Reversing Unknown Qubit-Unitary Operation, Deterministically and Exactly

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We report a deterministic and exact protocol to reverse any unknown qubit-unitary operation, which simulates the time inversion of a closed qubit system. To avoid known no-go results on universal deterministic exact unitary inversion, we consider the most general class of protocols transforming unknown unitary operations within the quantum circuit model, where the input unitary operation is called multiple times in sequence and fixed quantum circuits are inserted between the calls. In the proposed protocol, the input qubit-unitary operation is called 4 times to achieve the inverse operation, and the output state in an auxiliary system can be reused as a catalyst state in another run of the unitary inversion. We also present the simplification of the semidefinite programming for searching the optimal deterministic unitary inversion protocol for an arbitrary dimension presented by M. T. Quintino and D. Ebler [Quantum **6**, 679 (2022)]. We show a method to reduce the large search space representing all possible protocols, which provides a useful tool for analyzing higher-order quantum transformations for unitary operations.

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Introduction.—Time flows from the past toward the future, and the direction of time cannot be changed [1]. Time evolution of a closed quantum system is represented by a reversible operation, namely, a *unitary operation* corresponding to a unitary operator $U = e^{-iHt}$ using a Hamiltonian H and time t [2]. Then, we may simulate the inverse operation corresponding to $U^{-1} = e^{iHt}$ by preparing the system with Hamiltonian $-H$ if we know the full description of H. However, a physical system in nature does not tell us the full description of H *a priori*. Process tomography may be used to estimate the full description, but it may destroy the original state and introduces an extra resource overhead [3,4]. To simulate the time inversion $t \mapsto -t$ of a physical system, one needs to simulate the inverse operations of unitary operations given as *black boxes*. In this Letter, we consider the following task called "unitary inversion": Given a d-dimensional unknown unitary operation represented by a unitary operator U_{in}, the task is to implement the inverse operation U_{in}^{-1}. Simulation of the inverse operation of unitary operations plays an important role not only for foundational problems [5] but also for practical problems such as controlling quantum systems [6] and measurement of the out-of-time-order correlators [7–10]. Unitary inversion has also been investigated as one of the most important transformations of quantum operations, namely *higher-order quantum transformations* [11], which are studied to aim for a quantum version of functional programming [12].

In general, it is difficult to develop a protocol implementing a given functionality. It is nontrivial whether such a protocol exists or not in quantum regime. As often is the case with universal protocols (e.g., state cloning [13] and universal NOT [14]), we cannot implement the inverse operation U_{in}^{-1} deterministically and exactly with a single use of U_{in} [15]. To avoid this no-go theorem, protocols utilizing n calls of U_{in} to implement U_{in}^{-1} have been investigated. One trivial protocol is to perform a quantum process tomography [3,4] of U_{in} and then implement the inverse operation of the estimated operation. However, this protocol needs a large number of calls of U_{in}, and the implemented operation is nonexact. More efficient nonexact or exact but probabilistic protocols have been considered. A nonexact unitary inversion protocol is proposed in Ref. [16] inspired by the refocusing in NMR [17,18]. A probabilistic exact protocol for qubit-unitary inversion is proposed in Ref. [19]. This protocol is generalized to an arbitrary dimension in Refs. [20,21] by utilizing unitary complex conjugation [22,23] and port-based teleportation [24–26]. Nonexact protocols using a similar strategy are proposed in Refs. [23,27]. Probabilistic exact protocols to reverse uncontrolled Hamiltonian dynamics are presented in Refs. [6,28–30]. Yet, the proposed protocols so far are either *probabilistic* or *nonexact*, i.e., the output operation is obtained probabilistically or nonexactly even if all the operations in the protocol are error-free. This property limits the power of unitary inversion as a subroutine in practical problems since even a small failure probability or a small error will accumulate to destroy the whole computational result if we concatenate transformations of unitary operations.

Some works have investigated the fundamental limits of unitary inversion. The limits of probabilistic exact or deterministic nonexact unitary inversion have been investigated using semidefinite programming (SDP) [21,27], but the obtained numerical results are limited to small d and n since we need to search within a large space including all possible protocols. The limits have also been analyzed on the restricted set of protocols (e.g., exact [20] or deterministic [27] protocol utilizing n calls of $U_{\rm in}$ in parallel, exact "store-and-retrieve" protocol [19], and clean protocol [31]). Deterministic exact unitary inversion is shown to be impossible using parallel or "store-and-retrieve" protocols, and clean protocols of exact unitary inversion do not exist when $n \neq -1 \bmod d$, even if probabilistic. However, it has been an open problem whether deterministic exact unitary inversion is possible or not using more general protocols.

In this Letter, we report a *deterministic* and *exact* protocol of qubit-unitary inversion. This protocol utilizes $n = 4$ calls of a qubit unitary $U_{\rm in} \in \mathrm{SU}(2)$ in sequence with fixed quantum operations (see Fig. 1). The output state in the auxiliary system depends on the input unitary operation $U_{\rm in}$, which can be used as a catalyst state in another run of the unitary inversion [see Eq. (1)]. To search unitary inversion protocols for an arbitrary dimension d, we use an SDP to obtain the optimal deterministic unitary inversion, presented in Ref. [27]. We reduce the size of the search space by utilizing a certain symmetry, and obtain the numerical results for $n \leq 5$ and $d \leq 6$.

Main result.—We present the main result of this Letter, the existence of deterministic exact qubit-unitary inversion.

Theorem 1: There exists a quantum circuit transforming 4 calls of *any* qubit-unitary operation $U_{\rm in}$ into its inverse operation $U_{\rm in}^{-1}$ *deterministically* and *exactly*.

We show Theorem 1 by constructing a deterministic exact qubit-unitary inversion shown in Fig. 1. It is implemented using 4 calls of an arbitrary input qubit-unitary operation $U_{\rm in}$ with fixed quantum operations (unitary operations $V^{(1)}$ and $V^{(2)}$ and preparation of the antisymmetric state $|\psi^-\rangle \coloneqq (|01\rangle - |10\rangle)/\sqrt{2}$). The unitary operations $V^{(1)}$ and $V^{(2)}$ are constructed using the Clebsch-Gordan transforms [41,42] (see Supplemental Material [32] for the detail). This quantum circuit outputs $U_{\rm in}^{-1}|\phi_{\rm in}\rangle$ for an arbitrary input qubit-unitary operation $U_{\rm in}$ and an arbitrary input qubit state $|\phi_{\rm in}\rangle$ with additional quantum states $|\psi_{U_{\rm in}}\rangle \coloneqq (U_{\rm in} \otimes \mathbb{1})|\psi^-\rangle$ and $|0\rangle^{\otimes 4}$, where $\mathbb{1}$ is the identity operator on a qubit system. The simulation of this quantum circuit in QISKIT [43] is available at Ref. [44].

The quantum state $|\psi_{U_{\rm in}}\rangle$ can be used as a catalyst in the qubit-unitary inversion. Since the first call of $U_{\rm in}$ in Fig. 1 can be replaced by the quantum state $|\psi_{U_{\rm in}}\rangle$, we can transform 3 calls of $U_{\rm in}$ and the quantum state $|\psi_{U_{\rm in}}\rangle$ to the inverse operation $U_{\rm in}^{-1}$ and the quantum state $|\psi_{U_{\rm in}}\rangle$. This transformation can be schematically written as

$$|\phi_{\rm in}\rangle \otimes |\psi_{U_{\rm in}}\rangle \otimes |0\rangle^{\otimes 4} \mapsto U_{\rm in}^{-1}|\phi_{\rm in}\rangle \otimes |\psi_{U_{\rm in}}\rangle \otimes |0\rangle^{\otimes 4}, \qquad (1)$$

by using 3 calls of $U_{\rm in}$. Therefore, qubit-unitary inversion is implemented using 3 calls of the input unitary operation $U_{\rm in}$ and the catalyst state $|\psi_{U_{\rm in}}\rangle$, which can be reused to another run of qubit-unitary inversion of the same input unitary operation $U_{\rm in}$.

Proof sketch of Theorem 1:—The quantum circuit shown in Fig. 1 applies a unitary operation $f_{U_{\rm in}} \coloneqq V^{(2)}_{1\cdots 7}[\mathbb{1}^{\otimes 6}_{13\cdots 7} \otimes (U_{\rm in})_2]V^{(1)}_{1\cdots 7}[\mathbb{1}^{\otimes 6}_{13\cdots 7} \otimes (U_{\rm in})_2]$ twice on the quantum state $|\psi_{\rm in}\rangle \coloneqq |\phi_{\rm in}\rangle_1 \otimes |\psi^-\rangle_{23} \otimes |0\rangle^{\otimes 4}_{4\cdots 7}$, where the subscripts represent indices of the qubits on which the corresponding

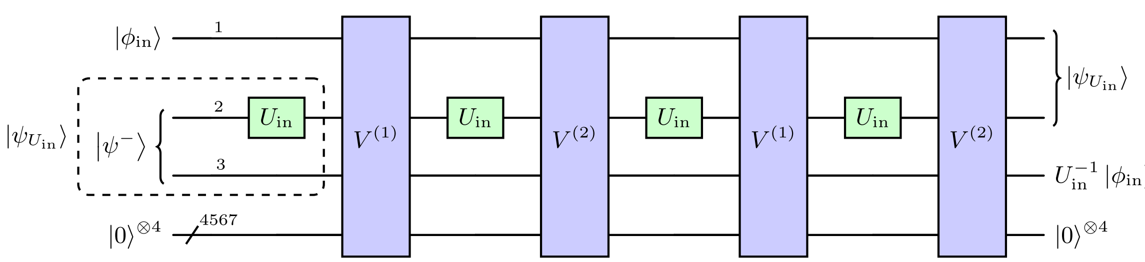

FIG. 1. Deterministic exact qubit-unitary inversion protocol using 4 calls of an input qubit-unitary operation $U_{\rm in}$, which implements the inverse operation $U_{\rm in}^{-1}$ on an arbitrary input quantum state $|\phi_{\rm in}\rangle$ with additional quantum states $|\psi_{U_{\rm in}}\rangle \coloneqq (U_{\rm in} \otimes \mathbb{1})|\psi^-\rangle$ and $|0\rangle^{\otimes 4}$. Here, each wire without a slash represents a qubit system, each wire with a slash represents a multiqubit system, numbers on wires represent the indices of the corresponding systems, $|\psi^-\rangle$ is the antisymmetric state defined as $|\psi^-\rangle \coloneqq (|01\rangle - |10\rangle)/\sqrt{2}$, and $V^{(1)}$ and $V^{(2)}$ are fixed unitary operations [32].

quantum operations act. It is sufficient to show that the output quantum state of the quantum circuit is given by $|\psi_{\mathrm{out}}\rangle \coloneqq -|\psi_{U_{\mathrm{in}}}\rangle_{12} \otimes U_{\mathrm{in}}^{-1}|\phi_{\mathrm{in}}\rangle_3 \otimes |0\rangle_{4\cdots 7}^{\otimes 4}$, i.e.,

$$f_{U_{\mathrm{in}}}^2|\psi_{\mathrm{in}}\rangle = |\psi_{\mathrm{out}}\rangle \quad \forall\ |\phi_{\mathrm{in}}\rangle \in \mathbb{C}^2, \quad U_{\mathrm{in}} \in \mathrm{SU}(2) \qquad (2)$$

holds.

This equation is equivalent to

$$g_{U_{\mathrm{in}}}^2|v_\phi\rangle = -|w_\phi\rangle \quad \forall\ |\phi\rangle \in \mathbb{C}^2, \quad U_{\mathrm{in}} \in \mathrm{SU}(2), \qquad (3)$$

where $g_{U_{\mathrm{in}}}$, $|v_\phi\rangle$ and $|w_\phi\rangle$ are defined by $g_{U_{\mathrm{in}}} \coloneqq [(U_{\mathrm{in}})_1 \otimes \mathbb{1}_{2\cdots 7}^{\otimes 6}]^\dagger (f_{U_{\mathrm{in}}})_{1\cdots 7}[(U_{\mathrm{in}})_1 \otimes \mathbb{1}_{2\cdots 7}^{\otimes 6}]$, $|v_\phi\rangle \coloneqq |\phi\rangle_1 \otimes |\psi^-\rangle_{23} \otimes |0\rangle_{4\cdots 7}^{\otimes 4}$, and $|w_\phi\rangle \coloneqq |\psi^-\rangle_{12} \otimes |\phi\rangle_3 \otimes |0\rangle_{4\cdots 7}^{\otimes 4}$, respectively. To show this relation, we investigate the action of $g_{U_{\mathrm{in}}}$ on a 4-dimensional subspace $\mathcal{H} \subset (\mathbb{C}^2)^{\otimes 7}$ defined by $\mathcal{H} \coloneqq \mathrm{span}\{|v_\phi\rangle, |w_\phi\rangle \,|\, |\phi\rangle \in \mathbb{C}^2\}$. We show that the action of $g_{U_{\mathrm{in}}}$ on the Hilbert space $\mathcal{H}$ is given by

$$g_{U_{\mathrm{in}}}(|v_\phi\rangle, |w_\phi\rangle) = (|v_\phi\rangle, |w_\phi\rangle)G \quad \forall\ |\phi\rangle \in \mathbb{C}^2, \qquad (4)$$

$$G \coloneqq \begin{pmatrix} -\frac{1}{\sqrt{3}} & -\frac{1}{\sqrt{3}} \\ \frac{1}{\sqrt{3}} & -\frac{2}{\sqrt{3}} \end{pmatrix}, \qquad (5)$$

if we define $V^{(1)}$ and $V^{(2)}$ properly using the Clebsch-Gordan transforms. Thus, we obtain Eq. (3) since

$$g_{U_{\mathrm{in}}}^2|v_\phi\rangle = g_{U_{\mathrm{in}}}^2(|v_\phi\rangle, |w_\phi\rangle)(1,0)^T \qquad (6)$$

$$= (|v_\phi\rangle, |w_\phi\rangle)G^2(1,0)^T \qquad (7)$$

$$= -|w_\phi\rangle \qquad (8)$$

holds. See Supplemental Material [32] for the definitions of $V^{(1)}$ and $V^{(2)}$ and the detail of the calculations.

SDP approach toward generalization for $d > 2$.—We consider the problem to find deterministic exact d-dimensional unitary inversion protocols for general d. Reference [27] showed the optimal deterministic unitary inversion circuit is obtained by the following SDP:

$$\max\ \mathrm{Tr}(C\Omega)$$
$$\text{s.t. } C \text{ is a quantum comb.} \qquad (9)$$

The solution of the SDP (9) gives the optimal average-case channel fidelity of unitary inversion using a quantum comb, namely, transformations of quantum operations realized by a quantum circuit shown in Fig. 2. The operator C is a matrix representation of a quantum comb called the Choi matrix of a quantum comb, and it is characterized by positivity and linear constraints [45]. Once the Choi matrix C is obtained, a quantum circuit implementing the corresponding quantum comb can be derived [46]. The operator Ω is a $d^{2(n+1)} \times d^{2(n+1)}$ positive matrix called the performance operator [27]. In particular, if the solution equals 1, deterministic exact unitary inversion is obtained (see Supplemental Material [32] for the detail).

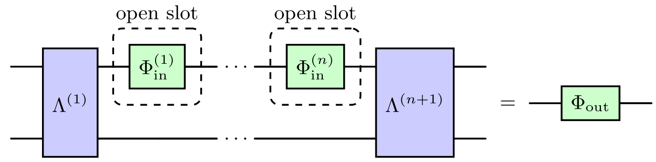

FIG. 2. Quantum combs are composed of a sequence of quantum operations $\Lambda^{(1)}, \ldots, \Lambda^{(n+1)}$ with open slots. Input quantum operations $\Phi_{\mathrm{in}}^{(1)}, \ldots, \Phi_{\mathrm{in}}^{(n)}$ can be inserted to the open slots to obtain an output operation Φ_{out}.

However, the numerical calculation of the SDP (9) in Ref. [27] is limited to $n \leq 3$ for $d = 2$ and $n \leq 2$ for $d = 3$ since the size of the matrix C is $d^{2(n+1)} \times d^{2(n+1)}$, which grows exponentially with respect to n. We present the simplification of the SDP (9) in Supplemental Material [32]. The main idea is to utilize the $\mathrm{SU}(d) \times \mathrm{SU}(d)$ symmetry of the operator Ω given by

$$[\Omega, V^{\otimes n+1} \otimes W^{\otimes n+1}] = 0 \quad \forall\ V, W \in \mathrm{SU}(d). \qquad (10)$$

Because of this symmetry, the SDP (9) can be solved without loss of generality by imposing an additional constraint given by

$$[C, V^{\otimes n+1} \otimes W^{\otimes n+1}] = 0 \quad \forall\, V, W \in \mathrm{SU}(d). \qquad (11)$$

The constraint (11) enables us to reduce the size of the SDP (9). For instance, when $n = 1$, any matrix C satisfying Eq. (11) can be written as

$$C = \sum_{\mu,\nu \in \{\mathrm{sym},\mathrm{antisym}\}} c^{\mu\nu}\Pi_\mu \otimes \Pi_\nu, \qquad (12)$$

where $c^{\mu\nu}$ are complex coefficients and Π_{sym} and Π_{antisym} are orthogonal projectors onto symmetric and antisymmetric subspaces of $(\mathbb{C}^d)^{\otimes 2}$, respectively. Then, the degree of freedom in the matrix C reduces from d^8 to 4. For a general n, we derive a block diagonalization of C using a group-theoretic relation called the Schur-Weyl duality [47,48] to obtain the simplified SDP.

We calculate the simplified SDP in MATLAB [49] using the interpreter CVX [50,51] with the solvers SDPT3 [52–54] and SEDUMI [55], and obtain the optimal values for $n \leq 5$ and $d \leq 6$ (see Table I). Group-theoretic calculations to write down the simplified SDP are done with SAGEMATH [56]. By estimating the analytical formula for the Choi matrix from the numerical result, we can derive the corresponding unitary inversion circuit [46]. In fact, the deterministic exact qubit-unitary inversion circuit shown in

TABLE I. The optimal value of the SDP (9) is numerically obtained for $n \leq 5$ and $d \leq 6$, which is the optimal fidelity of a deterministic transformation from n calls of an unknown unitary operation $U_{\mathrm{in}} \in \mathrm{SU}(d)$ to its inverse operation U_{in}^{-1}.

	$n = 1$	$n = 2$	$n = 3$	$n = 4$	$n = 5$
$d = 2$	0.5000	0.7500	0.9330	1.0000	1.0000
$d = 3$	0.2222	0.3333	0.4444	0.5556	0.6667
$d = 4$	0.1250	0.1875	0.2500	0.3125	0.3750
$d = 5$	0.0800	0.1200	0.1600	0.2000	0.2400
$d = 6$	0.0556	0.0833	0.1111	0.1389	0.1667

Fig. 1 is derived from the numerical result for the case $d = 2$ and $n = 4$.

We also present the SDP to obtain the optimal fidelity of unitary inversion using the input unitary operations in parallel, which is simplified compared to Ref. [27]. Our calculation allows us to obtain the numerical results beyond the previous work [27], which exhibits the coincidence between parallel and sequential optimal protocols for $n \leq d - 1$ [32]. The codes are available at Ref. [44] under the MIT license [57].

Discussions.—We compare the deterministic exact unitary inversion with the previously known protocols for qubit-unitary inversion. We consider the required number of calls of the input unitary operation to achieve success probability $p = 1 - \eta$ and/or average-case channel fidelity $F = 1 - \epsilon$, i.e., η and ϵ represent a failure probability and an approximation error of the protocol, respectively. The best-known protocol for probabilistic exact unitary inversion uses a "success-or-draw" strategy [20,21,58], which requires $n = O(\log \eta^{-1})$ calls of the input unitary operation to achieve the success probability $p = 1 - \eta$. We can convert this protocol to a deterministic nonexact protocol [27], which requires $n = O(\log \epsilon^{-1})$ to achieve the average-case channel fidelity $F = 1 - \epsilon$. On the other hand, the qubit-unitary inversion protocol presented in this Letter achieves $\eta = \epsilon = 0$ with $n = O(1)$. Therefore, our protocol is superior to the protocols in the previous works regarding the scaling of n with respect to failure probability η and approximation error ϵ (see Table II and Supplemental Material [32] for the detail).

As shown in Refs. [21,27], any protocol using 3 calls of a qubit-unitary operation cannot implement unitary inversion deterministically and exactly. Thus, the protocol shown in this Letter uses the minimum number of calls of a qubit-unitary operation. However, this fact does not mean that all information on the input unitary operation U_{in} is "consumed" in the unitary inversion protocol. Protocols "consuming" all information of the input unitary operations are analyzed as *clean* protocols, namely, the protocols where the auxiliary system used for the protocol does not depend on the input unitary operation, in Ref. [31]. As shown in Ref. [31], clean protocols of exact unitary inversion using n calls of an input d-dimensional unitary operation do not exist when $n \neq -1 \bmod d$. The protocol shown in this Letter avoids this no-go theorem by removing the restriction that the protocols be clean. In fact, the output state of the auxiliary system is given by $|\psi_{U_{\mathrm{in}}}\rangle \otimes |0\rangle^{\otimes 4}$, which stores some information about U_{in}. As shown in Eq. (1), the quantum state $|\psi_{U_{\mathrm{in}}}\rangle$ can be used as a catalyst, i.e., it can be reused in another run of the unitary inversion of the same unitary operation U_{in}. This is a possible application of the stored information about the input operation in output auxiliary states of nonclean protocols.

On the other hand, our qubit-unitary inversion protocol can be made clean by adding an extra call of the input unitary operation U_{in}. We can remove the information of U_{in} stored in the quantum state $|\psi_{U_{\mathrm{in}}}\rangle$ by applying U_{in} since $(\mathbb{1} \otimes U_{\mathrm{in}})|\psi_{U_{\mathrm{in}}}\rangle = U_{\mathrm{in}}^{\otimes 2}|\psi^-\rangle = |\psi^-\rangle$ holds. Since nonclean protocols require a thermodynamic cost to erase the information [59,60], the clean unitary inversion protocol has the potential to reduce the thermodynamic cost of quantum computation.

Conclusion.—In this Letter, we constructed a deterministic exact unitary inversion protocol using 4 calls of input qubit unitary operation $U_{\mathrm{in}} \in \mathrm{SU}(2)$ in sequence. This transformation can be regarded as a transformation from 3 calls of U_{in} to its inverse operation U_{in}^{-1} with a catalyst state $|\psi_{U_{\mathrm{in}}}\rangle$ as shown in Eq. (1), and we can make the protocol clean by adding an extra use of U_{in}. We leave it a future work to investigate general higher-order quantum transformations with catalyst states.

TABLE II. Comparison of our deterministic exact qubit-unitary inversion with previous works. The query complexity is the number of calls of the input operation with respect to failure probability η and/or approximation error ϵ.

	Deterministic	Exact	Query complexity
Universal refocusing [16]	×	×	$O(\eta^{-5} \log^2 \epsilon^{-1})$
Optimal parallel protocol (probabilistic exact) [19–21]	×	✓	$O(\eta^{-1})$
Optimal parallel protocol (deterministic nonexact) [27]	✓	×	$O(\epsilon^{-1/2})$
Success-or-draw (probabilistic exact) [20,21,58]	×	✓	$O(\log \eta^{-1})$
Success-or-draw (deterministic nonexact) [27]	✓	×	$O(\log \epsilon^{-1})$
Universal rewinding [28,29]	×	✓	$O(\log \eta^{-1})$
This Letter	✓	✓	$O(1)$

We also presented the SDP approach to seek deterministic exact unitary inversion for $d > 2$. We showed the simplification of the SDP using the $\mathrm{SU}(d) \times \mathrm{SU}(d)$ symmetry, which enables numerical calculation up to $n \leq 5$. Reference [61] presents the reduction of SDPs with $\mathrm{SU}(d)$ symmetry and additional symmetry to linear programming. It is an interesting future work to invent a similar technique for the SDP of unitary inversion, which will be applied to seek deterministic exact unitary inversion for $d > 2$.

We can also extend the qubit-unitary inversion protocol presented in this Letter to a protocol reversing any qubit-encoding isometry operations, namely, quantum operations transforming qubit pure states to *qudit* pure states. This extension is done by constructing a quantum circuit transforming unitary inversion protocols to isometry inversion protocols, which will be presented in another work [62].

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