordering $\{7,0,6,5,3,2,4,1\}$.) At the *j*th step $(j=1,\ldots,d-1)$, create the tree T_i , rooted at node j, from the portion of the spanning tree defined by nodes j, \ldots, d . (Note that T_i is connected due to the way we numbered the nodes.) Then, until only the root of \mathcal{T}_i remains, choose a leaf k, use a rotation defined by its edge to eliminate element (k,j) of U, and delete node k from T_i . The result of applying these steps is an upper triangular matrix (and therefore, since U is unitary, a diagonal matrix) computed by using d(d-1)/2 allowed rotations.

Suppose \mathcal{G} is not connected and consider a matrix $U \in \mathrm{SU}(d)$ that has no zero elements. Choose an arbitrary node to call node 1. Then we can at best eliminate all but one of the nonzeros in column 1 of the disconnected piece, but there is no allowed rotation that will eliminate the last nonzero. Repeating the argument for each choice of node 1, we conclude that we cannot reduce U to diagonal form using only allowed rotations.

III. MULTIQUDIT UNIVERSAILITY

Suppose in addition to being allowed local Hamiltonians $\{H_{jk}^{x,y}\}$ with a connected coupling graph, the physical system also allows for a two-qudit phase Hamiltonian

$$H_{\text{int}} = -\hbar\Omega |d-1, d-1\rangle \langle d-1, d-1|, \tag{10}$$

where $|m,n\rangle \equiv |m\rangle \otimes |n\rangle$. This interaction generates the singly-controlled one qudit phase gate

$$\Lambda_1(P(\phi)) = \exp[-iH_{\rm int}\phi/(\hbar\Omega)]. \tag{11}$$

For qubits, the controlled-phase gate $\Lambda_1(P(\pi))$ together with arbitrary single qubit rotations is sufficient for exactly universal quantum computation [15]. In many situations, the interaction between qudits will contain more than one term on the diagonal. For instance, the actual Hamiltonian may be

$$H'_{\text{int}} = \sum_{m,n=0}^{d-1} \hbar \Omega_{mn} |m,n\rangle \langle m,n|.$$
 (12)

In this case the evolution generated by H_{int} over a time t is entangling if the following is true [8]:

$$t(\Omega_{mn} + \Omega_{pq}) \neq t(\Omega_{mq} + \Omega_{pn}) \mod 2\pi \text{ for some } m, n, p, q.$$
(13)

When the interaction H'_{int} is entangling, it is always possible to map it to H_{int} using multiple applications of H'_{int} conjugated by single qudit gates. In practice, some multiqudit operations may be done more efficiently using H'_{int} directly.

There are several proposals for realizing diagonal coupling gates in real physical systems. For example, in trapped atoms possible coupling mechanisms include pairwise interactions via dipole-dipole interactions [16,17], and controlled ground state-ground state collisions [18]. The later proposal has been realized recently between atoms trapped in an optical lattice [19]. These proposals were originally made with the goal of engineering two qubit controlled-phase gates. As such, a naive adaptation to encoding over all magnetic hyperfine levels would fail due to off diagonal couplings between basis states. However, it should be possible to modify one or more proposals to realize a differential shift on a single product state. For instance, in Ref. [20] it was proposed to realize a quantum gate using the ground stateground state collisional shift in a trap induced shape resonance. Here one can tune a magnetic field such that a single molecular state is on resonance with a bound motional state of an external trap for both atoms. Because the resonance is dependent on the internal states, a unique phase is accumulated on a single product state. Provided the atoms are sufficiently separated, the other basis state pairs do not interact and a Hamiltonian of the form H_{int} is realized (up to local unitaries).

We describe a bootstrap technique using the interaction $H_{\rm int}$ and one-qudit unitaries which allows for universal quantum computation. Before presenting the generic discussion, we describe a particular example of a two-qubit operation. First, label as $(\oplus 1)$ the map which carries $k \mapsto (k+1) \mod d$. Then the controlled-increment gate, denoted Λ_1 (INC), is defined by extending the following rule linearly:

$$\Lambda_{1}(\text{INC})|j,k\rangle = \begin{cases} |j,k\rangle, & j \neq d-1, \\ |j,k \oplus 1\rangle, & j = d-1. \end{cases}$$
 (14)

The controlled-increment gate has been used in the literature for building a generic k-controlled computation $\Lambda_k(V)$ [9] as well as for constructing quantum error correction codes [21].

We may explicitly realize Λ_1 (INC) from the Hamiltonian H_{int} as follows. We write $(j_1j_2\cdots j_l)$ for the cyclic permutation of the single qudit basis states with $j_1\mapsto j_2$, $j_2\mapsto j_3,\cdots,j_{l-1}\mapsto j_l,\ j_l\mapsto j_1$, and all other set elements fixed. The permutation will also be identified implicitly with the associated permutation matrix $\pi_{(j_1j_2\cdots j_l)}\in U(d)$. Hence, given $(01)(12)\cdots(d-2d-1)=\oplus 1$, we see that $\Lambda_1(\text{INC})=\Lambda_1[(01)\times(12)\cdots(d-2d-1)]$. The construction of Λ_1 (INC) then takes place in the following steps:

Using Givens rotations, the gate $\Lambda_1(I_{j-1} \oplus \sigma^z \oplus I_{d-1-j})$ is constructed as

$$\Lambda_1(I_{j-1} \oplus \sigma^z \oplus I_{d-1-j}) = I_d \otimes U_{j+1,d-1}(\pi/2,0) \Lambda_1(P(\pi))$$

$$\times I_d \otimes U_{j+1,d-1}(-\pi/2,0), \qquad (15)$$

then

$$\Lambda_{1}[(jj+1)] = I_{d} \otimes U_{j+1,j+2}(-\pi/4,\pi/2)\Lambda_{1}(I_{j} \oplus \sigma^{z} \oplus I_{d-2-j})
\times I_{d} \otimes U_{j+1,j+2}(\pi/4,\pi/2).$$
(16)

This leads to the realization of Λ_1 (INC) using d-1 controlled operations, given that Λ_1 (INC) = $\Lambda_1(01)\Lambda_1(12)\cdots\Lambda_1(d-2d-1)$.

Finally, we count the number of gates needed to implement an arbitrary two-qudit unitary using one-qudit Givens rotations $U_{j,k}$ and the controlled-phase gate $\Lambda_1(P(\phi))$. A helpful tool is the controlled one-qudit Householder gate $\Lambda_1(X(|\psi\rangle))$ defined as a unitary extension of the mapping $|d-1\rangle \rightarrow e^{-i\chi}|\psi\rangle$ conditioned on the control qudit in state $|d-1\rangle$. In the Appendix we show that this gate can be constructed with 2(d-1) controlled-phase gates $\Lambda_1(P(\phi))$ and 2(d-1) one-qudit Givens rotations. Using the techniques in Ref. [22], d-1 singly controlled Householder gates suffice to synthesize an arbitrary two-qudit state $|\beta\rangle \in \mathbb{C}^{d^2}$, i.e., to realize the mapping $|d-1,d-1\rangle \rightarrow |\beta\rangle$.

Any two-qudit unitary $U \in U(d^2)$ can be written in a spectral decomposition $U = \sum_{j=0}^{d^2-1} e^{i\phi_j} |\lambda_j\rangle\langle\lambda_j|$, where $\{e^{i\phi_j}\}$ and $\{|\lambda_j\rangle\}$ are the sets of eigenvalues and eigenvectors of U. The unitary can then be decomposed into the product [23]

$$U = \prod_{j=0}^{d^2 - 1} W_j \Lambda_1(P_j(\phi_j)) W_j^{\dagger}, \tag{17}$$

where W_j is any unitary extension of the two-qudit mapping $|j\rangle \rightarrow |\lambda_j\rangle$, and the diagonal gate $\Lambda_1(P_j(\phi_j)) = I_{d^2} + (\mathrm{e}^{i\phi_j} - 1)|j\rangle\langle j|$ is locally equivalent to the singly controlled phase gate $\Lambda_1(\phi_j)$. Using controlled-Householders to construct the gates W_j , the total gate count for simulating $U \in U(d^2)$ is then $4d^2(d-1)^2 + d^2$ controlled-phase gates and $O(d^4)$ one-qudit Givens rotations. In Ref. [22] we derive a construction of an arbitrary n qudit unitary using $O(d^{2n})$ two-qudit gates. That construction uses a QR decomposition and is asymptotically optimal.

IV. CONCLUSIONS

We have identified the criteria for exact quantum computation in qudits. Our method is constructive and relies on the QR decomposition of unitaries on qudits using a gate library generated by a fixed set of single qudit Hamiltonians and a one parameter singly controlled phase gate. Using the concept of a coupling graph we are able to show that universal computation is possible if the nodes (equivalently logical basis states) are connected. Further we give a prescription for efficient single qudit computation by demanding that at each stage of the QR decomposition the graph remains connected. Using the gate library generated by the couplings in Eq. (1)

the worst case gate count is k=3d(d+1)/2-3. In the case that $H_{j,k}^x$ and $H_{j,k}^y$ can be turned on at the same time for a fixed pair of states (j,k) [as in Eq. (5)], the gate count is k=d(d-1)/2+3(d-1). If, in addition, one is allowed the set of diagonal generators $\{H_{jk}^z\}$, the gate count is optimal at k=d(d+1)/2-1. The technique for computation is exemplified with a d=8 qudit using the Raman coupled magnetic sublevels of ⁸⁷Rb. It is shown that arbitary single qudit computation is possible with at most 49 laser pulse sequences. A construction of an arbitrary two-qudit unitary is given using $O(d^4)$ controlled-phase gates and Givens rotations. Arbitrary computation on n qudits can then be done using $O(d^{2n})$ two-qudit gates [22].

We note that while the results herein have focused on the construction of unitaries, the ideas can be extended to simulating nonunitary processes such as generalized measurements. Generalized measurements on a system s can be thought of as orthogonal measurements on an extended system $H_s \oplus H_s^{\perp}$, which may not be orthogonal in s alone. Applications including precision measurement [24], quantum communication in the context of entanglement purification [25], and quantum error correction [26]. To realize a positive operator valued measurement (POVM), one can perform a unitary operation on $H_s \oplus H_s^{\perp}$ followed by a projective measurement on H_s^{\perp} alone. For example, nonorthogonal measurements on a qubit can be realized by appending ancillary qubits, performing unitary operations on the joint system, and measuring the ancillae. The requirement of using two qubit gates can be obviated if the ancillary degrees of freedom come from orthogonal states within the same system. For example, one can use the d-2 states of a qudit to implement POVMs on a qubit subspace. These ideas are explored in the context of quantum optical systems in Refs. [27,28]. The techniques reported here indicate that the requisite operations on the appended Hilbert space can be done efficiently.

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APPENDIX: THE CONTROLLED HOUSEHOLDER GATE

We describe the construction of the singly controlled Householder gate using one-qudit Givens rotations and the controlled-phase gate. The Householder gate is a unitary extension of the mapping of an arbitrary one-qubit superposition state $|\psi\rangle = \sum_{j=0}^{d-1} c_j |j\rangle$ to the logical basis state $|d-1\rangle$ (up to a global phase χ). For our convenience we describe the inverse controlled operation defined $\Lambda_1(X(|\psi\rangle))$ that maps $|d-1\rangle \to e^{-i\chi} |\psi\rangle$ on the target qudit iff the control is in state $|d-1\rangle$ and applies 1 to the target otherwise

$$\Lambda_{1}(X(|\psi\rangle)) = \sum_{k \neq d-1, k'} |kk'\rangle\langle kk'| + |d-1\rangle\langle d-1|$$

$$\otimes \left(e^{-i\chi}|\psi\rangle\langle d-1| + \sum_{k \neq d-1} |\beta_{k}\rangle\langle k|\right), \quad (A1)$$

where $\langle \psi | \beta_k \rangle = 0$ and $\langle \beta_i | \beta_k \rangle = \delta_{i,k}$. The singly controlled

Householder is then just $\Lambda_1(X(|\psi\rangle))^{\dagger}$. Because the gate $\Lambda_1(X(|\psi\rangle))$ is allowed to implement any unitary extension of $|\psi\rangle_t\langle d-1|$, it only depends on the 2d-2 parameters of the state $|\psi\rangle$ (two parameters are fixed by the norm $\langle\psi|\psi\rangle=1$ and setting the global phase to zero). This gate plays prominently in the contruction of universal computation in qudits by Muthukrishnan and Stroud [9]. They give an example of how such a gate could be designed using a specific Hamiltonian in an ion trap. Our construction is general for any system encoding qudits with a connected coupling graph.

First, expand the state $|\psi\rangle$ in the single qudit basis: $|\psi\rangle = e^{i\chi} \sum_{j=0}^{d-1} c_j |j\rangle$, where the global phase χ is chosen so that $\arg(c_{d-1}) = 0$. The conditional mapping $|d-1\rangle \rightarrow e^{-i\chi} |\psi\rangle$, can be realized as a sequence of d-1 controlled unitaries that couple two target qudit basis states at a time

$$\Lambda_1(X(|\psi\rangle)) = \prod_{j=0}^{d-2} \Lambda_1(U_{j,d-1}(\gamma_j, \phi_j)). \tag{A2}$$

The arguments (θ_j, ϕ_j) for each controlled unitary must satisfy the following relations:

$$c_{d-2} \equiv \langle d-2|U_{d-2,d-1}|d-1\rangle = -ie^{i\phi_{d-2}}\sin \gamma_{d-2},$$

$$\begin{split} c_{d-3} &\equiv \langle d-3 | U_{d-3,d-1} U_{d-2,d-1} | d-1 \rangle = \langle d-3 | U_{d-3,d-1} | d-1 \rangle \\ &= \langle d-1 | U_{d-2,d-1} | d-1 \rangle = -ie^{\phi_{d-3}} \sin \gamma_{d-3} \cos \gamma_{d-2}, \dots, \end{split}$$

$$c_k = -ie^{i\phi_k} \sin \gamma_k \prod_{l=k+1}^{d-2} \cos \gamma_l \quad (k < d-2).$$
 (A3)

Now it only remains to demonstrate that each controlled rotation $\Lambda_1(U_{j,d-1})$ can be simulated with just the controlled-phase gate and rotations on the target qudit. Four elementary gates suffice:

$$\begin{split} \Lambda_1(U_{j,d-1}(\gamma_j,\phi_j) &= \Lambda_1(P(\pi))[\mathbf{1} \otimes U_{j,d-1}(-\gamma_j/2,\phi_j)] \\ &\times \Lambda_1(P(\pi))[\mathbf{1} \otimes U_{j,d-1}(\gamma_j/2,\phi_j)]. \end{split} \tag{A4}$$

Following this construction, 2(d-1) controlled-phase gates and 2(d-1) single qudit Givens rotations suffice to exactly simulate $\Lambda_1(X(|\psi\rangle))$. The mapping of an arbitrary single qudit basis state $|k\rangle \rightarrow e^{-i\chi}|\psi\rangle$ is realized by substituting the Givens rotations $U_{j,k}$ in the product Eq. (A2) and conjugating the controlled-phase gates by the one-qudit state swap $[\oplus (d-1-j)]$, where \oplus denotes addition modulo d.

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