

Universal simulation of Markovian quantum dynamics

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Although the conditions for performing arbitrary unitary operations to simulate the dynamics of a closed quantum system are well understood, the same is not true of the more general class of quantum operations (also known as superoperators) corresponding to the dynamics of open quantum systems. We propose a framework for the generation of Markovian quantum dynamics and study the resources needed for universality. For the case of a single qubit, we show that a single nonunitary process is necessary and sufficient to generate all unital Markovian quantum dynamics, whereas a set of processes parametrized by one continuous parameter is needed in general. We also obtain preliminary results for the unital case in higher dimensions.

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I. INTRODUCTION

The idea of simulating one quantum system with another was first suggested in the early 1980s by Manin [1] and Feynman [2]. A universal quantum computer can perform such simulation because of its ability to apply arbitrary unitary transformations to arbitrary quantum states. The only necessary resources are single-qubit gates and the controlled-NOT (CNOT) two-qubit gate [3]. In fact, the CNOT may be replaced by nearly any two-qubit interaction [4], and the single-qubit gates can be reduced to a finite set [5]. Finiteness of the gate set is desirable because it reduces the necessary computational resources and simplifies the construction of fault tolerant gates.

Using a universal gate set, a quantum computer may simulate the time sequence of operations corresponding to any unitary dynamics. Such simulation is provably efficient [6] and has been implemented in the context of nuclear magnetic resonance quantum computation [7].

However, quantum systems may undergo interesting processes that are not unitary due to interactions with their environments. The evolution of such *open quantum systems* is described by *quantum operations* (or superoperators). Understanding such dynamics is important for studying quantum noise processes [8], designing quantum error correcting codes [9], and performing simulations of open quantum systems, such as of thermal equilibration [10].

Clearly, creation of arbitrary quantum operations and simulation of arbitrary quantum dynamics using a simple set of primitives are desirable goals. However, it is more difficult to describe a notion of universality for general quantum operations than for unitary operations alone. Unlike unitary operations, which form a Lie group, quantum operations comprise a semigroup due to their irreversibility. The lack of inverse operations for semigroups is troublesome, and it is

less obvious how best to combine quantum operations to form new ones.

A simple recipe for implementing a general quantum operation follows from its unitary representation: any quantum operation may be written as a unitary operation on an extended system with a trace over the extra degrees of freedom. As is well known, this procedure only requires an ancillary system of dimension equal to the square of the dimension of the system of interest to produce arbitrary quantum operations. However, our goal is to consider as a resource a small subset of nonunitary quantum dynamics applied to the system only, without the need to control the extra degrees of freedom. Such restrictions are important in many applications, including the experimental simulation of quantum systems. For this reason, we exclude the technique arising from the unitary representation when building arbitrary nonunitary quantum dynamics.

In this paper, we begin to study possible methods for simulating the dynamics of open quantum systems by some time sequence of operations. We take the approach of considering only processes that result from interaction with a Markovian environment in the Born approximation. We refer to this class of dynamics as *Markovian quantum dynamics* and refer to the semigroup they comprise as a *Markovian semigroup*. Such processes have a convenient description in terms of their *generators*, a concept analogous to the Hamiltonian of unitary dynamics. Therefore, simulation of Markovian quantum dynamics is reduced to building generators for Markovian semigroups.

We define two allowed procedures for transforming semigroup generators, *linear combination* and *unitary conjugation*. Using these procedures, we show how to build more complicated generators from simple ones, and we explore in detail the required resources for the case of a single quantum bit.

The structure of the paper is as follows. In Sec. II we present representations of quantum operations and the description of Markovian quantum dynamics in terms of semigroups. Then, in Sec. III, we describe the procedures of linear combination and unitary conjugation. Using these procedures, we present universal sets of generators for unital Markovian quantum dynamics on a qubit in Sec. IV and for general Markovian quantum dynamics on a qubit in Sec. V. Finally, we conclude with some open questions and directions for further investigation.

II. QUANTUM OPERATIONS AND MARKOVIAN SEMIGROUPS

A quantum state is described by a density matrix ρ , which is positive semidefinite and has $\text{tr}\rho = 1$. The most general state change of a quantum system, a quantum operation, is a linear map \mathcal{E} that is trace preserving and completely positive. \mathcal{E} acts on ρ to produce a state $\mathcal{E}(\rho)$. There are many representations for such a map. The operator sum representation

$$\mathcal{E}(\rho) = A_k \rho A_k^\dagger \quad (1)$$

(note that we use Einstein summation where appropriate)—and its corresponding fixed-basis form [11]—is convenient because the constraints of trace preservation and complete positivity may be simply expressed. For example, complete positivity is inherent in Eq. (1) and trace preservation is equivalent to $A_k^\dagger A_k = I$, where I is the identity matrix. However, the composition of two operator sum representations is complicated, usually resulting in a rapidly increasing number of terms. On the other hand, a manifestly linear representation

$$(\mathcal{E}(\rho))_{ab} = M_{(ab)(cd)} \rho_{cd} \quad (2)$$

(where M is a matrix with composite indices) makes the composition of operations trivial, yet obfuscates the constraints [12].

Instead of considering all possible dynamics, we will simplify the problem by focusing on Markovian quantum dynamics. We describe these processes informally here, saving a more complete presentation based on [14–16] for Appendix A. Every such process corresponds to some interaction, which, if applied for a duration t , induces a quantum operation \mathcal{E}_t . The class of quantum operations \mathcal{E}_t forms a Markovian semigroup. The time t may vary continuously. The operations must be stationary and Markovian, such that

$$\mathcal{E}_s \mathcal{E}_t = \mathcal{E}_{s+t}. \quad (3)$$

Here $\mathcal{E}_s \mathcal{E}_t$ denotes composition of the operations, i.e., $\mathcal{E}_s \circ \mathcal{E}_t$. Each Markovian semigroup describes the dynamics resulting from some interaction with a Markovian environment in the Born approximation.

Note that this terminology differs slightly from that used elsewhere. For example, Davies does not include the constraint of trace preservation when defining a Markov semigroup in [14] and, curiously, uses “Markov” to mean “uni-

tal” in [15]. For a precise definition of Markovian semigroups as used in this paper, see Appendix A.

The advantage of considering only Markovian semigroups is that they are uniquely determined by their generators. The generator \mathcal{Z} of \mathcal{E}_t is defined by its action on an arbitrary input ρ ,

$$\mathcal{Z}(\rho) = \lim_{t \downarrow 0} \frac{\mathcal{E}_t(\rho) - \rho}{t}. \quad (4)$$

In a sense, \mathcal{Z} can be thought of as the “Hamiltonian” corresponding to \mathcal{E}_t . Exponentiation gives

$$\mathcal{E}_t = e^{\mathcal{Z}t} \equiv \lim_{n \rightarrow \infty} \left(\mathcal{I} - \frac{t}{n} \mathcal{Z} \right)^{-n}, \quad (5)$$

where \mathcal{I} is the identity quantum operation. The generator also satisfies the differential equation

$$\frac{\partial \rho(t)}{\partial t} = \mathcal{Z}(\rho(t)), \quad (6)$$

which is known as a *master equation*. Through this analysis, simulating $\mathcal{E}_t \forall t \geq 0$ is reduced to simulating its generator.

Gorini, Kossakowski, and Sudarshan have shown that \mathcal{Z} is the generator of a Markovian semigroup on an N -dimensional Hilbert space if and only if it can be written in the form [17]

$$\mathcal{Z}(\rho) = -i[H, \rho] + a_{\alpha\beta}([F_\alpha \rho, F_\beta^\dagger] + [F_\alpha, \rho F_\beta^\dagger]), \quad (7)$$

where $a_{\alpha\beta}$ is an $(N^2 - 1) \times (N^2 - 1)$ positive matrix (with $\alpha, \beta \in [1, N^2 - 1]$) and $\{F_\alpha\}$ is a linear basis of traceless operators on the density matrices. We refer to the matrix $a_{\alpha\beta}$ as the “GKS matrix.” For related formulations, such as the “diagonal” form introduced by Lindblad (which also applies to countably infinite-dimensional systems), see [16, 18]. Physically, H corresponds to unitary dynamics that can be produced by a system Hamiltonian, as well as unitary dynamics induced by a coupling between the system and the bath—the so-called Lamb shift.

It will greatly simplify the discussion to choose a Hermitian basis that is orthonormal under the trace norm. Such a basis is assumed for the rest of the paper. Therefore,

$$\text{tr}(F_\alpha F_\beta^\dagger) = \delta_{\alpha\beta}, \quad (8)$$

and $\text{tr}(F_\alpha) = 0$. Note that we can always reduce a GKS matrix, which is expressed in an overcomplete or nonorthonormal traceless basis, to a representation involving a linearly independent orthonormal traceless basis.

There are other ways to describe the generator of a Markovian semigroup. For example, $\mathcal{Z}(\rho)$ may always be written as an affine transformation of ρ , just as any quantum operation can be written as a linear transformation as in Eq. (2). In this paper, we find it simplest to represent generators by the GKS matrix, and we describe the relationship between the GKS matrix and the affine representation in Appendix B.

To make our description of Markovian quantum dynamics concrete, we present some important examples of qubit noise

processes [19]. We choose the basis $\{F_\alpha\}$ to be the normalized Pauli operators $(1/\sqrt{2})\{\sigma_x, \sigma_y, \sigma_z\}$, and we write the density matrix of a qubit as

$$\rho = \begin{pmatrix} \rho_{00} & \rho_{01} \\ \rho_{10} & \rho_{11} \end{pmatrix}. \quad (9)$$

The first process, *phase damping*, acts on a qubit as

$$\mathcal{E}_t^{\text{PD}}(\rho) = \begin{pmatrix} \rho_{00} & e^{-\gamma t} \rho_{01} \\ e^{-\gamma t} \rho_{10} & \rho_{11} \end{pmatrix}, \quad (10)$$

where γ is a decay constant and t is the duration of the process. The generator has a GKS matrix with $a_{33}^{\text{PD}} = \gamma/2$ and all other $a_{\alpha\beta}^{\text{PD}} = 0$. The second example is the *depolarizing channel*, which acts on a qubit as

$$\mathcal{E}_t^{\text{DEP}}(\rho) = \begin{pmatrix} \frac{1 + e^{-\tilde{\gamma}t}(\rho_{00} - \rho_{11})}{2} & e^{-\tilde{\gamma}t} \rho_{01} \\ e^{-\tilde{\gamma}t} \rho_{10} & \frac{1 + e^{-\tilde{\gamma}t}(\rho_{11} - \rho_{00})}{2} \end{pmatrix}. \quad (11)$$

Its GKS matrix has the nonzero elements $a_{11}^{\text{DEP}} = a_{22}^{\text{DEP}} = a_{33}^{\text{DEP}} = \tilde{\gamma}/4$. Our final example is *amplitude damping*, which acts on a qubit as

$$\mathcal{E}_t^{\text{AD}}(\rho) = \begin{pmatrix} \rho_{00} + (1 - e^{-\Gamma t})\rho_{11} & e^{-\Gamma t/2} \rho_{01} \\ e^{-\Gamma t/2} \rho_{10} & e^{-\Gamma t} \rho_{11} \end{pmatrix}. \quad (12)$$

The GKS matrix $a_{\alpha\beta}^{\text{AD}}$ is given by

$$\frac{\Gamma}{4} \begin{pmatrix} 1 & -i & 0 \\ i & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}. \quad (13)$$

Note that the GKS matrix is real and diagonal for phase damping and the depolarizing channel and has rank 1 for phase damping and amplitude damping.

III. COMPOSITION FRAMEWORK: LINEAR COMBINATION AND UNITARY CONJUGATION

Recall that our goal is to find a simple way of combining as few primitive \mathcal{E}^i as possible to produce all possible \mathcal{E} via some time sequence of operations. To make this problem well posed, we must choose reasonable methods for composing quantum operations to make new ones. We have not found a simple way to express the composition of two semigroup processes of finite duration, and such composition need not preserve Markovity. However, a natural way to combine semigroup processes is by a procedure we call *linear combination*: the processes act one after another for small amounts of time. In the limit of infinitesimal time steps, two processes \mathcal{E}_t^a and \mathcal{E}_t^b can be combined to produce

$$\mathcal{E}_t^{a+b} \equiv \lim_{n \rightarrow \infty} (\mathcal{E}_{t/n}^a \mathcal{E}_{t/n}^b)^n, \quad (14)$$

where \mathcal{E}_t^{a+b} forms a Markovian semigroup if \mathcal{E}_t^a and \mathcal{E}_t^b do. Moreover, if \mathcal{E}_t^a and \mathcal{E}_t^b have generators \mathcal{A} and \mathcal{B} , then applying the Lie product formula to the generators,

$$\lim_{n \rightarrow \infty} (e^{At/n} e^{Bt/n})^n = e^{(A+B)t}. \quad (15)$$

In other words, the generator of a process formed by linear combination is the sum of the constituent generators. The generalization to produce a positive sum of any finite number of generators is straightforward. When all generators are expressed in the form of Eq. (7) using the same basis $\{F_\alpha\}$ (as we assume for the rest of the paper), linear combination corresponds to a positive sum of the GKS matrices of the constituent generators.

We also assume the capability to apply arbitrary unitary operations to the system, since these tasks are feasible and well understood. Using linear combination, we may produce the two terms in Eq. (7) separately. Assuming the ability to create any unitary dynamics, it remains to generate the second term under the assumption $H=0$.

We now turn to the second procedure to transform the GKS matrix, called *unitary conjugation*. This procedure transforms \mathcal{E} according to

$$\mathcal{U}^\dagger \mathcal{E} \mathcal{U}, \quad (16)$$

where $\mathcal{U}(\rho) = U\rho U^\dagger$ for some unitary operator U . Note that unitary conjugation preserves all the Markovian semigroup properties. We will see that the effect of unitary conjugation is to apply \mathcal{E} in a different basis, producing a new operation that may be used on its own or in linear combination. To understand how the GKS matrix transforms, we prove the following theorem.

Theorem 1. For an N -dimensional system, unitary conjugation by $U \in \text{SU}(N)$ results in conjugation of the GKS matrix by a corresponding element in the adjoint representation of $\text{SU}(N)$.

Proof. Suppose the Markovian semigroup has generator \mathcal{A} and a GKS matrix $a_{\alpha\beta}$. Conjugation by U results in the evolution

$$\mathcal{U}^\dagger e^{At} \mathcal{U} = \lim_{n \rightarrow \infty} \mathcal{U}^\dagger \left(\mathcal{I} - \frac{t}{n} \mathcal{A} \right)^{-n} \mathcal{U} \quad (17)$$

$$= \lim_{n \rightarrow \infty} \left(\mathcal{I} - \frac{t}{n} \mathcal{U}^\dagger \mathcal{A} \mathcal{U} \right)^{-n}. \quad (18)$$

In other words, the new generator is $\mathcal{A}' = \mathcal{U}^\dagger \mathcal{A} \mathcal{U}$. Expressed in the form of Eq. (7) (with $H=0$), we find

$$\mathcal{A}'(\rho) = a_{\alpha\beta} ([U^\dagger F_\alpha U \rho, U^\dagger F_\beta^\dagger U] + [U^\dagger F_\alpha U, \rho U^\dagger F_\beta^\dagger U]). \quad (19)$$

Evidently this unitary conjugation induces a change of basis $F_\alpha \rightarrow U^\dagger F_\alpha U$, which is still Hermitian, orthonormal, and traceless. We can expand the new basis in terms of the old one,

$$U^\dagger F_\alpha U = c_{\alpha\gamma} F_\gamma. \quad (20)$$

This implies

$$U^\dagger F_\alpha F_\beta^\dagger U = c_{\alpha\gamma} c_{\beta\nu}^* F_\gamma F_\nu^\dagger. \quad (21)$$

Taking the trace of Eq. (21), and using the orthonormality of the F_α [Eq. (8)],

$$c_{\alpha\gamma} c_{\beta\gamma}^* = \delta_{\alpha\beta}. \quad (22)$$

In other words, $c_{\alpha\gamma}$ is a unitary matrix. Further, by substituting Eq. (20) into Eq. (19), we obtain the transformed GKS matrix

$$a'_{\gamma\nu} = c_{\alpha\gamma} a_{\alpha\beta} c_{\beta\nu}^*. \quad (23)$$

Denoting the matrices $a_{\alpha\beta}$ and $c_{\alpha\beta}$ by A and C , $A' = C^T A C^*$. The effect of unitary conjugation is to conjugate the original GKS matrix by C^T .

Note that C is not arbitrary, but is determined by U in the following manner. Suppose we choose $\{F_\alpha\}$ to be the generators of $SU(N)$. Then we have

$$[F_\alpha, F_\beta] = i f_{\alpha\beta\gamma} F_\gamma, \quad (24)$$

where $f_{\alpha\beta\gamma}$ are the real structure constants for the Lie algebra generated by $\{F_\alpha\}$. Setting $U = e^{ir_\gamma F_\gamma}$, we find to first order in an infinitesimal r_γ that

$$\begin{aligned} U^\dagger F_\alpha U &= (I - ir_\gamma F_\gamma) F_\alpha (I + ir_\gamma F_\gamma) \\ &= F_\alpha - ir_\gamma [F_\gamma, F_\alpha] \\ &= F_\alpha - ir_\gamma (i f_{\gamma\alpha\beta} F_\beta). \end{aligned} \quad (25)$$

Thus

$$(C^T)_{\alpha\beta} = \delta_{\alpha\beta} + ir_\gamma (i f_{\gamma\alpha\beta}) \quad (26)$$

is in a Lie group generated by the matrices $(G_\gamma)_{\alpha\beta} = i f_{\gamma\alpha\beta}$.

It is an elementary fact of group theory that these G_γ are the generators of the adjoint representation of the F_α algebra. Therefore, $U = e^{ir_\gamma F_\gamma} \in SU(N)$ induces conjugation of the GKS matrix by $C^T = e^{ir_\gamma G_\gamma}$ in the adjoint representation of $SU(N)$. ■

As an example of an application of these two methods, we can perform linear combination of amplitude damping, \mathcal{E}^{AD} [Eq. (12)], and damping in the opposite direction, $\mathcal{X}^\dagger \mathcal{E}^{\text{AD}} \mathcal{X}$, where $\mathcal{X}(\rho) = \sigma_x \rho \sigma_x$, to simulate generalized amplitude damping with an arbitrary mixture of the ground and excited states as the fixed point.

IV. UNITAL MARKOVIAN QUANTUM DYNAMICS

We now use the resources we have defined to simulate Markovian quantum dynamics. We first consider *unital* processes, those that fix the identity. Well-known unital processes on a qubit include phase damping and the depolarizing channel.

We first characterize unitality for GKS matrices. \mathcal{Z} is the generator of a unital Markovian semigroup iff $\mathcal{Z}(I) = 0$. Us-

ing Eq. (7) (with $H=0$), Eq. (24), and the antisymmetry of $f_{\alpha\beta\gamma}$, we find

$$\begin{aligned} \mathcal{Z}(I) &= 2a_{\alpha\beta} [F_\alpha, F_\beta^\dagger] = 2a_{\alpha\beta} [F_\alpha, F_\beta] \\ &= 2ia_{\alpha\beta} f_{\alpha\beta\gamma} F_\gamma = 2i \sum_{\alpha < \beta} (a_{\alpha\beta} - a_{\beta\alpha}) f_{\alpha\beta\gamma} F_\gamma \\ &= -4 \sum_{\alpha < \beta} \text{Im}(a_{\alpha\beta}) f_{\alpha\beta\gamma} F_\gamma. \end{aligned} \quad (27)$$

By orthonormality of the F_α , $\mathcal{Z}(I) = 0$ iff

$$\sum_{\alpha < \beta} \text{Im}(a_{\alpha\beta}) f_{\alpha\beta\gamma} = 0 \quad \forall \gamma. \quad (28)$$

In general, reality of the GKS matrix is a sufficient condition for unitality. When $N=2$, the sum has only one term, so that this condition is also necessary. Thus the unital Markovian semigroups on a qubit are exactly those generated by real GKS matrices.

For $N > 2$, reality of the GKS matrix is not necessary for the corresponding process to be unital. In Appendix C, we give an example of a unital operation of dimension $N=3$ for which the GKS matrix is not real. Since $SU(N)$ for $N \geq 3$ contains an isomorphic copy of $SU(3)$, it follows that there are unital Markovian semigroups generated by complex GKS matrices for all $N \geq 3$. The set of Markovian semigroups generated by real GKS matrices is a *proper* subset of the set of all unital Markovian semigroups.

We now focus on Markovian quantum dynamics on a qubit and consider the effects of unitary conjugation. We take $F_{1,2,3} = \sigma_{x,y,z}$ as before. The generators are represented by real positive semidefinite GKS matrices A . The transformations induced by unitary conjugation are simply

$$A' = e^{ir_\gamma G_\gamma} A e^{-ir_\gamma G_\gamma}, \quad (29)$$

where

$$\begin{aligned} G_1 &= i \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & -1 & 0 \end{pmatrix}, \\ G_2 &= i \begin{pmatrix} 0 & 0 & -1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}, \\ G_3 &= i \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \end{aligned} \quad (30)$$

can be found using $f_{\alpha\beta\gamma} = \epsilon_{\alpha\beta\gamma}$ for the Pauli matrices. Note that the G_γ 's are simply the generators of $SO(3)$ —as is well known, $SO(3)$ is the adjoint representation of $SU(2)$.

Having characterized unital Markovian quantum dynamics on a qubit, we are ready to state the following.

Theorem 2. All unital Markovian quantum dynamics on a single qubit can be simulated with linear combination and unitary conjugation given phase damping as a primitive operation.

Proof. When A is positive semidefinite and real, $A = ODO^T$ for some $O \in \text{SO}(3)$ and D diagonal with diagonal entries $d_i \geq 0$. Let A^{PD} denote the GKS matrix for phase damping. Then

$$A = \frac{2}{\gamma} (d_1 O e^{i(\pi/2)G_2} A^{\text{PD}} e^{-i(\pi/2)G_2} O^T + d_2 O e^{i(\pi/2)G_1} A^{\text{PD}} e^{-i(\pi/2)G_1} O^T + d_3 O A^{\text{PD}} O^T). \quad (31)$$

Thus the GKS matrix for any unital Markovian semigroup can be simulated using linear combination of the unitary conjugates of phase damping. ■

Note that any unital Markovian semigroup with rank 1 GKS matrix can be used in place of phase damping.

V. GENERAL MARKOVIAN QUANTUM DYNAMICS ON A QUBIT

We now consider general Markovian quantum dynamics on a single qubit. We prove the following.

Theorem 3. To simulate arbitrary Markovian quantum dynamics on a qubit with linear combination and conjugation by unitaries, it is necessary and sufficient to be able to perform all operations with GKS matrix $A(\theta) = \vec{a}(\theta)\vec{a}(\theta)^\dagger$, where $\vec{a}(\theta) = (\cos \theta, i \sin \theta, 0)^T$ and $\theta \in [0, \pi/4]$.

Sufficiency. Let A be the GKS matrix to be simulated. Since A is positive semidefinite, we apply the spectral decomposition to express A as a positive sum of outer products,

$$A = \sum_k \lambda_k \vec{a}_k \vec{a}_k^\dagger, \quad (32)$$

where $\lambda_k \geq 0$ and \vec{a} 's are normalized to unit length. By linear combination, it suffices to simulate all $\vec{a}\vec{a}^\dagger$. Separating into real and imaginary parts, we may write any such vector as

$$\vec{a} = \vec{a}^R + i\vec{a}^I. \quad (33)$$

Because \vec{a} only appears in outer products, the overall phase of \vec{a} is irrelevant. In other words, we have $\vec{a}'\vec{a}'^\dagger = \vec{a}\vec{a}^\dagger$, where

$$\vec{a}' = e^{i\psi} \vec{a} = (\vec{a}^R \cos \psi - \vec{a}^I \sin \psi) + i(\vec{a}^R \sin \psi + \vec{a}^I \cos \psi). \quad (34)$$

This transformation maps the two parameters

$$k_1 \equiv |\vec{a}^R|^2 - |\vec{a}^I|^2, \quad (35)$$

$$k_2 \equiv 2\vec{a}^R \vec{a}^I \quad (36)$$

according to

$$\begin{pmatrix} k'_1 \\ k'_2 \end{pmatrix} = \begin{pmatrix} \cos 2\psi & -\sin 2\psi \\ \sin 2\psi & \cos 2\psi \end{pmatrix} \begin{pmatrix} k_1 \\ k_2 \end{pmatrix}. \quad (37)$$

Because we may choose ψ arbitrarily, we make the choice

$$\tan 2\psi = -k_2/k_1, \quad (38)$$

such that $k'_2 = 0$, in which case \vec{a}'^R and \vec{a}'^I are orthogonal. Moreover, we can choose $k'_1 = k_1/\cos 2\psi \geq 0$ such that $|\vec{a}'^R| \geq |\vec{a}'^I|$. Thus, without loss of generality, we may assume that \vec{a} has a real part no shorter than its imaginary part, and that the two parts are orthogonal.

Performing a unitary transformation on the operation effects conjugation by $G \in \text{SO}(3)$,

$$\vec{a}\vec{a}^\dagger \rightarrow G\vec{a}\vec{a}^\dagger G^T = (G\vec{a})(G\vec{a})^\dagger. \quad (39)$$

Because G is real, it does not mix the real and imaginary parts of \vec{a} in $G\vec{a}$. In other words, G simultaneously rotates the two vectors \vec{a}^R and \vec{a}^I . Therefore, G can always be chosen to align \vec{a}^R with the $+x$ axis and \vec{a}^I with the $+y$ axis, so that we can write

$$G\vec{a} = \vec{a}(\theta) = (\cos \theta, i \sin \theta, 0)^T, \quad (40)$$

where $\theta \in [0, \pi/4]$.

Necessity. The $A(\theta)$, being rank 1, are extreme in the convex cone of all the positive matrices. Thus linear combination cannot be used to compose a new $A(\theta')$.

Because scalar multiplication of \vec{a} by a phase commutes with an $\text{SO}(3)$ transformation, it suffices to show that given a phase ψ and rotation G such that $G e^{i\psi} \vec{a}(\theta) = \vec{a}(\theta')$ with $\theta, \theta' \in [0, \pi/4]$, then $\theta = \theta'$. To see this, note that given $k_2 = k'_2 = 0$ and $k_1, k'_1 \geq 0$ in Eq. (37), the phase transformation must be trivial. Thus the real and imaginary parts are unchanged by $e^{i\psi}$, and have to be unchanged by G to remain aligned with the $+x$ and $+y$ axes. Therefore, $\theta' = \theta$. ■

Note that the set of required operations includes amplitude damping, with $\vec{a}^{\text{AD}} = \vec{a}(\pi/4) = (1, i, 0)^T/\sqrt{2}$, and phase damping about the x axis, with $\vec{a}^{\text{PD}'} = \vec{a}(0) = (1, 0, 0)^T$.

We have seen that a one parameter set of generators is necessary and sufficient to simulate all Markovian quantum dynamics on a qubit. With this result in mind, we can estimate the number of parameters in the universal set of generators needed for an N -dimensional quantum system. Generating the $(N^2 - 1) \times (N^2 - 1)$ GKS matrix can be reduced to generating all those with rank 1 by linear combination. Thus we have to obtain all (normalized) complex $(N^2 - 1)$ -dimensional vectors \vec{a} up to a phase, with $2(N^2 - 1) - 2$ free parameters. As there are $N^2 - 1$ degrees of freedom in $\text{SU}(N)$, unitary conjugation will eliminate at most $N^2 - 1$ parameters, leaving $N^2 - 3$ parameters to be obtained, perhaps by a continuous set of primitives. In the case of a qubit ($N = 2$), we have seen that this bound is tight.

VI. CONCLUSIONS AND OPEN QUESTIONS

In the search for a way to simulate the dynamics of open quantum systems using a simple set of primitives, we have set up a framework to study the notion of universality for Markovian quantum dynamics. We have shown how the generators of Markovian semigroups transform under the composition procedures of linear combination [Eq. (15)] and unitary conjugation (Theorem 1). For the case of a single qubit, we have shown that one primitive unital operation suffices to simulate all other unital operations (Theorem 2), and we have exhibited a necessary and sufficient single-parameter universal set for general qubit Markovian quantum dynamics (Theorem 3).

The most immediate open questions are related to the corresponding results for higher dimensions. We have seen that for $N \geq 3$, unital operations no longer correspond to real GKS matrices. An interesting open question is whether there is still a *finite* generating set for unital Markovian quantum dynamics. It would also be interesting to see how the results for general processes scale to $N \geq 3$ dimensions and how many parameters are needed to describe the extreme points of the basis set. This will require an investigation of the specific adjoint representation of $SU(N)$ that acts on $(N^2 - 1) \times (N^2 - 1)$ GKS matrices.

Further open questions arise from other possible composition rules for quantum operations. If we lift the restriction to Markovian quantum dynamics, it is reasonable to include composition procedures other than linear combination and unitary conjugation. For instance, we might allow direct composition of operations. Or we might consider implementing adaptive methods of quantum control, as suggested by Lloyd and Viola [20]. We might also combine processes probabilistically (either by tossing coins or by performing different operations on different parts of the sample in a bulk quantum computer), giving a convex combination $p^i \mathcal{E}^i$ of quantum operations. Such combination does not preserve Markovity in general, but it has other attractive properties; for example, any unital operation on a qubit can be written as a convex sum of *unitary* operations (although this does not hold for higher-dimensional systems [21]). The characterization of the extremal operations on a qubit presented in [13] can be used to extend this to nonunital operations.

Finally, we might consider a formulation of the problem that requires only that we be able to come arbitrarily close to a given quantum operation [22]. This would be more in line with the usual notion of universality for unitary operations, and might prove fruitful as a way of finding smaller basis sets for general quantum operations.

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APPENDIX A: FORMAL PROPERTIES OF MARKOVIAN SEMIGROUPS

A strongly continuous one-parameter semigroup on a complex Banach space B is defined as a family \mathcal{E}_t of bounded linear operators $\mathcal{E}_t: B \rightarrow B$ parametrized by real $t \geq 0$, which satisfy (a) $\mathcal{E}_0 = \mathcal{I}$; (b) $\mathcal{E}_s \mathcal{E}_t = \mathcal{E}_{s+t}$; and (c) the fact that the map $(t, \rho) \rightarrow \mathcal{E}_t(\rho)$ from $[0, \infty) \times B$ to B is jointly continuous.

The generator \mathcal{Z} of a strongly continuous one-parameter semigroup is determined by

$$\mathcal{Z}(\rho) = \lim_{t \downarrow 0} \frac{\mathcal{E}_t(\rho) - \rho}{t}. \quad (\text{A1})$$

The domain of \mathcal{Z} , $\text{Dom}(\mathcal{Z})$, is defined to be the space for which the above limit exists. $\text{Dom}(\mathcal{Z})$ is a dense linear subspace of B . If $\rho \in \text{Dom}(\mathcal{Z})$,

$$\frac{\partial \rho(t)}{\partial t} = \mathcal{Z}(\rho(t)) \quad \forall t \geq 0, \quad (\text{A2})$$

and the semigroup is defined by its generator according to

$$\mathcal{E}_t = e^{\mathcal{Z}t} \equiv \lim_{n \rightarrow \infty} \left(\mathcal{I} - \frac{t}{n} \mathcal{Z} \right)^{-n}, \quad (\text{A3})$$

the inverse being a bounded operator for sufficiently large n .

A one-parameter semigroup is norm continuous if and only if the generator is bounded, in which case

$$\mathcal{E}_t = \lim_{n \rightarrow \infty} \sum_{n=0}^{\infty} \frac{\mathcal{Z}^n t^n}{n!}. \quad (\text{A4})$$

Continuous one-parameter semigroups capture the Markovian and stationarity features of the Markovian quantum dynamics of interest. The remaining features to be incorporated are complete positivity and trace preservation. This leads to our definition: *A Markovian semigroup is a norm continuous one-parameter semigroup of completely positive, trace-preserving linear maps.*

APPENDIX B: THE AFFINE REPRESENTATION AND THE GKS MATRIX

Following the discussion in Sec. II, consider a basis for traceless operators $\{F_\alpha\}$ that is Hermitian and trace orthonormal. Then we can express a density matrix as $\rho = \rho_0 I + \sum_\alpha \rho_\alpha F_\alpha$, where ρ_0, ρ_α are real numbers. Due to trace preservation, the linear representation of the generator \mathcal{Z} of a Markovian semigroup can be reduced to an affine map on the traceless components only,

$$\dot{\rho}_\alpha = L_{\alpha\beta} \rho_\beta + p_\alpha. \quad (\text{B1})$$

In Eq. (B1), $L_{\alpha\beta}$ are entries of an $(N^2 - 1) \times (N^2 - 1)$ matrix L , and p_α are entries of an $(N^2 - 1)$ -dimensional vector.

In the qubit case, let $\{F_{\alpha}\} = (1/\sqrt{2})\{\sigma_x, \sigma_y, \sigma_z\}$. Using Eq. (7), we obtain a one-to-one correspondence between the GKS matrix A (with entries $a_{\alpha\beta}$) and $\{L, p\}$ in the affine representation,

$$L = \begin{pmatrix} -2(a_{22}+a_{33}) & a_{12}+a_{21} & a_{13}+a_{31} \\ a_{12}+a_{21} & -2(a_{11}+a_{33}) & a_{23}+a_{32} \\ a_{13}+a_{31} & a_{23}+a_{32} & -2(a_{11}+a_{22}) \end{pmatrix} \\ = A + A^T - (2 \operatorname{tr} A) I, \quad (\text{B2})$$

$$p = 4(\operatorname{Im}(a_{32}), \operatorname{Im}(a_{13}), \operatorname{Im}(a_{21}))^T. \quad (\text{B3})$$

As positivity of the GKS matrix is equivalent to the complete positivity of Eq. (7), the correspondence between A and $\{L, p\}$ allows complete positivity of the affine representation to be easily characterized.

For higher dimensions, the affine representation $\{L, p\}$ and the GKS matrix for a generator \mathcal{Z} are still in one-to-one correspondence. In particular, let $[F_{\alpha}, F_{\beta}] = i f_{\alpha\beta\gamma} F_{\gamma}$ and $\{F_{\alpha}, F_{\beta}\} = h_{\alpha\beta\gamma} F_{\gamma}$, where $f_{\alpha\beta\gamma}$ are the real structure constants and $h_{\alpha\beta\gamma}$ are real. Then the entries of L and p are given by

$$L_{\eta\gamma} = -h_{\alpha\gamma\lambda} f_{\lambda\beta\eta} \operatorname{Im}(a_{\alpha\beta}) - f_{\alpha\gamma\lambda} f_{\lambda\beta\eta} \operatorname{Re}(a_{\alpha\beta}), \quad (\text{B4})$$

$$p_{\gamma} = -4 \sum_{\alpha < \beta} f_{\alpha\beta\gamma} \operatorname{Im}(a_{\alpha\beta}). \quad (\text{B5})$$

Conversely, given $\{L, p\}$, \mathcal{Z} is uniquely determined. For a fixed basis $\{F_{\alpha}\}$, a unique decomposition in the form of Eq. (7) exists, so that the GKS matrix is uniquely determined. In other words, the linear system of equations (B4) and (B5) can be inverted. Thus the $\{L, p\}$ that represent Markovian semigroups are those for which a solution to Eqs. (B4) and (B5) exists and corresponds to a positive semidefinite GKS matrix.

APPENDIX C: A UNITAL PROCESS WITH COMPLEX GKS MATRIX

A convenient set of generators for $SU(3)$, known as the Gell-Mann matrices, are defined as

$$\begin{aligned} \sqrt{2}\lambda_1 &= \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, & \sqrt{2}\lambda_2 &= \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \\ \sqrt{2}\lambda_3 &= \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, & \sqrt{2}\lambda_4 &= \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}, \\ \sqrt{2}\lambda_5 &= \begin{pmatrix} 0 & 0 & -i \\ 0 & 0 & 0 \\ i & 0 & 0 \end{pmatrix}, & \sqrt{2}\lambda_6 &= \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \\ \sqrt{2}\lambda_7 &= \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix}, & \sqrt{6}\lambda_8 &= \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -2 \end{pmatrix}. \end{aligned} \quad (\text{C1})$$

The only nonvanishing structure constants are $f_{321} = -\sqrt{2}$, $f_{651} = 1/\sqrt{2}$, $f_{642} = f_{741} = f_{752} = -1/\sqrt{2}$, $f_{854} = f_{876} = -\sqrt{3}/\sqrt{2}$ together with cyclic permutations of the indices.

The following process defined over the Gell-Mann matrices is unital, although A is complex:

$$A = \frac{1}{2} \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & i & 0 \\ 0 & 0 & 0 & 0 & 1 & i & 0 & 0 \\ 0 & 0 & 0 & 0 & -i & 1 & 0 & 0 \\ 0 & 0 & 0 & -i & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}. \quad (\text{C2})$$

The eigenvalues are 2 and 0 with degeneracies 2 and 6, so the process is well defined. To show that it is unital, we need to show $\sum_{\alpha < \beta} a_{\alpha\beta} f_{\alpha\beta\gamma} = 0 \forall \gamma$. First, $a_{\alpha\beta} = 0$ for all $\alpha < \beta$ except for $a_{47} = a_{56} = i$. The criterion reduces to $f_{47\gamma} + f_{56\gamma} = 0 \forall \gamma$. But $f_{47\gamma} = f_{56\gamma} = 0 \forall \gamma \neq 1$, and $f_{471} = 1/2$, $f_{561} = -1/2$. Therefore, the process is unital.

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