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Choi's proof as a recipe for quantum process tomography

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Quantum process tomography is a procedure by which an unknown quantum operation can be fully experimentally characterized. We reinterpret Choi's proof [Linear Algebr. Appl. **10**, 285 (1975)] of the fact that any completely positive linear map has a Kraus representation as a method for quantum process tomography. The analysis for obtaining the Kraus operators is extremely simple. We discuss the systems in which this tomography method is particularly suitable. © 2003 American Institute of Physics. [DOI: 10.1063/1.1518554]

I. INTRODUCTION

The formalism of quantum operation can be used to describe a very large class of dynamical evolution of quantum systems, including quantum algorithms, quantum channels, noise processes, and measurements. The task to fully characterize an unknown quantum operation \mathcal{E} by applying it to carefully chosen input state(s) and analyzing the output is called quantum process tomography. The parameters characterizing the quantum operation are contained in the density matrices of the output states, which can be measured using quantum state tomography.¹ Recipes for quantum process tomography have been proposed.^{2–6} In earlier methods,^{2–4} \mathcal{E} is applied to different input states each of exactly the input dimension of \mathcal{E} . In Refs. 5 and 6, \mathcal{E} is applied to part of a fixed bipartite entangled state. In other words, the input to \mathcal{E} is entangled with a reference system, and the joint output state is analyzed.

Quantum processing tomography is an essential tool in reliable quantum information processing, allowing error processes and possibly imperfect quantum devices such as gates and channels to be characterized. The method in Ref. 3 has been experimentally demonstrated and used to benchmark the fidelities of teleportation⁷ and the controlled-NOT gate,⁸ and to verify a core assumption in fault tolerant quantum computation.⁸

The minimum experimental resource for quantum process tomography is determined by the number of parameters characterizing a quantum operation \mathcal{E} , and is fixed by the input and output dimensions of \mathcal{E} . However, different methods that consume the same quantity of resource can require different types of resources, and be suitable for different physical systems. Furthermore, each method defines a procedure to convert the measured output density matrices to a desired representation of \mathcal{E} , and a simpler procedure will enhance the necessary error analysis.

In this paper, we describe in detail the method initially reported in Ref. 6, which is derived as a simple corollary of a mathematical proof reported in Ref. 9. Our goal is twofold. We hope to make this interesting proof more accessible to the quantum information community, as well as to provide a simple recipe for obtaining the Kraus operators of an unknown quantum operation. In the rest of the paper, we review the different approaches of quantum operations, describe Choi's proof and the recipe for quantum process tomography in Secs. II, III, and IV. We discuss the relative merits of various tomography methods in Sec. V.

II. EQUIVALENT APPROACHES FOR QUANTUM OPERATIONS

A quantum state is usually described by a density matrix ρ that is positive semidefinite ($\rho \geq 0$, i.e., all eigenvalues are non-negative) with $\text{tr}(\rho)=1$. A quantum operation \mathcal{E} describes the evolution of one state ρ to another $\rho' = \mathcal{E}(\rho)$.

More generally, let \mathcal{H}_1 and \mathcal{H}_2 denote the input and output Hilbert spaces of \mathcal{E} . A density matrix can be regarded as an operator acting on the Hilbert space (but it evolves as a state rather than as an operator). Let $\mathcal{B}(\mathcal{H}_i)$ denote the set of all bounded linear operators acting on \mathcal{H}_i for $i=1,2$. We can consider $\mathcal{E}(M)$ for any $M \in \mathcal{B}(\mathcal{H}_1)$ without restricting the domain to density matrices. A map \mathcal{E} from $\mathcal{B}(\mathcal{H}_1)$ to $\mathcal{B}(\mathcal{H}_2)$ is a quantum operation if it satisfies the following equivalent sets of conditions:

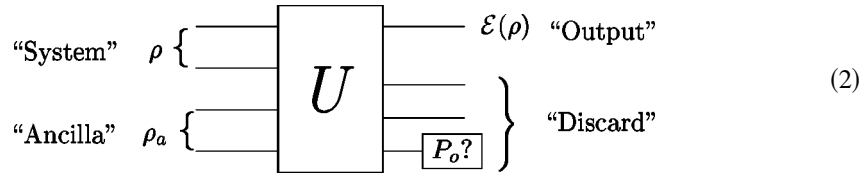
- (1) \mathcal{E} is (i) linear, (ii) trace nonincreasing for all $M \geq 0$ ($\text{tr}(\mathcal{E}(M)) \leq \text{tr}(M)$), and (iii) *completely positive*.¹⁰ The map \mathcal{E} is *positive* if $M \geq 0$ in $\mathcal{B}(\mathcal{H}_1)$ implies $\mathcal{E}(M) \geq 0$ in $\mathcal{B}(\mathcal{H}_2)$. It is completely positive if, for any auxiliary Hilbert space \mathcal{H}_a , $\tilde{M} \geq 0$ in $\mathcal{B}(\mathcal{H}_1 \otimes \mathcal{H}_a)$ implies $(\mathcal{E} \otimes \mathcal{I})(\tilde{M}) \geq 0$ in $\mathcal{B}(\mathcal{H}_2 \otimes \mathcal{H}_a)$ where \mathcal{I}_a is the identity operation on $\mathcal{B}(\mathcal{H}_a)$.
- (2) \mathcal{E} has a *Kraus representation* or an *operator sum representation*:^{11,9,12}

$$\mathcal{E}(M) = \sum_k A_k M A_k^\dagger, \quad (1)$$

where $\sum_k A_k^\dagger A_k \leq I$, and I is the identity operator in $\mathcal{B}(\mathcal{H}_1)$. The A_k operators are called the Kraus operators or the operation elements of \mathcal{E} .

- (3) $\mathcal{E}(M) = \text{Tr}_0[U(M \otimes \rho_a)U^\dagger(I \otimes P_0)]$ for some unitary U in $\mathcal{B}(\mathcal{H}_1 \otimes \mathcal{H}_a)$. Here, $\rho_a \in \mathcal{B}(\mathcal{H}_a)$ is a density matrix of the initial state of the ancilla, I is the identity operator in $\mathcal{B}(\mathcal{H}_2)$, $\mathcal{H}_2 \otimes \mathcal{H}_0 = \mathcal{H}_1 \otimes \mathcal{H}_a$, $P_0 \in \mathcal{B}(\mathcal{H}_0)$ is a projector, and Tr_0 is a partial trace over \mathcal{H}_0 .

Each set of conditions represents an approach to quantum operation when the input is a density matrix ($M = \rho$). The first approach puts down three axioms any quantum operation should satisfy. Completely positivity requires that if the input is entangled with some other system (described by the Hilbert space \mathcal{H}_a), the output after \mathcal{E} acts on \mathcal{H}_1 should still be a valid state. The second approach describes a noise process in which A_k is applied to the state at random, which is particularly convenient in quantum information theory (see Ref. 13 for a review). The third approach describes system-ancilla (or system-environment) interaction. Each evolution results from a unitary interaction of the system with a fixed ancilla state ρ_a , followed by a measurement on a subsystem \mathcal{H}_0 with measurement operators $\{P_0, I - P_0\}$, post-selection of the first outcome, and removal of \mathcal{H}_0 [see (2)].



The fact that the third approach is equivalent to the first is nontrivial—the operations in the third approach are actually all that satisfy the three basic axioms.

The earliest proof of the equivalence of the three approaches is due to Ref. 11. Summaries and simplified proofs can be found in Refs. 6, 14, and 15. There are four major steps, showing that the first set of conditions implies the second set and vice versa, and similarly for the second and third sets of conditions. The most nontrivial step is to show that every linear and completely positive map has a Kraus representation. We will describe a proof due to Choi,⁹ which is independent of Ref. 11 and is much simpler and elementary.

III. CHOI'S PROOF

The precise statement to be proved is that, if \mathcal{E} is a completely positive linear map from $\mathcal{B}(\mathcal{H}_1)$ to $\mathcal{B}(\mathcal{H}_2)$, then $\mathcal{E}(M) = \sum_k A_k M A_k^\dagger$ for some $n_2 \times n_1$ matrices A_k , where n_i is the dimension of \mathcal{H}_i . Let $|\Phi\rangle = (1/\sqrt{n_1}) \sum_i |i\rangle \otimes |i\rangle$ be a maximally entangled state in $\mathcal{H}_1 \otimes \mathcal{H}_1$. Here, $\{|i\rangle\}_{i=1, \dots, n_1}$ is a basis for \mathcal{H}_1 . Consider $(\mathcal{I} \otimes \mathcal{E})(\tilde{M})$ where

$$\tilde{M} = n_1 |\Phi\rangle\langle\Phi| = \sum_{i,j=1}^{n_1} |i\rangle\langle j| \otimes |i\rangle\langle j|. \quad (3)$$

\tilde{M} is an $n_1 \times n_1$ array of $n_1 \times n_1$ matrices. The (i,j) block is exactly $|i\rangle\langle j|$:

$$\tilde{M} = \begin{bmatrix} \begin{matrix} 1 & 0 & \cdot & 0 \\ 0 & 0 & \cdot & 0 \\ \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & \cdot & 0 \end{matrix} & \begin{matrix} 0 & 1 & \cdot & 0 \\ 0 & 0 & \cdot & 0 \\ \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & \cdot & 0 \end{matrix} & \begin{matrix} \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \end{matrix} & \begin{matrix} 0 & 0 & \cdot & 1 \\ 0 & 0 & \cdot & 0 \\ \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & \cdot & 0 \end{matrix} \\ \hline \begin{matrix} 0 & 0 & \cdot & 0 \\ 1 & 0 & \cdot & 0 \\ \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & \cdot & 0 \end{matrix} & \begin{matrix} 0 & 0 & \cdot & 0 \\ 0 & 1 & \cdot & 0 \\ \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & \cdot & 0 \end{matrix} & \begin{matrix} \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \end{matrix} & \begin{matrix} 0 & 0 & \cdot & 0 \\ 0 & 0 & \cdot & 1 \\ \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & \cdot & 0 \end{matrix} \\ \hline \begin{matrix} \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \end{matrix} & \begin{matrix} \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \end{matrix} & \begin{matrix} \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \end{matrix} & \begin{matrix} \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \end{matrix} \\ \hline \begin{matrix} 0 & 0 & \cdot & 0 \\ 0 & 0 & \cdot & 0 \\ \cdot & \cdot & \cdot & \cdot \\ 1 & 0 & \cdot & 0 \end{matrix} & \begin{matrix} 0 & 0 & \cdot & 0 \\ 0 & 0 & \cdot & 0 \\ \cdot & \cdot & \cdot & \cdot \\ 0 & 1 & \cdot & 0 \end{matrix} & \begin{matrix} \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \end{matrix} & \begin{matrix} 0 & 0 & \cdot & 0 \\ 0 & 0 & \cdot & 0 \\ \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & \cdot & 1 \end{matrix} \end{bmatrix} \quad (4)$$

When $\mathcal{I} \otimes \mathcal{E}$ is applied to \tilde{M} , the (i,j) block becomes $\mathcal{E}(|i\rangle\langle j|)$, and

$$(\mathcal{I} \otimes \mathcal{E})(\tilde{M}) = \begin{bmatrix} \mathcal{E} \begin{pmatrix} 1 & 0 & \cdot & 0 \\ 0 & 0 & \cdot & 0 \\ \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & \cdot & 0 \end{pmatrix} & \mathcal{E} \begin{pmatrix} 0 & 1 & \cdot & 0 \\ 0 & 0 & \cdot & 0 \\ \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & \cdot & 0 \end{pmatrix} & \begin{matrix} \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \end{matrix} & \mathcal{E} \begin{pmatrix} 0 & 0 & \cdot & 1 \\ 0 & 0 & \cdot & 0 \\ \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & \cdot & 0 \end{pmatrix} \\ \hline \mathcal{E} \begin{pmatrix} 0 & 0 & \cdot & 0 \\ 1 & 0 & \cdot & 0 \\ \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & \cdot & 0 \end{pmatrix} & \mathcal{E} \begin{pmatrix} 0 & 0 & \cdot & 0 \\ 0 & 1 & \cdot & 0 \\ \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & \cdot & 0 \end{pmatrix} & \begin{matrix} \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \end{matrix} & \mathcal{E} \begin{pmatrix} 0 & 0 & \cdot & 0 \\ 0 & 0 & \cdot & 1 \\ \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & \cdot & 0 \end{pmatrix} \\ \hline \begin{matrix} \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \end{matrix} & \begin{matrix} \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \end{matrix} & \begin{matrix} \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \end{matrix} & \begin{matrix} \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \end{matrix} \\ \hline \mathcal{E} \begin{pmatrix} 0 & 0 & \cdot & 0 \\ 0 & 0 & \cdot & 0 \\ \cdot & \cdot & \cdot & \cdot \\ 1 & 0 & \cdot & 0 \end{pmatrix} & \mathcal{E} \begin{pmatrix} 0 & 0 & \cdot & 0 \\ 0 & 0 & \cdot & 0 \\ \cdot & \cdot & \cdot & \cdot \\ 0 & 1 & \cdot & 0 \end{pmatrix} & \begin{matrix} \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \end{matrix} & \mathcal{E} \begin{pmatrix} 0 & 0 & \cdot & 0 \\ 0 & 0 & \cdot & 0 \\ \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & \cdot & 1 \end{pmatrix} \end{bmatrix} \quad (5)$$

which is an $n_1 \times n_1$ array of $n_2 \times n_2$ matrices.

We now express $(\mathcal{I} \otimes \mathcal{E})(\tilde{M})$ in a manner completely independent of Eq. (5). Since \tilde{M} is positive and \mathcal{E} is completely positive, $(\mathcal{I} \otimes \mathcal{E})(\tilde{M})$ is positive, and can be expressed as $(\mathcal{I} \otimes \mathcal{E})(\tilde{M}) = \sum_k |a_k\rangle\langle a_k|$, where $|a_k\rangle$ for $k=1, \dots, n_1 n_2$ are the eigenvectors of $(\mathcal{I} \otimes \mathcal{E})(\tilde{M})$, normalized to the respective eigenvalues. One can represent each $|a_k\rangle$ as a column vector and each $\langle a_k|$ as a row vector. We can divide the column vector $|a_k\rangle$ into n_1 segments each of length n_2 , and define a matrix A_k with the i th column being the i th segment, so that the i th segment is exactly $A_k|i\rangle$. Then

$$(\mathcal{I} \otimes \mathcal{E})(\tilde{M}) = \sum_k \left[\begin{array}{c} \boxed{} \\ \boxed{} \\ \boxed{} \\ \boxed{} \end{array} \right] \times \left[\begin{array}{cccc} \langle 1|A_k^\dagger & \langle 2|A_k^\dagger & \cdots & \langle n_1|A_k^\dagger \end{array} \right] \quad (6)$$

$A_k|1\rangle$
 $A_k|2\rangle$
 $A_k|n_1\rangle$

$$(\mathcal{I} \otimes \mathcal{E})(\tilde{M}) = \sum_k \left[\begin{array}{cccc} A_k|1\rangle\langle 1|A_k^\dagger & A_k|1\rangle\langle 2|A_k^\dagger & \cdots & A_k|1\rangle\langle n_1|A_k^\dagger \\ A_k|2\rangle\langle 1|A_k^\dagger & A_k|2\rangle\langle 2|A_k^\dagger & \cdots & A_k|2\rangle\langle n_1|A_k^\dagger \\ \cdots & \cdots & \cdots & \cdots \\ A_k|n_1\rangle\langle 1|A_k^\dagger & A_k|n_1\rangle\langle 2|A_k^\dagger & \cdots & A_k|n_1\rangle\langle n_1|A_k^\dagger \end{array} \right] \quad (7)$$

Comparing Eqs. (5) and (7) block by block $\mathcal{E}(M) = \sum_k A_k M A_k^\dagger$ for $\forall M = |i\rangle\langle j|$, and thus $\forall M \in \mathcal{B}(\mathcal{H}_1)$ by linearity.

IV. RECIPE FOR QUANTUM PROCESS TOMOGRAPHY

The basic assumptions in quantum process tomography are as follows. The unknown quantum operation \mathcal{E} is available as an “oracle” or a “blackbox” without information about its internal mechanism. One prepares certain input states and *measures* the corresponding output density matrices to learn about \mathcal{E} systematically. The task to measure the density matrix of a quantum system is called quantum state tomography.¹ To obtain a Kraus representation for \mathcal{E} , one needs an experimental procedure that specifies the input states to be prepared, and a numerical method for obtaining the Kraus operators from the measured output density matrices.

A method follows immediately from the proof in Sec. III. We retain all the previously defined notation. The crucial observation is that $(1/n_1)\tilde{M}$ and $(1/n_1)(\mathcal{I} \otimes \mathcal{E})(\tilde{M})$ correspond to the input and output physical states $|\Phi\rangle\langle\Phi|$ and $(\mathcal{I} \otimes \mathcal{E})(|\Phi\rangle\langle\Phi|)$ which can be prepared and measured. Therefore, the procedure is as follows.

- (1) Prepare a maximally entangled state $|\Phi\rangle$ in $\mathcal{H}_1 \otimes \mathcal{H}_1$.
- (2) Subject one system to the action of \mathcal{E} , keeping the other system from evolving.
- (3) Measure the joint output density matrix $(\mathcal{I} \otimes \mathcal{E})(|\Phi\rangle\langle\Phi|) = (1/n_1)(\mathcal{I} \otimes \mathcal{E})(\tilde{M})$, multiply by n_1 , obtain the eigen-decomposition $\sum_k |a_k\rangle\langle a_k|$. Divide $|a_k\rangle$ (of length $n_1 n_2$) into n_1 equal segments each of length n_2 . A_k is the $n_2 \times n_1$ matrix having the i th segment as its i th column.

The maximally entangled state in the above procedure can be replaced by any pure state with maximum Schmidt number, $|\phi\rangle = \sum_i \alpha_i (U|i\rangle) \otimes (V|i\rangle)$ where $\alpha_i > 0$ are real and $\sum_i \alpha_i^2 = 1$. The output density matrix ρ_{out} is equal to $(\mathcal{I} \otimes \mathcal{E})(|\phi\rangle\langle\phi|) = \sum_{i,j} \alpha_i \alpha_j (U|i\rangle\langle j|U^\dagger) \otimes \mathcal{E}(V|i\rangle\langle j|V^\dagger)$. One computes $(U^\dagger \otimes I)\rho_{\text{out}}(U \otimes I)$, divides the (i,j) block by $\alpha_i \alpha_j$, and performs eigen-decomposition to obtain a set of A_k operators. The Kraus operators of \mathcal{E} are given by $A_k V^\dagger$.

V. DISCUSSION

We have provided an experimental and analytic procedure for obtaining a set of Kraus operators A_k for an unknown quantum operation \mathcal{E} . The set of A_k is called “canonical” in Ref. 9, meaning that the A_k are linearly independent. We remark that any other Kraus representation can be obtained from A_k using the fact that $\mathcal{E}(\rho) = \sum_k A_k \rho A_k^\dagger = \sum_k B_k \rho B_k^\dagger$ if and only if $A_k = \sum_j u_{kj} B_k$ when u_{kj} are the entries of an isometry.⁹ Alternatively, one can replace the eigen-decomposition of $(\mathcal{I} \otimes \mathcal{E})(|\Phi\rangle\langle\Phi|)$ by any decomposition into a positive sum to obtain other valid sets of Kraus operators.

Previous methods of quantum process tomography^{2–4} involve preparing a set of physical input states ρ_i that form a basis of $\mathcal{B}(\mathcal{H}_1)$, and measuring $\mathcal{E}(\rho_i)$ to determine \mathcal{E} . Since the input ρ_i are physical states, they are not trace orthonormal, causing complications in the analysis. [A set of $n \times n$ matrices $\{O_{ij}\}$ is trace orthonormal if $\text{tr}(O_i^\dagger O_j) = \delta_{ij}$.] In contrast, the output state in the current method automatically contains complete information on $\mathcal{E}(|i\rangle\langle j|)$ for the unphysical orthonormal basis for operators $|i\rangle\langle j|$ [see Eq. (5)], which greatly simplifies the analysis to obtain the Kraus operators.

Both previous and current methods require state tomography. The current method requires the preparation of an entangled input state and the ability to stop the evolution of the reference system while \mathcal{E} is being applied. In systems such as the optical system, these requirements are all straightforward, and process tomography can be realized with current experimental techniques. In solution NMR,^{16,17} the method still applies to an effective pure maximally entangled input state,¹⁶ if the evolution of the reference system can be stopped. This is possible using decoupling techniques though at the risk of increased error rates due to the decoupling procedure. In general, the current method is suitable for any system in which a maximally entangled can be easily prepared with a controllable reference system (such as one physically separated from the original system).

Any efficient quantum process tomography procedure consumes approximately the same amount of resources, which is determined by the number of degrees of freedom in the quantum operation. In general, to measure an $n \times n$ density matrix, n^2 ensemble measurements are needed, requiring $\approx \mathcal{O}(n^2)$ steps. The previous methods require the determination of n_1^2 density matrices each $n_2 \times n_2$ and take $\approx \mathcal{O}(n_1^2 n_2^2)$ steps. The current method requires the determination of one $n_1 n_2 \times n_1 n_2$ density matrix which also requires $\approx \mathcal{O}(n_1^2 n_2^2)$ steps. In both cases, the number of steps is of the same order as the number of degrees of freedom in the quantum operation and are optimal in some sense.

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