# Simulating quantum operations with mixed environments

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We study the physical quantum resources required to implement general quantum operations, and provide bounds on the minimum possible size which an environment must be in order to perform certain quantum operations. We prove that contrary to a previous conjecture, not all quantum operations on a single qubit can be implemented with a single-qubit environment, even if that environment is initially prepared in a mixed state. We show that a mixed single-qutrit environment is sufficient to implement a special class of operations, the generalized depolarizing channels. [S1050-2947(99)04107-4]

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## I. INTRODUCTION

Future quantum computers may be useful in studying the behavior of open quantum systems and the nature of decoherence [1,2]. Instead of performing real experiments on quantum systems, a single quantum computer can be used as an efficient, multiple-purpose simulator for a wide variety of physical systems. In general, an important goal of such investigations will be to understand the effects arising from interactions between the system of interest $S$ and another quantum system $E$. For example, a quantum computer can be used to simulate quantum systems $S$ in thermal equilibrium [3], but such a simulation requires an additional quantum system $E$, coupled in a particular way to $S$, to mimic the thermal bath of the system. In other applications involving the simulation of nonequilibrium quantum properties, $S$ could, for molecules whose isomerization dynamics we wish to study, represent the relevant conformational states, which couple to other molecules $E$ through long-range electronic dipolar interactions. In all these applications, we wish to implement $E$ with the smallest quantum resources possible, and this paper investigates the most efficient implementation of such quantum environments.

Suppose $S$ exists in a Hilbert space $\mathcal{H}_n$ of dimension $n$, and $E$ is in $\mathcal{H}_r$ of dimension $r$. It is well known that any *quantum operation* [4] on $\mathcal{H}_n$, resulting from some interaction with $E$ in $\mathcal{H}_r$ with arbitrary $r$, can be performed by appending a state in $\mathcal{H}_{n^2}$, evolving unitarily, and then tracing over $\mathcal{H}_{n^2}$. The difference between $r$ and $n^2$ can represent a significant reduction, since $E$ can be a large bath (for example, of harmonic oscillators), and $r$ can be infinite.

Can a general quantum operation be implemented with an environment even smaller than $n^2$ dimensions? Lloyd conjectured [2] that it is possible to implement a general quantum operation on $k$ quantum bits (qubits) with a $k$-qubit environment, if one prepares the environment not in a pure state, as is usually the case, but rather in an arbitrary *mixed* state.

Here we provide a specific counterexample to this conjecture for $k=1$, although we find that at least for some operations, fewer resources are required than was previously known. Our counterexample is part of a class known as the generalized depolarizing channels, for which we show that a three-dimensional environment is sufficient for simulation. The proof of the counterexample is established by the technique of computing Gröbner bases.

Our results also address the following question: suppose a physical system is given as a black box—we can prepare $S$ in an arbitrary initial state, and then measure the final state of $S$ after a fixed evolution period. What is the smallest environment $E$ with which $S$ might have interacted in this system? A method to completely determine the quantum operation $\chi$ performed by this system is known [5]. This work goes one step further, by showing a way to turn knowledge about $\chi$ into bounds on the nature of $E$.

It is important to realize that an environment that is less than $n^2$ dimensional does truly represent a gain in spatial quantum resources over an environment of dimension $n^2$, even if that smaller environment is mixed. One can prepare any mixed state of a $d$ dimensional system by using no additional quantum spatial resources in the following way: Choosing any pure-state ensemble to represent the mixed state [6], one prepares the environment in one of these pure states at random based on the outcome of a random-number generator. Thus, while more resources are needed (the apparatus generating the random numbers) they are only classical, not needing to be protected from decoherence, for example.

## II. QUANTUM OPERATIONS

We begin by summarizing the mathematical formalism of quantum operations. The most general transformation allowed by quantum mechanics for an initially isolated quantum system is a linear, trace-preserving, completely positive map. Such a map $\chi:\mathcal{A}_n\rightarrow\mathcal{A}_m$, where $\mathcal{A}_n$ is the set of (bounded) operators on a Hilbert space $\mathcal{H}_n$, can be decomposed into a set of at most $nm$ $m\times n$ matrices $A_i$ [7] (which we shall refer to as ''operation elements'') as

 

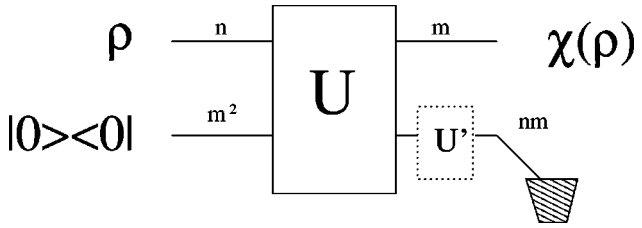


FIG. 1. Implementation of the map $\chi$ using a pure state environment.

$$\chi(\rho)=\sum_{i=1}^{nm} A_i \rho A_i^\dagger . \tag{1}$$

$n$ and $m$ are the dimensions of the input and output Hilbert spaces, respectively. The trace-preserving property implies that the $A_i$ obey the constraint

$$\sum_{i=1}^{nm} A_i^\dagger A_i = \mathbf{1}_n , \tag{2}$$

with $\mathbf{1}_n$ the identity matrix on $\mathcal{H}_n$. Following Choi [7], the set of all such maps $\chi:\mathcal{A}_n\rightarrow\mathcal{A}_m$ we call trace-preserving, completely positive (TCP)$[n,m]$. A physical implementation of these maps is represented in Fig. 1: A unitary operation on the state $\rho\otimes|0\rangle\langle 0|$ (where $|0\rangle$ represents some pure state in an $m^2$-dimensional environment) is performed, and then $nm$ ''degrees of freedom'' are traced out,

$$\chi(\rho)=\sum_{k=1}^{nm} \langle e_k|U[\rho\otimes|0\rangle\langle 0|]U^\dagger|e_k\rangle. \tag{3}$$

Here $\{|e_k\rangle\}_{k=1}^{nm}$ is a set of basis vectors for $\mathcal{H}_{nm}$. As there are at most $nm$ operation elements, it follows that one can implement any map in TCP$[n,m]$ with an environment of dimension $m^2$. To determine the dimension of the parameter space of TCP$[n,m]$ we note that the map $\chi$ does not uniquely determine the set $\{A_i\}_{i=1}^{nm}$. Any set of $m\times n$ matrices $\{B_i\}_{i=1}^{nm}$ and $\{A_j\}_{j=1}^{nm}$ that are related by a unitary transformation

$$B_i=\sum_j^{nm} U'_{ij}A_j \tag{4}$$

implement the same map $\chi$. This freedom corresponds to a unitary rotation $U'$ (see Fig. 1) of the environment qubits after the completion of the interaction $U$. It is shown in [4] that this unitary equivalence is the only freedom in the choice for the set of operators $\{A_i\}_{i=1}^{nm}$.

The dimension of the parameter space of all maps in TCP$[n,m]$ that can be implemented with a pure $d$-dimensional environment will therefore be

$$D_{\mathrm{pure},d}^{n\rightarrow m}=2n^2d-(nd/m)^2-n^2, \tag{5}$$

where the first term represents parameters in $\{A_i\}$, the second is the unitary freedom, the third term is the constraint (2), and where $d$ is such that $m$ divides $nd$. Thus we have $D_{\mathrm{TCP}[n,m]}=D_{\mathrm{pure},m^2}^{n\rightarrow m}=n^2(m^2-1)$.

In a more general physical implementation, however, the initial state of the environment can be an arbitrary density matrix. Consider the set of completely positive trace-preserving linear maps $\chi:\mathcal{A}_n\rightarrow\mathcal{A}_m$ that are implemented by an environment that is initially in some $d$-dimensional density matrix. We call this set $S_{\mathrm{mix}}[d,n,m]$. The action on the input state $\rho$ is

$$\chi(\rho)=\sum_{j=1}^{d}\lambda_j\sum_{k=1}^{dn/m}\langle e_k|U[\rho\otimes|j\rangle\langle j|]U^\dagger|e_k\rangle, \tag{6}$$

where $\{\lambda_j,|j\rangle\}_{j=1}^{d}$ are now the eigenvalues and eigenvectors of the mixed environment state. We identify a set of $m\times n$ matrices $\{A_{jk}\}_{j=1,k=1}^{d,dn/m}$ in the representation of Eq. (1),

$$A_{jk}=\sqrt{\lambda_j}\langle e_k|U|j\rangle. \tag{7}$$

Unitarity implies that these matrices are constrained,

$$\sum_k A_{ik}^\dagger A_{jk}=\delta_{ij}\lambda_i\mathbf{1}_n . \tag{8}$$

There is a residual unitary freedom in choosing the set of matrices $\{A_{jk}\}_{j=1,k=1}^{d,nd/m}$. The set $\{B_{jm}\}_{j=1,m=1}^{d,nd/m}$ with $B_{jm}=\Sigma_k U'_{mk}A_{jk}$, where the $dn/m$-dimensional unitary matrix $U'$ does not depend on the label $j$, implements the same quantum operation and also obeys constraint (8). As before, this freedom corresponds to a unitary transformation on the environment after the completion of the operation. The dimension of the parameter space of $S_{\mathrm{mix}}[d,n,m]$ can be bounded,

$$D_{\mathrm{pure},d}^{n\rightarrow m}\leqslant D_{\mathrm{mix},d}^{n\rightarrow m}\leqslant D_{\mathrm{pure},d^2}^{n\rightarrow m}. \tag{9}$$

The upper bound is given by the fact that one can always simulate a $d$-dimensional mixed environment with a $d^2$-dimensional pure environment.

From Eq. (5) and Eq. (9) it follows that an environment of dimension $d<m$ cannot be used to implment *all* maps in TCP$[n,m]$. In fact a large set of maps, the extremal maps in TCP$[n,m]$, cannot be simulated with $d<m$. A map $\chi$ that is decomposable in $m$ or fewer linearly-independent operation elements is extremal [7] in TCP$[n,m]$. These maps can be implemented with a pure-state environment of dimension $m$; moreover, we prove that there does not exist a more efficient implementation of these maps using a mixed-state environment.

Extremality implies that the map $\chi$ cannot be written as a convex combination of linearly independent maps $\chi^i$ that each have operation elements $\{A_j^i\}$ for which $\Sigma_j A_j^{i\dagger}A_j^i=\mathbf{1}_n$ for each $i$. This ensures that only one of the eigenvalues in constraint (8) is nonzero, but this in fact corresponds to a pure-state environment of dimension $m$. An example of such an extremal map is a von Neumann measurement on a $n$-dimensional system. The set of projection operators $\{P_i\}_{i=1}^{n}$ can be implemented minimally by using an $n$-dimensional pure state.

We now turn to the question of whether all maps in TCP$[n,m]$ can be implemented with $d=m$. Note that our parameter count does not exclude this. In the following, we restrict ourselves to the case $n=m=2$. We study which

maps can be implemented using a single-qubit environment and provide a proof that a particular qubit channel, the two-Pauli channel, cannot be implemented in this way.

We consider a special set of maps, the generalized depolarizing channels [6], which are described by the set $\{(\epsilon_i, A_i)\}_{i=1}^4$, where

$$\chi(\rho) = \sum_i \epsilon_i A_i \rho A_i^\dagger, \tag{10}$$

such that $\epsilon_1+\epsilon_2+\epsilon_3+\epsilon_4=1$ and the operators $A_i$ are given by $A_1=\mathbf{1}_2$, $A_2=\sigma_x$, $A_3=\sigma_y$, $A_4=\sigma_z$. One can represent this family of maps geometrically as a tetrahedron, which is embedded in a cube with vertices at $(1,-1,-1)$, $(-1,1,-1)$, $(1,1,1)$, and $(-1,-1,1)$. The transformation that relates the parameters $\epsilon_1,\epsilon_2,\epsilon_3,\epsilon_4$ to the $(x,y,z)$ coordinates is given by $x=\epsilon_1+\epsilon_2-\epsilon_3-\epsilon_4$, $y=\epsilon_1-\epsilon_2+\epsilon_3-\epsilon_4$, and $z=\epsilon_1-\epsilon_2-\epsilon_3+\epsilon_4$. The vertices of the tetrahedron correspond to a single-operator map. Its edges are two-operator maps, the four faces represent all three-operator maps, and the points in the interior of the tetrahedron are all the four-operator maps of Eq. (10).

A computer search suggests that only a subset of these maps can be simulated by using a qubit environment. For this subset we are able to construct an explicit qubit solution. At the web address [8] one can find pictures of the three-dimensional volume that is described by the solution set and a picture of the solution set as generated by the computer search. The computer work also suggests that the dimension of $S_{\mathrm{mix}}[2,2,2]$ is equal the upper bound of Eq. (9), namely, $D^{2\to 2}_{\mathrm{pure},4}=12$. We find this by randomly sampling in the space of all superoperators; that is, we choose random orthonormal vectors that make up the columns of the unitary matrix $U$ of Eq. (3); a finite percentage could be implemented with a qubit environment. Thus there is enough ''room'' for a solution, but it is not in the right place, as we will see.

This solution is constructed in the following way. We start with the center of mass of the tetrahedron, the point $(\epsilon_1,\epsilon_2,\epsilon_3,\epsilon_4)=(1/4,1/4,1/4,1/4)$. This channel has the property that it maps every input state $\rho$ onto $\frac{1}{2}\mathbf{1}_2$. It can thus be easily implemented by performing a SWAP gate on an environment qubit that is initially in the $\frac{1}{2}\mathbf{1}_2$ state and the input qubit. The SWAP gate on two registers $|a\rangle|b\rangle$ gives $|b\rangle|a\rangle$. Then one considers the line that departs from a vertex, say the point $(\epsilon_1,\epsilon_2,\epsilon_3,\epsilon_4)=(1,0,0,0)$, and goes through the center of mass. This one-dimensional set of channels is characterized by $\epsilon_2=\epsilon_3=\epsilon_4$ and represents the regular depolarizing channel [6]. Performing a $(\mathrm{SWAP})^{1/m}$ (obtained by turning on for time $t/m$ a two-bit interaction that, over time $t$, gives the SWAP transformation) on a $\frac{1}{2}\mathbf{1}_2$ environment and the input qubit implements these channels, up to $\epsilon_1=1/4$. The integer $m$ is related to the $\epsilon$ parameters by $\epsilon_2=\epsilon_3=\epsilon_4=\sin^2(\pi/2m)/4$. One extra step of generalization gives us an even larger set of channels. The unitary matrix is a somewhat generalized form of $(\mathrm{SWAP})^{1/m}$,

$$U=\begin{pmatrix} e^{i\theta}\cos\phi_1 & 0 & 0 & ie^{i\theta}\sin\phi_1 \\ 0 & \cos\phi_2 & i\sin\phi_2 & 0 \\ 0 & i\sin\phi_2 & \cos\phi_2 & 0 \\ ie^{i\theta}\sin\phi_1 & 0 & 0 & e^{i\theta}\cos\phi_1 \end{pmatrix}, \tag{11}$$

and the environment is again prepared in state $\frac{1}{2}\mathbf{1}_2$. We can determine the operation elements and express these as linear (unitary) combinations of the Pauli matrices. This leads to an expression of the parameters $\epsilon_i$ in terms of $(\theta,\phi_1,\phi_2)\in[0,2\pi]\times[0,2\pi]\times[0,2\pi]$,

$$\begin{aligned}
\epsilon_1&=\frac{1}{4}(\cos^2\phi_1+\cos^2\phi_2+2\cos\phi_1\cos\phi_2\cos\theta),\\
\epsilon_2&=\frac{1}{4}(\sin^2\phi_1+\sin^2\phi_2+2\sin\phi_1\sin\phi_2\cos\theta),\\
\epsilon_3&=\frac{1}{4}(\sin^2\phi_1+\sin^2\phi_2-2\sin\phi_1\sin\phi_2\cos\theta),\\
\epsilon_4&=\frac{1}{4}(\cos^2\phi_1+\cos^2\phi_2-2\cos\phi_1\cos\phi_2\cos\theta).
\end{aligned} \tag{12}$$

Alternatively the solution set can be expressed as a set of inequalities on the parameters $\epsilon_i$,

$$S=S_1\cup S_2\cup S_3\cup S_4, \tag{13}$$

where

$$S_i=\{(\epsilon_1,\epsilon_2,\epsilon_3,\epsilon_4)\,|\,\epsilon_1\epsilon_2\geqslant\epsilon_3\epsilon_4\wedge\epsilon_1\epsilon_3\geqslant\epsilon_2\epsilon_4\wedge\epsilon_1\epsilon_4\geqslant\epsilon_2\epsilon_3\}. \tag{14}$$

and

$$S_2=S_1(\epsilon_1\leftrightarrow\epsilon_2), S_3=S_1(\epsilon_1\leftrightarrow\epsilon_3) \text{ and } S_4=S_1(\epsilon_1\leftrightarrow\epsilon_4).$$

In the Appendix we prove that the volume described by Eqs. (13) and (14) and the one given by Eq. (12) coincide.

## III. TWO-PAULI CHANNEL

We now turn to another set of maps, the two-Pauli channel, which is given by the three operators,

$$A_1=\mathbf{1}_2\sqrt{x},\quad A_2=\sigma_x\sqrt{(1-x)/2},\quad A_3=i\sigma_y\sqrt{(1-x)/2}. \tag{15}$$

We will prove that for $0<x<1$, there is no qubit environment which simulates this channel. For $x=0$ or $x=1$ there is a two-dimensional environment that can simulate the channel as the channel has two operation elements when $x=0$ and only one operator when $x=1$.

Any unitary linear combination of the $A_1$, $A_2$, and $A_3$ may be written as

$$B_k=\begin{pmatrix} b_k\sqrt{x} & (c_k-a_k)\sqrt{\frac{1}{2}(1-x)} \\ (c_k+a_k)\sqrt{\frac{1}{2}(1-x)} & b_k\sqrt{x} \end{pmatrix}, \tag{16}$$

with appropriate constraints resulting from unitarity on the coefficients $a_k,b_k,c_k$. This new set of operators $\{B_k\}_{k=1}^4$ will implement the same channel due to Eq. (4). Furthermore, these operators $B_k$ are constrained through Eq. (8). For notational convenience, we define

$$|u_0\rangle=\frac{1}{\sqrt{2}}\begin{pmatrix}a_0+c_0\\ a_1+c_1\end{pmatrix},\quad |u_1\rangle=\frac{1}{\sqrt{2}}\begin{pmatrix}a_2+c_2\\ a_3+c_3\end{pmatrix},$$

$$|w_0\rangle=\frac{1}{\sqrt{2}}\begin{pmatrix}c_0-a_0\\ c_1-a_1\end{pmatrix},\quad |w_1\rangle=\frac{1}{\sqrt{2}}\begin{pmatrix}c_2-a_2\\ c_3-a_3\end{pmatrix},\qquad (17)$$

$$|v_0\rangle=\begin{pmatrix}b_0\\ b_1\end{pmatrix},\quad |v_1\rangle=\begin{pmatrix}b_2\\ b_3\end{pmatrix}.$$

Using the assumption $0\neq x\neq 1$ and by linearly combining all the equations we obtain:

$$\langle v_0|w_0\rangle+\langle u_0|v_0\rangle=:g_1=0, \qquad (18)$$

$$\langle v_1|w_1\rangle+\langle u_1|v_1\rangle=:g_2=0, \qquad (19)$$

$$\langle v_0|w_1\rangle+\langle u_0|v_1\rangle=:g_3=0, \qquad (20)$$

$$\langle w_0|v_1\rangle+\langle v_0|u_1\rangle=:g_4=0, \qquad (21)$$

$$\langle u_0|u_0\rangle-\langle w_0|w_0\rangle=:g_5=0, \qquad (22)$$

$$\langle u_1|u_1\rangle-\langle w_1|w_1\rangle=:g_6=0, \qquad (23)$$

$$\langle u_0|u_0\rangle+\langle u_1|u_1\rangle-1=:g_7=0, \qquad (24)$$

$$\langle v_0|v_0\rangle+\langle v_1|v_1\rangle-1=:g_8=0, \qquad (25)$$

$$\langle u_0|v_0\rangle+\langle u_1|v_1\rangle=:g_9=0, \qquad (26)$$

$$\langle u_0|w_0\rangle+\langle u_1|w_1\rangle=:g_{10}=0, \qquad (27)$$

$$\langle u_0|u_1\rangle-\langle w_0|w_1\rangle=:g_{11}=0. \qquad (28)$$

Writing each of the coefficients $a_k$, $b_k$, and $c_k$ in the form $x_j+ix_{j+1}$ (where $i^2=-1$), we get a system of polynomial equations $\mathrm{Re}(g_1)=\mathrm{Im}(g_1)=\ldots=\mathrm{Im}(g_{11})=0$, where $\mathrm{Re}(g_k)$ and $\mathrm{Im}(g_k)$ are polynomials in the variables $x_1,\ldots,x_{24}$ with real coefficients. To show that this system of equations has no solution we make use of Gröbner bases (see, e.g., [9]). The computation of a Gröbner basis with Buchberger's algorithm generalizes the Euclidean algorithm to compute the greatest common divisor (GCD) of univariate polynomials $p_1(x)$ and $p_2(x)$. In that case, the GCD $g(x)$ can be written as a ''linear'' combination $g(x)=f_1(x)p_1(x)+f_2(x)p_2(x)$. The two univariate polynomials $p_1$ and $p_2$ have a common root if and only if their GCD is nontrivial, i.e., $g(x)\neq 1$.

For multivariate polynomials, a common solution exists if and only if the Gröbner basis of the ideal generated by them is nontrivial, i.e., does not contain a constant. In our case, using the computer algebra system MAGMA [10] we have shown that there exist polynomials $f_1,\ldots,f_{11}$ such that $\Sigma_{j=1}^{11}f_j(x_1,\ldots,x_{24})g_j(x_1,\ldots,x_{24})=1$, i.e., the Gröbner basis contains 1 and there is no solution of Eqs. (18)–(28).

## IV. QUTRIT SOLUTION

Despite the above proof, it turns out that the class of channels we have been studying do not require a two qubit environment ($d=4$) for their simulation; a mixed *qutrit* ($d=3$) suffices. For generalized depolarizing channels, there will be nine operators, $\{A_{ij}\}_{i,j=1}^{3}$. We set one eigenvalue $\lambda_3=0$ and thus $A_{31}=A_{32}=A_{33}=0$. If $\epsilon_1\epsilon_2\geqslant\epsilon_3\epsilon_4$ the solution is $A_{11}=0$, $A_{21}=\sqrt{\epsilon_2-\epsilon_3\epsilon_4/\epsilon_1}\sigma_x$, $A_{12}=\sqrt{\epsilon_3}\sigma_z$, $A_{22}=\sqrt{\epsilon_4}\sigma_y$, $A_{13}=\sqrt{\epsilon_1}\mathbf{1}_2$, and $A_{23}=-i\sqrt{\epsilon_3\epsilon_4/\epsilon_1}\sigma_x$. Otherwise, we take $A_{11}=0$, $A_{21}=\sqrt{\epsilon_4-\epsilon_1\epsilon_2/\epsilon_3}\sigma_y$, $A_{12}=\sqrt{\epsilon_1}\mathbf{1}_2$, $A_{22}=\sqrt{\epsilon_2}\sigma_x$, $A_{13}=\sqrt{\epsilon_3}\sigma_z$, and $A_{23}=i\sqrt{\epsilon_1\epsilon_2/\epsilon_3}\sigma_y$. One can check that this set implements any generalized depolarizing channel and satisfies Eq. (8).

On the basis of the computer work we conjecture that *any* map in TCP[2,2] can be simulated with a qutrit environment. Also, the numerics suggest that one can always set one eigenvalue to zero. Furthermore, we have some numerical evidence that channels that have three linearly independent operation elements can never be simulated with a qubit environment.

## V. DISCUSSION

Our results provide additional bounds on the size of an environment needed to simulate certain quantum operations on single qubits. However, we have only addressed simple mappings on the smallest input space. Many questions now arise: how do these results generalize to mappings on $n$-dimensional systems? A relevant scenario might be $n$ uses of the generalized depolarizing channel, where the environment can be shared between the channels. In such a case, might a qubit environment per channel suffice for large $n$? A nice extension of the generalized depolarizing channels are the channels that are defined with the Heisenberg group elements [11]. These channels on $n$-dimensional inputs are mixtures of a set of $n^2$ unitary matrices $U(i,j)$. However, it is not straightforward to construct solutions, as in the qutrit case, for a general ''Heisenberg channel,'' and we have no insight at the moment of what gain one can get by using mixed states here. The number of additional constraints of Eq. (8) for a mixed environment grows as $n^2$; therefore, our expectation is that the minimal dimension of the environment needed for a general Heisenberg channel on a $n$-dimensional input, will be of order $n^2$.

The questions we have formulated also apply to the construction of generalized measurements: how large an environment is needed for the minimal-size construction of arbitrary generalized measurements on an $n$-dimensional system? We hope our results and the questions they motivate will be useful in future quantum computing applications, and provide fundamental insights into the often strange properties of quantum systems.

## ACKNOWLEDGMENT

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## APPENDIX: $P_1=P_2$

We prove that the volume given by the parametrization of $(x,y,z)$ in terms of $(\phi_1,\phi_2,\theta)$, Eq. (12), which we call $P_1$, is equal to the volume described by the inequalities of Eqs. (13) and (14), which we call $P_2$.

The volume $P_1$ is generated by a mapping of a three-

dimensional torus specified by coordinates $(\phi_1,\phi_2,\theta)$ to $(x,y,z)$. The Jacobian determinant $|\det\partial(x,y,z)/\partial(\phi_1,\phi_2,\theta)|$ will vanish on a set of points which we call $R_{P_1}$ that include the surface of $P_1$ denoted as $\Sigma_{P_1}$. $R_{P_1}$ might include points interior to $P_1$, but we will rule this out. We will show that $R_{P_1}=\Sigma_{P_2}$. Then, by inspection of the volume $P_2$ we can conclude that $R_{P_1}$ can only be the surface $\Sigma_{P_1}$.

### 1. $R_{P_1}=\Sigma_{P_2}$

The Jacobian determinant of the transformation is

$$J=|4\cos\theta\sin\theta(\cos^2\phi_1\sin^2\phi_1-\cos^2\phi_2\sin^2\phi_2)|. \tag{A1}$$

First we show that the volume $P_1$ is unchanged under all permutations of the $\epsilon_1,\ldots,\epsilon_4$. The permutations are generated by transpositions of two elements $\epsilon_i$ and $\epsilon_j$. Transposition $(\epsilon_1\epsilon_2)(\epsilon_3)(\epsilon_4)$ will map $(x,y,z)$ onto $(x,-z,-y)$, and similarly, the other transpositions interchange $x$, $y$, and $z$ and add minus signs. The Jacobian determinant is invariant under these transformations, thus the surface is a symmetric function of $\epsilon_1,\epsilon_2,\epsilon_3,\epsilon_4$. This implies that the volume itself is symmetric in $\epsilon_1,\epsilon_2,\epsilon_3,\epsilon_4$.

We will show that the Jacobian vanishes for points $(x,y,z)$ if and only if $(x,y,z)\in\Sigma_{P_2}$, where $\Sigma_{P_2}$ denotes the surface of $P_2$.

$\Rightarrow$ The Jacobian vanishes when

$\cdot\cos\theta=0\Rightarrow\epsilon_1\epsilon_3=\epsilon_2\epsilon_4$,

$\cdot\sin\theta=0\Rightarrow\epsilon_1\epsilon_2=\epsilon_3\epsilon_4$,

$\cdot\cos^2\phi_1\sin^2\phi_1-\cos^2\phi_2\sin^2\phi_2=0\Rightarrow\epsilon_1\epsilon_4=\epsilon_2\epsilon_3$.

These resulting equalities define points on $\Sigma_{P_2}$. Note that the surface is connected (see [8]), i.e., there is a way to reach any point on the surface from any starting point and thus the volume $P_1$ is (edge) connected.

$\Leftarrow$ Take section $S_1$ [Eq. (14)], for which there are three parts of the surface $C_1,C_2,C_3$, with $C_1=\{\epsilon_1\epsilon_3=\epsilon_2\epsilon_4,\epsilon_1\epsilon_2\geqslant\epsilon_3\epsilon_4,\epsilon_1\epsilon_4\geqslant\epsilon_2\epsilon_3\}$ and $C_2=C_1(\epsilon_2\leftrightarrow\epsilon_3)$ $C_3=C_1(\epsilon_3\leftrightarrow\epsilon_4)$. The Jacobian vanishes for $\epsilon_1\epsilon_3=\epsilon_2\epsilon_4$. As $C_2$ and $C_3$ are obtained by permutations, the Jacobian will also vanish on these surfaces. Now by interchanging $\epsilon_1$ with $\epsilon_2$ we obtain $S_2$ etc., but again because the Jacobian is invariant under this transposition, we know that the Jacobian will vanish also on the surface of $S_2$, $S_3$, and $S_4$.

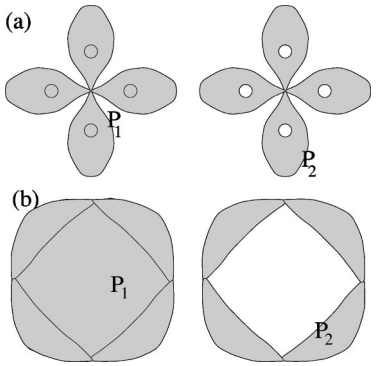


FIG. 2. Schematic examples of volumes $P_1$ and $P_2$ that do not coincide, even though $R_{P_1}=\Sigma_{P_2}$.

### 2. $P_2$ has no holes or noncontractible surfaces

We must rule out the possibility that $R_{P_1}$ includes points in the interior of $P_1$. In Fig. 2 a couple of example-volumes are given for which $R_{P_1}=\Sigma_{P_2}$ but $P_1\neq P_2$. The volume $P_2$ consists of four sections. Any two sections intersect on a line. For volumes $S_1$ and $S_2$ this is the line given by $(\epsilon_1=\epsilon_2,\epsilon_3=\epsilon_4)$. Inspection of each section shows that that it has no holes, as in Fig. 2(a).[1]

Inspection also shows that joining the four sections does not introduce a noncontractible surface on the total volume $P_2$, as shown in Fig. 2(b). Thus the set of points $R_{P_1}$ that coincides with $\Sigma_{P_2}$ cannot contain points that lie inside the volume $P_1$. From this we can conclude that $\Sigma_{P_1}=\Sigma_{P_2}$.

To conclude, we note that there exists a point which is both inside $P_1$ and inside $P_2$, for example, the point $\epsilon_1=5/8$, $\epsilon_2=\epsilon_3=\epsilon_4=1/8$, and $P_1$ is (edge) connected; therefore, $P_1$ and $P_2$ coincide.

[1] A rigorous proof could be established, say for section $S_1$, by showing that rays emanating from points on the line $\epsilon_2=\epsilon_3=\epsilon_4, 1/4\leqslant\epsilon_1\leqslant 1$ cross the surface of $S_1$ only once.

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