

Simulating Hamiltonian dynamics using many-qudit Hamiltonians and local unitary control

Michael J. Bremner,^{1,2,*} Dave Bacon,^{2,3,†} and Michael A. Nielsen^{1,2,4,‡}

¹*School of Physical Sciences, The University of Queensland, Queensland 4072, Australia*

²*Institute for Quantum Information, California Institute of Technology, Pasadena, California 91125, USA*

³*Department of Physics, California Institute of Technology, Pasadena, California 91125, USA*

⁴*School of Information Technology and Electrical Engineering, The University of Queensland, Queensland 4072, Australia*

(Received 31 May 2004; published 9 May 2005)

When can a quantum system of finite dimension be used to simulate another quantum system of finite dimension? What restricts the capacity of one system to simulate another? In this paper we complete the program of studying what simulations can be done with entangling many-qudit Hamiltonians and local unitary control. By *entangling* we mean that every qudit is coupled to every other qudit, at least indirectly. We demonstrate that the only class of finite-dimensional entangling Hamiltonians that are not universal for simulation is the class of entangling Hamiltonians on *qubits* whose Pauli operator expansion contains only terms coupling an *odd* number of systems, as identified by Bremner *et al.* [Phys. Rev. A **69**, 012313 (2004)]. We show that in all other cases entangling many-qudit Hamiltonians are universal for simulation.

DOI: 10.1103/PhysRevA.71.052312

PACS number(s): 03.67.Mn, 03.65.-w

I. INTRODUCTION

A. Overview

One remarkable aspect of Nature is that it can be modeled by equations whose solution may be obtained by algorithmic means. This empirically observed fact allows us to construct physical theories that make predictions as to how Nature will behave. Of course, while we can simulate Nature, our capacity to do so is limited by the way we choose to perform the simulation and the complexity of the system to be simulated. Feynman's landmark paper on quantum computation [1] discussed the apparent inability of classical computers to efficiently simulate quantum systems and suggested that a quantum computer might succeed where classical computers fail. In this paper we study a class of simulation protocols motivated by the example of quantum computation. In particular, we examine the following question: given a composite system with a finite-dimensional Hamiltonian and the ability to perform arbitrary local unitary operations, what other Hamiltonians can we simulate?

The simulation of quantum systems by quantum computers is a topic that has attracted considerable attention. A considerable literature (see [2] and references therein) addresses the question of how to adequately simulate physically interesting closed quantum systems. Issues of particular interest include the complexity of protocols for simulating initial states, simulating evolutions, and for extracting physically important information from the final state of the computer. Each of these issues must be addressed in any comparative study of quantum and classical computers, and their capacity to simulate Nature.

While state preparation and measurement are vital elements of any simulation of a quantum system, we focus in

this paper on the simulation of *evolutions* of systems. Hamiltonian simulation protocols using single-qudit unitary operations as an additional resource have received considerable attention in recent years due to their relationship with various models of quantum computation. One of the more noteworthy advances was the discovery that all two-body Hamiltonians can simulate all other Hamiltonians on the set of qudits that they entangle, when combined with single-qudit unitary operations [3–12]. This body of work also demonstrated that these Hamiltonians could be used to *efficiently* simulate any other two-body Hamiltonian that acts on the network of qudits they entangle. This includes a Hamiltonian that can implement the CNOT operation, thus implying that all entangling two-body Hamiltonians combined with single-qubit unitary operations are universal for quantum computation.

The results and tools used to study two-body Hamiltonian simulation have been applied fruitfully to several related problems. There is now a considerable literature on time-optimal strategies for simulating two-qubit Hamiltonians and quantum gates; see, for example, [5,13–27], and references therein. This body of investigation has led to interest in applying these theoretical results to practical proposals for quantum computation [28].

More recently, studies have focused on using systems with many-qubit interactions for Hamiltonian simulation and gate-synthesis [21,27,29–31]. A number of these papers have investigated the structure of systems with many-body interactions for the purposes of gate synthesis and algorithm design [21,27,30,31]. Several authors have recently examined the effects of many-body interactions in quantum dot [32] and optical lattice [33,34] systems.

For the purposes of this paper we are most concerned with the work in [29], where the authors established which Hamiltonians with many-qubit interactions are universal when combined with the ability to perform arbitrary single-qubit unitary operations. In a similar vein we examine which Hamiltonians with many-*qudit* interactions are universal when combined with arbitrary single-*qudit* unitary operations. Our final result is a striking generalization of the con-

*Electronic address: bremner@physics.uq.edu.au

†Electronic address: dabacon@cs.caltech.edu

‡Electronic address: nielsen@physics.uq.edu.au

clusion in [29]. [29] showed that the only class of non-universal entangling Hamiltonians on qubits are the *odd* entangling Hamiltonians, i.e., those Hamiltonians whose Pauli operator expansion contains only terms coupling an odd number of qubits. Furthermore, [29] showed that the odd entangling Hamiltonians can all simulate one another, so there is a sense in which there are only two types of many-qubit entangling Hamiltonian. Remarkably, in this paper we will see that when the systems involved are not all qubits, this structure actually *simplifies*, with *all* entangling Hamiltonians capable of simulating all other entangling Hamiltonians, i.e., we show that apart from the many-*qubit* case, there is only one type of many-body entangling Hamiltonian.

Our primary concern in this paper is with questions of universality in many-qudit systems, without regard to the issue of complexity. Thus, when we say a set of resources is *universal* on a set of qudits, we are stating that these resources can be used to simulate any Hamiltonian on those qudits, without implication that this simulation is efficient or inefficient. This is in contrast to the notion of *universality for quantum computation* which requires that any universal set of resources can simulate a standard gate set with a polynomial overhead in the number of qubits used. That said, it is often possible to exploit the structure of certain classes of many-body Hamiltonians to develop efficient simulation algorithms. For instance much headway can be made in developing efficient Hamiltonian simulation protocols that use *k*-local Hamiltonians by adapting the methods developed for systems of qubits in [29] to systems of qudits.

B. Terminology and statement of results

Before turning to the discussion and proof of the main results of this paper it is helpful to introduce some terminology. Generally, we will use the term *qudit* to describe any quantum system with a finite-dimensional state space. As an example of our usage, a three-qudit system might contain a two-dimensional system (a qubit), a five-dimensional system, and a four-dimensional system.

We are interested in the properties of the Hamiltonian dynamics of an *n*-qudit system. As we will see, a great deal can be said about the properties of a Hamiltonian simply by examining its structure in a suitable representation. In [29], the authors found that the universality properties of a many-body Hamiltonian acting on qubits could be identified by expanding it in the Pauli-operator basis, i.e., tensor products of *X*, *Y*, *Z* and *I*. In this paper we expand upon this analysis by examining the properties of an *n*-qudit Hamiltonian written in a *d*-dimensional generalization of the Pauli basis.

An arbitrary Hamiltonian on *n* qudits can be uniquely written as

$$H = \sum_{\alpha} h_{\alpha} H_{\alpha}, \tag{1}$$

where h_{α} are real coefficients and each H_{α} in the expansion is a tensor product of Hermitian operators acting on the individual qudits,

$$H_{\alpha} = \bigotimes_{j=1}^n H_{\alpha}^{(j)}, \tag{2}$$

where $H_{\alpha}^{(j)}$ acts on qudit *j*, and is either the identity operator, or one of a set of traceless Hermitian matrices known as the *Gell-Mann matrices*. The Gell-Mann matrices generalize the Pauli matrices, and thus this expansion is a generalization of the expansion for qubits used in [29]. The Gell-Mann matrices for a *d*-dimensional quantum system consist of (a) *d*−1 matrices of the form

$$W_m = \frac{1}{\sqrt{m(m-1)}} \left(\sum_{b=1}^{m-1} |b\rangle\langle b| - (m-1)|m\rangle\langle m| \right), \tag{3}$$

where $2 \leq m \leq d$, and (b) the Pauli-like matrices:

$$X_{ab} = \frac{1}{\sqrt{2}} (|a\rangle\langle b| + |b\rangle\langle a|), \tag{4}$$

$$Y_{ab} = \frac{-i}{\sqrt{2}} (|a\rangle\langle b| - |b\rangle\langle a|), \tag{5}$$

where $1 \leq a < b \leq d$. These act as the Pauli *X* and *Y* on the two-dimensional subspace spanned by the vectors $|a\rangle$ and $|b\rangle$. We sometimes refer to the W_m matrices as *Cartan subalgebra* elements of the Gell-Mann matrices, since they span a Cartan subalgebra of the Lie algebra *su*(*d*) generated by the Gell-Mann matrices. However, it is worth emphasizing that we do not use any special properties of Cartan subalgebras, and the reader does not need to be familiar with the properties of Cartan subalgebras to follow the details of the paper; our use of the term is a convenience of nomenclature only. Note that the Gell-Mann matrices are traceless and Hermitian, and form a complete basis for traceless Hermitian matrices.

The representation Eq. (1) is useful as it highlights which qudits interact and which do not. In particular, given a term H_{α} let S_{α} be the set of qudits upon which H_{α} acts non-trivially, that is, the set of qudits for which $H_{\alpha}^{(j)}$ is traceless. We say that the qudits in S_{α} are *coupled* by H_{α} and refer to H_{α} as a *coupling term*. We also say that H_{α} is *entangling* on the set S_{α} . More generally, we say that a Hamiltonian H is *entangling* on some set of qudits if it is not possible to partition this set of qudits into two nontrivial sets S and \bar{S} such that every term H_{α} in the expansion of H couples either a subset of S or of \bar{S} . In graph-theoretic language, if the qudits corresponded to vertices on a hypergraph and the couplings corresponded to hyperedges, the condition that the Hamiltonian is entangling on a set of qudits is simply that the hypergraph connects this set. As such we say that a Hamiltonian *connects* the set of qudits it entangles.

Our strategy for demonstrating universality in this paper is to show that some set of resources is capable of simulating another set already known to be universal. In particular, we make reference to two theorems that categorize large classes of Hamiltonians as universal up to single-qudit unitary operations. The first was mentioned in the Introduction: two-

body entangling Hamiltonians are universal for quantum computation [10]. Using the terminology just introduced, this theorem may be stated as follows [10].

Theorem 1. Suppose H is a two-body Hamiltonian, that is, every coupling term in the Gell-Mann expansion of H couples at most two qudits. If H is entangling on a set of n qudits (that is, the coupling terms in H connect these qudits) then evolutions of H together with single-qudit unitary operations are universal for quantum computation on these n qudits.

The second universality theorem that we use involves Hamiltonians acting on sets of qubits that have coupling terms that may couple more than two qubits. This theorem is stated [29] as follows.

Theorem 2. Suppose H is an arbitrary entangling Hamiltonian on a set of n qubits. Evolutions of H and single-qubit unitary operations are universal on those n qubits if and only if the Gell-Mann (i.e., Pauli) expansion of H contains at least one coupling term that couples an even number of qubits.

Theorem 2 tells us that for a Hamiltonian acting on qubits alone to be universal, it must have a coupling term acting on an even number of qubits. If H does not contain such a coupling term then we shall call it an *odd* Hamiltonian, since all its terms couple an odd number of qubits. What can the odd Hamiltonians simulate? This question was also answered in [29].

Theorem 3. Let H be an odd entangling Hamiltonian, that is, every term in the Gell-Mann expansion of H couples an odd number of qubits. Then H and single-qubit unitaries can simulate any other odd Hamiltonian on the n qubits.

Reference [29] also demonstrated that the Lie algebra generated by the odd entangling Hamiltonians on n qubits (and local unitaries) corresponds to the Lie algebras $so(2^n)$ and $sp(2^n)$, for even or odd n respectively. Furthermore, [29] showed that the odd Hamiltonians can be made universal with appropriate encodings.

In this paper we demonstrate that if a Hamiltonian is entangling on a set of qudits, then this Hamiltonian is universal on those qubits, when assisted by local unitary operations. The only exception to this result is the special case when the Hamiltonian is an odd Hamiltonian acting on qubits only.

C. Outline

Theorem 1 shows that if a Hamiltonian connects a set of qudits with two-qudit couplings then this Hamiltonian is universal with single-qudit unitaries. Our strategy in this paper is to show that a many-body Hamiltonian (that is not one of the odd qubit-only Hamiltonians) connecting a set of n qudits can simulate a two-body Hamiltonian connecting the same set of qudits. This is done by defining a series of simulation protocols, each identifying broad classes of Hamiltonians that any entangling Hamiltonian can simulate, until we arrive at the eventual result.

The structure of the paper is as follows. In Sec. II we introduce some simple general simulation techniques that are used often in this paper. Section III introduces a simulation technique known as *term isolation*. This simulation technique allows us to simulate any particular coupling term, H_{α} ,

that is present in the Gell-Mann expansion of H , thus *isolating* the term. In Sec. IV we show that given some term coupling k qudits, we can simulate new coupling terms that couple fewer than k qudits. We also discuss the limitations on this type of simulation. Section V examines how we can use a term that couples k qudits to simulate a coupling between two qudits. Finally we prove the main result of the paper: that the only nonuniversal class of entangling Hamiltonians is the class of odd Hamiltonians. This is argued through an exhaustive demonstration that all n -qudit entangling Hamiltonians other than the odd many-qubit Hamiltonians are indeed universal.

II. SIMPLE SIMULATIONS

In this section, we review some simple Hamiltonian simulation techniques studied in previous papers [3–12], and that will form the basis for our later results. By a Hamiltonian simulation we mean a sequence of evolutions due to our system Hamiltonian, H , which is assumed fixed, interleaved with single-qudit unitary operations. The goal is to approximate (to arbitrary accuracy) evolution according to some other Hamiltonian. If that is possible for some desired Hamiltonian we say that Hamiltonian can be *simulated*. The theory of Lie algebras and Lie groups ensures that the techniques described in this section exhaust the set of possible simulations that can be performed given some Hamiltonian and single-qudit unitaries.

A. Conjugation by a unitary operator

A quantum system with Hamiltonian H evolves in time via the unitary operation e^{-iHt} . Say we are also given the ability to perform some unitary operation, U , and its inverse, U^\dagger . Then performing the sequence of unitary operations $Ue^{-iHt}U^\dagger = e^{-iUHU^\dagger t}$, we see that we can simulate an evolution according to the conjugated Hamiltonian UHU^\dagger . In this paper, as we have given ourselves the ability to perform arbitrary single-qudit unitaries, we will often conjugate a Hamiltonian by unitaries of the form $U = U_1 \otimes U_2 \otimes \cdots \otimes U_n$.

B. Simulating linear combinations

Suppose we can simulate two different Hamiltonians, H_1 and H_2 . Then we can simulate the sum of these Hamiltonians, since $e^{-iH_1\Delta}e^{-iH_2\Delta} \approx e^{-i(H_1+H_2)\Delta}$ for small Δ , and with successive evolutions we can simulate the Hamiltonian $H_1 + H_2$ for an arbitrary time t . Imagine that we could evolve our system by a whole set of Hamiltonians, \mathcal{H} , and their negatives.¹ It follows that we can simulate arbitrary linear combinations of any of the elements of \mathcal{H} .

¹Given that we can simulate H , it turns out always to be possible to simulate $-H$, using single-qudit unitary operations. This follows from Eq. (11), later in the paper, which shows how to express $-H$ as a sum of terms of the form UHU^\dagger , where U are local unitary operations. By the methods of simulation we've already introduced, it follows that $-H$ can be simulated.

C. Simulating commutators of Hamiltonians

Another simple simulation protocol that can be performed is the simulation of a commutator of two different Hamiltonians. This is possible as $e^{-iH_1\Delta}e^{iH_2\Delta}e^{iH_1\Delta}e^{-iH_2\Delta} \approx e^{-i([H_1,H_2])\Delta^2}$. So if we can simulate H_1, H_2 and their negations we can simulate the commutator of these Hamiltonians.

D. Simulating Hamiltonians that couple the same qudits

Consider the general expression for a Hamiltonian acting on a system of qudits in Eqs. (1) and (2), and recall that H_α couples a set of qudits S_α . We now introduce a theorem from [8] to show it is possible to use H_α and single-qudit unitaries to exactly simulate any other coupling term that couples the set of qudits S_α :

Theorem 4. Let A and B be any two traceless Hermitian operators in d dimensions and assume that $B \neq 0$. There is an algorithm to find a set of at most d^2 unitary operators, U_n , and constants $c_n > 0$ such that

$$A = \sum_n c_n U_n B U_n^\dagger. \quad (6)$$

Key to proving this theorem is a result from the theory of operator majorization, Uhlmann's theorem [35]. Although we do not need the theory of majorization in this paper, for the benefit of readers familiar with majorization, we make the following summary remarks. Recall that Uhlmann's theorem tells us that if $P < Q$ (that is, P is majorized by Q) then $P = \sum_n p_n U_n Q U_n^\dagger$, for some unitary operators U_n and some p_n that form a probability distribution. The proof of theorem 4 in [8] follows by showing that $A < cB$ for some positive constant c .

Any coupling term H_α in H is a tensor product of traceless terms acting on S_α . If we replace B in Theorem 4 by the individual tensor factors appearing in H_α , then we see that we can simulate any A that is a tensor product of traceless Hermitian operators acting on the same set S_α . This result will be extremely useful in the remainder of this paper. It tells us that if we can simulate some coupling H_α , we can simulate every other coupling on the same set of qudits.

III. TERM ISOLATION

In Sec. II D, we saw that any coupling term, H_α , in the expansion $H = \sum_\alpha h_\alpha H_\alpha$ [Eq. (1)], could be used to simulate any other coupling term that entangles the same set of qudits. If we have a Hamiltonian that is simply a coupling term on a given set of qudits, we can immediately say a great deal about what can be simulated with that Hamiltonian. In general we do not have this luxury of interpretation. Instead, some general Hamiltonian, $H = \sum_\alpha H_\alpha$, has many different coupling terms that couple many different sets of qudits. *Term isolation* is a simulation technique that uses H and single-qudit unitaries to simulate any particular term H_α in the expansion of H alone.

Term isolation allows us to think about H in a different way, showing that the ability to simulate H is *equivalent* to the ability to simulate the coupling terms $\{H_\alpha\}$ individually. Thus, we can perform our analysis entirely in terms of the set

$\{H_\alpha\}$ and still encapsulate all of the Hamiltonian simulation properties of H . Given that the elements of the set $\{H_\alpha\}$ have a much simpler structure than a general H , term isolation is a powerful tool for analysis.

We now show that term isolation can always be performed. If we demonstrate that we can use H and single-qudit unitaries to simulate some H_α coupling an arbitrarily chosen set of qudits, then we know from Sec. II D that it can be used to simulate any other term coupling the same qudits.

Without loss of generality we may assume that the term being isolated is of the form

$$H_\alpha = \bigotimes_{j=1}^k W_{b_j}^{(j)} \otimes I^{\otimes n-k}, \quad (7)$$

where k is the number of qudits in the set S_α . To see that there is no loss of generality in assuming this form, note that we can always relabel the qudits in S_α so that they are the first k qudits in the system, and any operators X_{ab} or Y_{ab} in H_α are equivalent under local unitaries to W_2 .

Any term in the expansion of H, H_β , that is not the term H_α that we wish to keep, is different from H_α in at least one of three ways.

Case 1: H_β has terms acting nontrivially on qudits outside of S_α , the set of qudits upon which H_α acts.

Case 2: H_β acts on a strict subset of S_α .

Case 3: H_β acts on the same qudits as H_α but is a tensor product of different elements of the Gell-Mann basis. That is, $H_\alpha \neq H_\beta$, even though H_β couples the set S_α .

Each of these cases identifies a special difference between H_α and H_β . In the following sections these differences are exploited to define simulations that remove undesirable terms.

As we have previously stated, every simulation in this section may be represented as a sequence of linear combinations, commutators and conjugations by local unitaries. We often denote a sequence of operations of this type on a Hamiltonian, H , by a scripted letter. For example, in Sec. III A we define the depolarizing channel, which is a linear combination of conjugations by local unitaries, and write $\mathcal{D}[H] = H_D$ to symbolize the depolarizing channel acting on H , resulting in the simulated Hamiltonian H_D . The action of \mathcal{D} on H defines a simulation. We can also compose simulation techniques, so, for example, in Sec. III B we define a simulation $\mathcal{T}[H_D] = H_T$.

A. Case 1

We begin by noting the identity

$$\sum_{U_p} U_p J U_p^\dagger = d \operatorname{tr}(J) I, \quad (8)$$

where J is an operator acting on some qudit of dimension d and the sum is over all d^2 elements of the d -dimensional Pauli group,² where we omit repeated summation when two

²The properties of the d -dimensional Pauli group were extensively studied in [36]. We will not use any further special properties of this group and refer the interested reader to [36] for further information.

elements in the Pauli group differ merely by a phase factor. We note there is a simple extension of Eq. (8) for multiple-qudit systems,

$$\sum_{U_p^{(j)}} (U_p^{(1)} \otimes \cdots \otimes U_p^{(n)}) J(U_p^{(1)} \otimes \cdots \otimes U_p^{(n)})^\dagger = D \operatorname{tr}(J) I^{\otimes n}, \quad (9)$$

where the superscripts indicate the different qudit systems, of respective dimension $d^{(j)}$, $D=d^{(1)}, \dots, d^{(n)}$ is the dimension of the combined system, I represents the appropriate identity operator for each subsystem, and the sum is over conjugations by all elements of the Pauli group for each qudit, again omitting repeated sums over elements that are the same up to a phase factor.

We define the simulation $\mathcal{D}[H]=H_D$ to be the multiple-qudit depolarizing channel acting on the $n-k$ qudits that are not coupled by H_α ,

$$\begin{aligned} \mathcal{D}[H] &= \sum_{U_p^{(j)}} (U_p^{(k+1)} \otimes \cdots \otimes U_p^{(n)}) H(U_p^{(k+1)} \otimes \cdots \otimes U_p^{(n)})^\dagger \\ &= H_D. \end{aligned} \quad (10)$$

H_α acts on the first k qudits of an n -qudit system, that is, the set S_α . If we examine the simulated Hamiltonian, H_D , we find from Equation (9) that any terms H_β in H that act non-trivially on qudits outside the set S_α are eliminated. The simulation leaves the coupling term H_α unchanged except for an unimportant positive scaling factor. Thus we have removed all the case 1 terms H_β from the Hamiltonian, and need only consider the remaining case 2 and case 3 terms.

B. Case 2

The Hamiltonian H_D is a linear combination of terms that couple the set of qudits S_α or some subset of S_α . It turns out that we can use another extension of Eq. (8) to simulate a Hamiltonian, H_T , that only has terms that couple the set S_α . In Eq. (8), if J is a traceless operator we find that the right-hand side of the equation is zero. Noting that I is an element of the Pauli group, we find

$$\sum_{U_p \neq I} U_p J U_p^\dagger = -J, \quad (11)$$

which always holds for traceless J . Using single-qudit unitaries from the Pauli group we consider the following summation:

$$\sum_{U_p^{(1)} \neq I, U_p^{(2)} \neq I} (U_p^{(1)} \otimes U_p^{(2)}) (J^{(1)} \otimes J^{(2)}) (U_p^{(1)} \otimes U_p^{(2)})^\dagger. \quad (12)$$

If $J^{(1)}$ and $J^{(2)}$ are traceless, this expression is equal to $J^{(1)} \otimes J^{(2)}$. If $J^{(2)}$ is traceless and $J^{(1)}$ is the identity, this expression is equal to $-(d^{(1)})^2 - 1 I \otimes J^{(2)}$. With this in mind we define a simulation:

$$\begin{aligned} \mathcal{T}^{(j)}[H] &\equiv ((d^{(j)})^2 - 1)H \\ &+ \sum_{U_p^{(1)}, U_p^{(j)} \neq I} (U_p^{(1)} \otimes U_p^{(j)}) H (U_p^{(1)} \otimes U_p^{(j)})^\dagger. \end{aligned} \quad (13)$$

Performing $\mathcal{T}^{(j)}$ for $j=2, \dots, k$, only terms that couple the same qudits as H_α are not eliminated. So performing the following sequence of simulations,

$$\mathcal{T}[H_D] = \mathcal{T}^{(k)}[\mathcal{T}^{(k-1)}[\cdots[\mathcal{T}^{(2)}[H_D]]\cdots]] = H_T \quad (14)$$

the simulated Hamiltonian, H_T , is a linear combination of terms that couple the same qudits as H_α .

C. Case 3

We have shown how to simulate a Hamiltonian H_T that only contains terms which couple the same qudits as H_α . To eliminate the remaining terms we define the following operators that are both unitary and Hermitian:

$$Z_a \equiv I - 2|a\rangle\langle a| = \sum_{j=1}^d |j\rangle\langle j| - 2|a\rangle\langle a|. \quad (15)$$

Notice that the Z_a operators commute with each of the Cartan subalgebra elements, W_m , in Eq. (3). Hence, each of the Z_a will also commute with H_α as it is a tensor product of elements of the Cartan subalgebra. Further notice that Z_a anti-commutes with X_{lm} and Y_{lm} if $a=l$ or $a=m$ and commutes otherwise. We can use this fact to define a simulation that eliminates terms with X_{lm} and Y_{lm} operators present in H_T . We define a simulation

$$\mathcal{Z}_a^{(j)}[H] = H + Z_a^{(j)} H Z_a^{(j)}, \quad (16)$$

where the superscript j indicates a Z_a operator acting on the j th qudit, with identities acting elsewhere. If there exists any term with an X_{lm} or Y_{lm} operator on the j th qudit, and such that $a=l$ or $a=m$, then this term will be eliminated from H_T by the simulation $\mathcal{Z}_a^{(j)}[H_T]$. Expanding on this idea we can eliminate every term on the j th qudit that has the form X_{lm} or Y_{lm} by performing the following simulation:

$$\mathcal{Z}^{(j)}[H_T] \equiv \mathcal{Z}_d^{(j)}[\mathcal{Z}_{(d-1)}^{(j)}[\cdots[\mathcal{Z}_1^{(j)}[H_T]]\cdots]], \quad (17)$$

where d is the dimension of the j th qudit. The effect of this simulation on H_α is simply to rescale it. Now, if we perform the simulation $\mathcal{Z}^{(j)}$ for each qudit in S_α ,

$$\mathcal{Z}[H_T] = \mathcal{Z}^{(k)}[\mathcal{Z}^{(k-1)}[\cdots[\mathcal{Z}^{(1)}[H_T]]\cdots]] = H_Z, \quad (18)$$

all that remains in the newly simulated Hamiltonian, H_Z , is a linear combination of terms that commute with the Cartan subalgebra elements. We have now simulated a Hamiltonian with no X - and Y -type terms.

H_Z is a linear combination of terms that are tensor products of operators from the Cartan subalgebra. Consider the unitary representation, $P^{(j)}(\pi)$, of the permutation group S_{b_j-1} that permutes the elements of the diagonal basis of the Cartan subalgebra, $|a\rangle$, for $a=1, \dots, b_j-1$ on the j th qudit. When $a \geq b_j$ we have $P^{(j)}(\pi) W_a P^{(j)\dagger}(\pi) = W_a$. When $a < b_j$,

we find that the effect of conjugating W_a by a permutation operation is to shift around the diagonal elements of W_a . Now, we can eliminate any terms in H_Z that contain an operator $W_a^{(j)}$ with $a < b_j$ by performing the simulation

$$\mathcal{P}^{(j)}[H_Z] = \sum_{\pi \in S_{b-1}} \mathcal{P}^{(j)} H_Z \mathcal{P}^{(j)\dagger}. \quad (19)$$

This works because $W_a^{(j)}$ is a diagonal, traceless operator and the permutation, $\mathcal{P}^{(j)}$, distributes each of the diagonal elements of $W_a^{(j)}$ equally. The effect of $\mathcal{P}^{(j)}$ on terms $W_a^{(j)}$ acting on the j th qudit and with $a \geq b_j$ is to simply scale them by a factor of $(b_j - 1)!$. Performing the following simulation,

$$\mathcal{P}[H_Z] = \mathcal{P}^{(k)}[\mathcal{P}^{(k-1)}[\dots[\mathcal{P}^{(1)}[H_Z]]\dots]] = H_P, \quad (20)$$

we produce a Hamiltonian H_P that is a linear combination of terms that couple the same qudits as H_α and are tensor products of operators W_a with $a \geq b_j$.

In Sec. II C we pointed out that it is possible to simulate a Hamiltonian proportional to the commutator of two Hamiltonians that are both simulatable. Now, we note that the commutator $-i[W_a^{(j)}, X_{b_j-1b_j}] = 0$ if $a > b_j$. If $a = b_j$ we find $-i[W_{b_j}^{(j)}, X_{b_j-1b_j}] = (\sqrt{b_j}/\sqrt{b_j-1})Y_{b_j-1b_j}$. We can make use of this distinction to find a way to remove the unwanted terms from H_P . We define the simulation

$$\mathcal{X}^{(j)}[H] \equiv -i[H, X_{b_j-1b_j}^{(j)}]. \quad (21)$$

Then if we perform the following sequence of simulations,

$$\mathcal{X}[H_P] = \mathcal{X}^{(k)}[\mathcal{X}^{(k-1)}[\dots[\mathcal{X}^{(1)}[H_P]]\dots]] = H_X, \quad (22)$$

we find that $H_X = (\otimes_{j=1}^k Y_{b_j-1, b_j}) \otimes I^{\otimes n-k}$, up to some unimportant but nonzero constant multiple. We have now simulated a single coupling term that couples the same qudits as H_α . Recall in Sec. II D we noted that a coupling term can be used with single-qudit unitaries to simulate any other term coupling the same set of qudits. So, we can use H_X and single-qudit unitaries to simulate H_α , the desired term. Thus we have demonstrated that it is possible to isolate H_α from H .

IV. SIMULATING NEW COUPLING TERMS

Term isolation shows that the ability to simulate a Hamiltonian $H = \sum_\alpha h_\alpha H_\alpha$ is equivalent to the ability to simulate the set of coupling Hamiltonians, $\{H_\alpha\}$, given single-qudit unitary operations. Additionally, we learned in Sec. II D that given H_α and single-qudit unitaries we can simulate any coupling term that couples the same qudits as H_α . So far we have not presented any way of simulating some coupling term that couples a different set of qudits than any of the terms in the set $\{H_\alpha\}$. In this section we will take a key step towards a proof of universality, showing how to use single-qudit unitaries and a term H_α coupling k qudits in order to simulate a term that couples $k-1$ qudits.

A. Evaluation of commutators

In [29] it was shown that if H_α coupled qubits, its capacity to simulate other coupling terms depended on the number of

qubits that it coupled. More specifically, it was shown that if H_α coupled k qubits and k was an odd number, then H_α could not be used with single-qubit unitaries to simulate a coupling term that coupled $k-1$ qubits. One way of seeing why this is true is to examine the commutator of two Hamiltonians, $[H_\alpha, H_\beta]$, that couple the same set of qubits S_α . It is easy to show that the commutator $[H_\alpha, H_\beta] \neq 0$ if and only if there are an odd number of locations in S_α where H_α and H_β differ. From this restriction it is possible to prove, as was done in [29], that coupling terms coupling an odd number of qubits can only ever simulate other Hamiltonians that have odd couplings.

What is different when not all the systems are qubits? The purpose of this subsection is to investigate the commutator of two specially chosen couplings H_α and H_β that couple the same set of qudits, S_α . In the case of qubits, it is not difficult to convince oneself that when S_α contains an *even* number of qubits, the commutator $[H_\alpha, H_\beta]$ is either zero, or else couples a set of qubits that is a *strict* subset of the original set S_α . We will show by an explicit calculation that when one or more of the systems is not a qubit, it is possible to choose H_α and H_β so that the commutator $[H_\alpha, H_\beta]$ contains terms coupling the entire set S_α . Remarkably, we will see in the remainder of the paper that this is the key fact that simplifies the study of universality when not all the systems are qubits.

We begin by choosing $H_\alpha = \otimes_{j=1}^k X_{ab}^{(j)}$ and $H_\beta = \otimes_{j=1}^k X_{ab'}^{(j)}$, where for all j we set $b \neq b'$. (We assume initially that all systems are of dimension 3 or greater.) Given these forms for H_α and H_β , what does $[H_\alpha, H_\beta]$ look like? We find

$$[H_\alpha, H_\beta] = \bigotimes_{j=1}^k \frac{1}{2\sqrt{2}} (X_{bb'}^{(j)} + iY_{bb'}^{(j)}) - \bigotimes_{j=1}^k \frac{1}{2\sqrt{2}} (X_{bb'}^{(j)} - iY_{bb'}^{(j)}). \quad (23)$$

This expression contains Hermitian and skew-Hermitian terms. Upon expansion of the above expression we find that all of the Hermitian terms sum to zero, leaving only a sum of skew-Hermitian terms remaining. These terms correspond to a sum of tensor product terms containing odd numbers of $Y_{bb'}$ terms. All of the terms couple the entire set S_α . It is easy to verify that this sum is always nonzero, simply by inspection of the coefficients of the relevant terms.

So far we have only considered the case where we could choose to simulate H_α and H_β for $X_{ab}^{(j)}$ and $X_{ab'}^{(j)}$, $b \neq b'$. We can only do this when each subsystem has dimension $d > 2$. If we have subsystems where $d=2$, the situation changes slightly, but the results are similar, provided not all of the subsystems are qubits.

For every j where the qudit has dimension $d > 2$ we choose $H_\alpha^{(j)} = X_{ab}^{(j)}$ and $H_\beta^{(j)} = X_{ab'}^{(j)}$, with $b \neq b'$. For every j where the qudit has dimension $d=2$, we choose $H_\alpha^{(j)} = X$, and $H_\beta^{(j)} = Y$. Provided H_α and H_β do not couple qubits exclusively, a straightforward calculation along lines similar to that already done shows that $[H_\alpha, H_\beta]$ is a nonzero sum of terms, each of which is skew-Hermitian and couples all k qudits. The only subtlety in the calculation is the need to analyze separately the cases where there are an *even* number

of qubits in the set S_α , which gives rise to a commutator which is a nonzero sum of tensor product terms containing an odd number of $Y_{bb'}$ terms, and the case where there are an *odd* number of qubits in the set S_α , which gives rise to a commutator which is a nonzero sum of tensor product terms containing an even number of $Y_{bb'}$ terms.

B. Simulating identity operators

Given some term, H_α , coupling a set of qudits S_α , we show how the results on commutators just obtained allow us to simulate other coupling term that couples a subset of S_α with just one qudit removed, more precisely, as follows.

Lemma 1. Given the ability to evolve via $H_\alpha = \otimes_{j=1}^n H_\alpha^{(j)}$, which couples k qudits, and local unitary operations, it is possible to simulate H' such that

$$H' = I \otimes H_\gamma, \quad (24)$$

provided H_α does not couple qubits exclusively. The coupling term H_γ may couple any $k-1$ qudit subset of S_α , subject to the constraint that the subset not be qubits exclusively.

Proof. Given H_α we can simulate any other coupling term, $H_\beta = \otimes_{j=1}^n H_\beta^{(j)}$, that acts nontrivially on the same set of k qudits, S_α . We label the qudits so that S_α consists of qudits $1, \dots, k$, and so that our goal is to simulate a coupling on qudits $2, \dots, k$, i.e., the goal is to remove qudit 1. To this end, we choose $H_\beta^{(1)}$ so that $H_\alpha^{(1)} = H_\beta^{(1)}$. Note that, by assumption, the set $2, \dots, k$ does not contain qubits exclusively. Evaluating the commutator, we find

$$i[H_\alpha, H_\beta] = i(H_\alpha^{(1)})^2 \otimes \left[\bigotimes_{j=2}^n H_\alpha^{(j)}, \bigotimes_{j=2}^n H_\beta^{(j)} \right]. \quad (25)$$

We note that $(H_\alpha^{(1)})^2$ is a positive operator and thus is not traceless. Hence, if we apply the depolarizing channel, Eq. (8), to the first qudit we can simulate an identity term acting on the first qudit. If we do this and set $N \equiv \otimes_{j=2}^n H_\alpha^{(j)}$, $N' \equiv \otimes_{j=2}^n H_\beta^{(j)}$ we simulate

$$H' = iI \otimes [N, N']. \quad (26)$$

Finally, we note that as N and N' don't act exclusively on qubits, our earlier results on commutators show that we can ensure that $[N, N']$ is a nonzero linear combination of terms that couple S_α , less the first qudit. Term isolation allows us to simulate one of the coupling terms in $[N, N']$ alone, i.e., $H'' = I \otimes H_\gamma$, as required. ■

V. UNIVERSALITY

Theorem 1 stated that if a set of qudits is *connected* by a Hamiltonian, H , with two-body interactions, then evolutions by H and single-qudit unitaries form a universal set of operations on that set of qudits [10]. A set of 2-qudit coupling terms connecting the same set of qudits is also universal as they can simulate a two-body Hamiltonian on the set of qudits. We prove in this section the main result of this paper: that a generic Hamiltonian, H , entangling a set of qudits can simulate a set of 2-qudit coupling terms connecting the qudits, and is thus universal. The only exception to this rule is

the case where H is a sum of odd coupling terms, as discussed in [29], and summarized in theorems 2 and 3 in the present paper.

We begin by proving theorem 5, which shows that a coupling term, H_α , that couples a set of k qudits, S_α , can be used to simulate a set of 2-qudit couplings that connect the set S_α . This implies that H_α and single-qudit unitaries are a universal set on the qudits S_α . We conclude with theorem 6, showing that an arbitrary entangling Hamiltonian on n qudits is universal for the qudits it entangles.

A. Theorem 5: Using a term coupling many qudits to simulate a term coupling two qudits

Theorem 5. Suppose $H_\alpha = \otimes_{j=1}^n H_\alpha^{(j)}$ couples k qudits. Then H_α and single-qudit unitary operations can be used to simulate a set of two-qudit couplings connecting every qudit coupled by H_α , provided H_α does not couple qubits exclusively, and $k > 1$. Thus H_α and single-qudit unitaries are universal on the set of qudits coupled by H_α .

Proof. Without loss of generality we may label the systems so that H_α couples systems 1 through k , and system 1 is not a qubit. Fix j in the range 2 through k . Applying lemma 1 repeatedly, we see that we can simulate a Hamiltonian coupling system 1 and system j . It follows that H_α and single-qudit unitaries are universal on the set of qudits coupled by H_α . ■

B. Theorem 6: Which Hamiltonians are universal?

With Theorem 5 in mind, we now prove that the only nonuniversal set of entangling Hamiltonians is the set of odd Hamiltonians acting on qubits alone.

Theorem 6. Single-qudit unitary operations, and evolutions via a Hamiltonian, H , that connects a set of n qudits, is a universal set of operations on those n qudits if and only if H is not an odd Hamiltonian acting on qubits alone.

Proof. The forward implication follows from Theorem 2, as does the reverse implication when all systems are qubits. Thus, all that needs proof is the reverse implication in the case when H is an entangling Hamiltonian that does not act exclusively on qubits. We will show how to construct a set of two-body couplings that connect all n qudits.

To construct this set, begin by picking a system that is not a qubit, and label it system 1. We will explain how to construct a set, S , of systems to which 1 can be coupled via a two-body interaction. We begin by setting $S = \{1\}$, and aim to add in other systems that can be coupled to 1 via two-body interactions. Our strategy is to show that provided S is not yet maximal, i.e., does not yet contain all n qudits, then it is always possible to add an extra qudit into S .

To see this, suppose S is not yet maximal. Then it is always possible to pick a qudit j inside S and a qudit k outside of S such that H contains a coupling term H_{jk} which couples systems j and k . (Other systems may also be coupled by H_{jk} .) In the case when either j or k is not a qubit, theorem 5 shows that a term coupling just j and k may be simulated. Theorem 1 implies that we can also simulate a term coupling system 1 and k , and so system k may be added to S .

The other possible case is when j and k are both qubits. In this case, suppose without loss of generality that H_{jk} has the form $X^{(j)} \otimes X^{(k)} \otimes \dots$, where the superscripts label the systems. We may also simulate the coupling $X_{12}^{(1)} \otimes Z^{(j)}$, since system j is in S . Taking the commutator of these two couplings, we see that we may simulate couplings of the form $X_{12}^{(1)} \otimes Y^{(j)} \otimes X^{(k)} \otimes \dots$. Applying Theorem 5, we see that it is possible to simulate a two-body coupling between system 1 and k , and thus system k may be added to S . ■

VI. CONCLUSION

We have demonstrated that many-qudit Hamiltonians combined with local unitary operations are always universal for simulation on any connected set of subsystems upon which the interactions act nontrivially, *provided* that Hamiltonian is not an odd Hamiltonian acting on qubits. This result is rather intriguing and elegant, especially in the light of the general lack of broad results for many-body (as opposed to two-body) problems in quantum information science. In the study of pure state bipartite entangled states, for example, a single unit of currency, the maximally entangled state, has been identified and the fungible nature of this currency has been established. On the other hand, a similar currency and set of fungible transformations has not been identified for systems consisting of more than two parties. Given this difficulty in understanding the structure of quantum states, it is

quite remarkable that, with the exception of odd entangling Hamiltonians, all of the different many-qudit interactions are equivalent. Even in the case of odd entangling Hamiltonians, universal simulation can be achieved using an encoding which wastes only a single extra qubit of space [29]. Thus there is a real sense in which, for simulation, all interactions have been created equal.

Part of the simplicity of our result stems from our focus on universality for simulation as opposed to universality for quantum computation, which requires that issues of *efficiency* be taken into account. When one adds the requirement of efficiency of simulation, then problems of universality become much more difficult: indeed this is perhaps one of the fundamental problems in the study of the computational complexity of quantum circuits. A well-developed theory of efficient simulation is a task of great importance and, judging from the difficulties encountered in proving lower bounds for problems in classical circuit complexity, this task is probably an immensely difficult problem. This paper can be seen, however, as a necessary precursor to any attempt to advance this program.

ACKNOWLEDGMENTS

We thank Jennifer Dodd, Henry Haselgrove, and Andrew Hines for checking this manuscript and helpful discussions. This work was supported in part by the National Science Foundation under Grant. No. EIA-0086038.

-
- [1] R. P. Feynman, *Int. J. Theor. Phys.* **21**, 467 (1982).
 - [2] R. Somma, G. Ortiz, J. E. Gubernatis, E. Knill, and R. Laflamme, *Phys. Rev. A* **65**, 042323 (2002).
 - [3] J. L. Dodd, M. A. Nielsen, M. J. Bremner, and R. T. Thew, *Phys. Rev. A* **65**, 040301(R) (2002).
 - [4] P. Wocjan, D. Janzing, and T. Beth, *Quantum Inf. Comput.* **2**, 117 (2002).
 - [5] C. H. Bennett, J. I. Cirac, M. S. Leifer, D. W. Leung, N. Linden, S. Popescu, and G. Vidal, *Phys. Rev. A* **66**, 012305 (2002).
 - [6] D. W. Leung, *J. Mod. Opt.* **49**, 1199 (2002).
 - [7] W. Dür, G. Vidal, J. I. Cirac, N. Linden, and S. Popescu, *Phys. Rev. Lett.* **87**, 137901 (2001).
 - [8] M. A. Nielsen, M. J. Bremner, J. L. Dodd, A. M. Childs, and C. M. Dawson, *Phys. Rev. A* **66**, 022317 (2002).
 - [9] P. Wocjan, M. Roetteler, D. Janzing, and T. Beth, *Quantum Inf. Comput.* **2**, 133 (2002).
 - [10] P. Wocjan, M. Rötteler, D. Janzing, and T. Beth, *Phys. Rev. A* **65**, 042309 (2002).
 - [11] G. Vidal and J. I. Cirac, *Phys. Rev. A* **66**, 022315 (2002).
 - [12] G. Vidal and J. I. Cirac, *Phys. Rev. Lett.* **88**, 167903 (2002).
 - [13] N. Khaneja, R. Brockett, and S. J. Glaser, *Phys. Rev. A* **63**, 032308 (2001).
 - [14] N. Khaneja, S. J. Glaser, and R. Brockett, *Phys. Rev. A* **65**, 032301 (2002).
 - [15] M. J. Bremner, C. M. Dawson, J. L. Dodd, A. Gilchrist, A. W. Harrow, D. Mortimer, M. A. Nielsen, and T. J. Osborne, *Phys. Rev. Lett.* **89**, 247902 (2002).
 - [16] G. Vidal, K. Hammerer, and J. I. Cirac, *Phys. Rev. Lett.* **88**, 237902 (2002).
 - [17] K. Hammerer, G. Vidal, and J. I. Cirac, *Phys. Rev. A* **66**, 062321 (2002).
 - [18] S. S. Bullock and I. L. Markov, *Phys. Rev. A* **68**, 012318 (2003).
 - [19] J. Zhang, J. Vala, S. Sastry, and K. B. Whaley, *Phys. Rev. Lett.* **91**, 027903 (2003).
 - [20] J. Zhang, J. Vala, S. Sastry, and K. B. Whaley, e-print quant-ph/0312193.
 - [21] H. L. Haselgrove, M. A. Nielsen, and T. J. Osborne, *Phys. Rev. A* **68**, 042303 (2003).
 - [22] A. M. Childs, H. L. Haselgrove, and M. A. Nielsen, *Phys. Rev. A* **68**, 052311 (2003).
 - [23] V. V. Schende, I. L. Markov, and S. S. Bullock, *Phys. Rev. A* **69**, 062321 (2004).
 - [24] V. V. Schende, S. S. Bullock, and I. L. Markov, *Phys. Rev. A* **70**, 012310 (2004).
 - [25] G. Vidal and C. M. Dawson, *Phys. Rev. A* **69**, 010301(R) (2004).
 - [26] F. Vatan and C. Williams, *Phys. Rev. A* **69**, 032315 (2004).
 - [27] R. Zeier, M. Grassl, and T. Beth, *Phys. Rev. A* **70**, 032319 (2004).
 - [28] C. D. Hill and H.-S. Goan, *Phys. Rev. A* **68**, 012321 (2003).
 - [29] M. J. Bremner, J. L. Dodd, M. A. Nielsen, and D. Bacon, *Phys. Rev. A* **69**, 012313 (2003).

- [30] S. S. Bullock and G. K. Brennen, *J. Math. Phys.* **45**, 2447 (2004).
- [31] S. S. Bullock, G. K. Brennen, and D. P. O'Leary, e-print quant-ph/0402051.
- [32] A. Mizel and D. A. Lidar, *Phys. Rev. Lett.* **92**, 077903 (2004).
- [33] J. K. Pachos and M. B. Plenio, *Phys. Rev. Lett.* **93**, 056402 (2004).
- [34] J. K. Pachos and E. Rico, *Phys. Rev. A* **70**, 053620 (2004).
- [35] A. Uhlmann, *Wiss. Z.-Karl-Marx-Univ. Leipzig, Math.-Naturwiss. Reihe* **20**, 633 (1971).
- [36] D. Gottesman, in *Quantum Computing and Quantum Communications: First NASA International Conference*, edited by C. P. Williams (Springer-Verlag, New York, 1999), e-print quant-ph/9802007.