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 four times to achieve the inverse operation. We present the qubit-unitary inversion protocol by deriving the corresponding Choi matrix with the SU(2) × SU(2) symmetry. We also present the semidefinite programming (SDP) for searching a deterministic exact unitary inversion protocol for an arbitrary dimension. By utilizing the SU(d) × SU(d) symmetry on the Choi matrix, 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.

Introduction.— Time flows from the past towards 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 \( t \rightarrow -t \) 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 \( U_d \), the task is to implement the inverse operation \( U_d^{-1} \). Simulation of the inverse operation of unitary operations plays an important role not only on foundational problems [5] but also on practical problems such as controlling quantum systems [6] and measurement of the out-of-time-order correlators (OTOCs) [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 \( U_d^{-1} \) deterministically and exactly with a single use of \( U_d \) [15]. To avoid this no-go theorem, protocols utilizing \( n \) calls of \( U_d \) to implement \( U_d^{-1} \) have been investigated. One trivial protocol is to perform a quantum process tomography [3, 4] of \( U_d \) and then implement the inverse operation of the estimated operation. However, this protocol needs a large number of calls of \( U_d \), and the implemented operation is non-exact. More efficient non-exact or exact but probabilistic protocols have been considered. A non-exact 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, 25]. Non-exact protocols using a similar strategy are proposed in Refs. [23, 24]. Probabilistic exact protocols to reverse uncontrolled Hamiltonian dynamics are presented in Refs. [6, 25, 30]. Yet, the proposed protocols so far are either probabilistic or non-exact, which limit 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.

Some works have investigated the fundamental limits of unitary inversion. The limits of probabilistic exact or deterministic non-exact 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
In this Letter, quantum operations are denoted with a tum combs are supermaps that can be implemented by a linear transformations of quantum operations. Quantum work of supermaps and quantum combs. Supermaps are SDP by imposing a similar symmetry on the Choi matrix. Deterministic exact unitary inversion protocols for an arbitrary dimension \( d \) have been analyzed on the restricted set of protocols (e.g., exact \([20]\) or deterministic \([27]\) protocol utilizing \( n \) calls of \( U_d \) 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 \( n \neq -1 \mod d \), 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 \( U_2 \) in sequence with fixed quantum operations \( \Lambda_i \) for \( i \in \{1, 2, 3, 4, 5\} \) (see FIG. 1).

To search unitary inversion protocols, we use the framework of supermaps and quantum combs. Supermaps are linear transformations of quantum operations. Quantum combs are supermaps that can be implemented by a quantum circuit using input operations in a fixed order. In this Letter, quantum operations are denoted with a tilde like \( \tilde{U} \), while supermaps are denoted with a double tilde like \( \tilde{\tilde{C}} \). We represent quantum combs using their Choi matrices \([32]\), and we search within the protocols whose Choi matrices have a certain symmetry to reduce the size of the search space. We also show an SDP searching deterministic exact unitary inversion protocols for an arbitrary dimension \( d \). We reduce the complexity of the SDP by imposing a similar symmetry on the Choi matrix.

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

**Theorem 1.** There exists a 4-slot quantum comb \( \tilde{C} \) transforming 4 calls of any qubit unitary operation \( \tilde{U}_2 \) into its inverse operation \( \tilde{U}_2^{-1} \) deterministically and exactly, i.e.,

\[
\tilde{C}(\tilde{U}_2^\otimes 4) = \tilde{U}_2^{-1} \tag{1}
\]

for all qubit unitary operations \( \tilde{U}_2 \).

**Choi matrix of quantum comb.**— To prove Theorem 1, we introduce the Choi matrix of quantum combs. A quantum comb \( \tilde{C} : \bigotimes_{i=1}^n [L(I_i) \rightarrow L(O_i)] \rightarrow [L(P) \rightarrow L(F)] \) can be characterized by the Choi matrix \( C \in L(\mathcal{P} \otimes \mathcal{I}^n \otimes \mathcal{O}^n \otimes \mathcal{F}) \), where \( L(\mathcal{H}) \) denotes the space of linear operators on \( \mathcal{H} \), \( [L(\mathcal{H}_1) \rightarrow L(\mathcal{H}_2)] \) denotes the space of linear operators from \( L(\mathcal{H}_1) \) to \( L(\mathcal{H}_2) \), and \( \mathcal{I}^n \) and \( \mathcal{O}^n \) are defined by \( \mathcal{I}^n := \bigotimes_{i=1}^n I_i \) and \( \mathcal{O}^n := \bigotimes_{i=1}^n O_i \), as shown in the following Lemma.

**Lemma 2.** \([32]\) Suppose a matrix \( C \in L(\mathcal{P} \otimes \mathcal{I}^n \otimes \mathcal{O}^n \otimes \mathcal{F}) \) satisfies

\[
C \geq 0, \tag{2}
\]

\[
\text{Tr}_\mathcal{I} C_i = C_{i-1} \otimes I_{O_{i-1}}, \tag{3}
\]

\[
C_0 = 1, \tag{4}
\]

for \( i \in \{1, \ldots, n+1\} \), where \( I_{\mathcal{H}} \) is the identity operator on \( \mathcal{H} \), \( C_{n+1} := C \), \( C_{i-1} := \text{Tr}_\mathcal{I} C_i \otimes C_i / d \), and \( I_{n+1} \), \( O_0 \) are defined by \( I_{n+1} := \mathcal{F} \), \( O_0 := \mathcal{P} \). Then, there exists a sequence of quantum operations \( \Lambda_i \) implementing the corresponding supermap \( \tilde{C} \).

In terms of the Choi matrix, the condition that a quantum comb \( \tilde{C} \) implements unitary inversion \([\text{Eq. } (1)]\) can be written as

\[
C \ast |U_2\rangle\langle U_2|_{\mathcal{P}\mathcal{I}^n} = |U_2^{-1}\rangle\langle U_2^{-1}|_{\mathcal{P}\mathcal{F}}, \tag{5}
\]

for all \( U_2 \in \mathcal{U}(2) \), where \( |U_2\rangle\langle U_2|_{\mathcal{I}O} := \sum_i |i\rangle \otimes (|U_2|i\rangle) \in \mathcal{I} \otimes \mathcal{O} \) is the Choi vector of a unitary operator \( U_2 \) for the computational basis \( \{|i\rangle\} \) of \( \mathcal{I} = \mathcal{O} = \mathbb{C}^2 \), and the link product \( A \ast B \) of two matrices \( A \in L(\mathcal{X} \otimes \mathcal{Y}) \) and \( B \in L(\mathcal{Y} \otimes \mathcal{Z}) \) is defined as \( A \ast B := \text{Tr}_\mathcal{Y}(A^T B) \) using the partial transpose of \( A \) in the system \( \mathcal{Y} \) denoted by \( A^T \).

In the following, we construct a Choi matrix \( C \in L(\mathcal{P} \otimes \mathcal{I}^4 \otimes \mathcal{O}^4 \otimes \mathcal{F}) \) satisfying the quantum comb conditions \([2]\)–\([4]\) and the unitary inversion condition \([5]\). We impose an additional constraint on \( C \) given by

\[
[C, U_2^\otimes 5 \otimes V_2^\otimes 5] = 0, \tag{6}
\]

for all \( U, V \in \mathcal{U}(2) \), where \([X, Y] := XY - YX\) is the commutator of \( X \) and \( Y \).

**Schur-Weyl duality and Young-Yamanouchi basis.**— To express the matrix satisfying the SU(\( d \)) \times SU(\( d \)) symmetry efficiently, we introduce a relationship between the special unitary group SU(\( d \)) and the symmetric group \( \mathfrak{S}_{n+1} \) called the Schur-Weyl duality. We consider the following representations on \( (\mathbb{C}^d)^{\otimes n+1} \):

\[
\text{SU}(d) \ni U \mapsto U^{\otimes n+1} \in L(\mathbb{C}^d)^{\otimes n+1}, \tag{7}
\]

\[
\mathfrak{S}_{n+1} \ni \sigma \mapsto P_{\sigma} \in L(\mathbb{C}^d)^{\otimes n+1}, \tag{8}
\]

where \( P_{\sigma} \) is a permutation operator defined as

\[
P_{\sigma} = \bigoplus_{\mu \in \mathfrak{S}_{n+1}} U_{\mu} \otimes I_{\mathfrak{S}_{n+1}}, \tag{9}
\]

\[
U^{\otimes n+1} = \bigoplus_{\mu \in \mathfrak{S}_{n+1}} U_{\mu} \otimes I_{\mathfrak{S}_{n+1}}, \tag{10}
\]

\[
P_{\sigma} = \bigoplus_{\mu \in \mathfrak{S}_{n+1}} I_{\mu} \otimes \sigma_{\mu}. \tag{11}
\]
where $\mu$ runs in the set of Young diagrams with $n+1$ boxes and at most depth $d$, denoted by $\mathcal{Y}_{n+1}^d$, and $\text{SU}(d) \ni U \mapsto U_{\mu} \in \mathcal{L}(U_{\mu})$ and $\mathcal{S}_{n+1} \ni \sigma \mapsto \sigma_{\mu} \in \mathcal{L}(S_{\mu})$ are irreducible representations. Due to Schur’s lemma, any operator commuting with $U^{\otimes n+1}$ can be written as a linear combination of the operators $E_{ij}^\mu$ defined by

$$E_{ij}^\mu := 1_{d_i} \otimes |\mu,i\rangle\langle\mu,j|_{S_{\mu}},$$

(12)

for $i,j \in \{1, \ldots, d_{\mu}\}$, where $\{|\mu,i\rangle\}$ is an orthonormal basis of $S_{\mu}$ and $d_{\mu} := \dim S_{\mu}$. In particular, we take the Young-Yamanouchi basis of $S_{\mu}$, whose element is associated with standard tableaux with frame $\mu$. The standard tableaux with $\mu$ index by $i = 1, \ldots, d_{\mu}$ and the $i$-th standard tableau is denoted by $s_{j}^{\mu}$. Each element in the Young-Yamanouchi basis $\{|\mu,i\rangle\}$ is associated with the standard tableau $s_{j}^{\mu}$.

Using the basis $\{E_{ij}^\mu\}$, any matrix $C$ satisfying Eq. (6) can be represented as

$$C = \sum_{\mu,\nu \in \mathcal{Y}^d} \sum_{i,j=1}^{d_{\mu}} \sum_{k,l=1}^{d_{\nu}} c_{ijkl}^{\mu\nu}(E_{ij}^\mu)_{\mu\nu} \otimes (E_{kl}^\nu)_{\mu\nu},$$

(13)

using complex coefficients $c_{ijkl}^{\mu\nu} \in \mathbb{C}$.

**Construction of unitary inversion comb.**—We consider the Choi matrix $C \in \mathcal{L}(\mathcal{P} \otimes \mathcal{I}^4 \otimes \mathcal{O}^4 \otimes \mathcal{F})$ for $\mathcal{P} = \mathcal{I}_1 = \mathcal{O}_1 = \mathbb{C}^4$ defined by

$$C = \frac{1}{2} \sum_{i,j=2}^{5} (-1)^{a_i + a_j} (E_{ii}^{i})_{\mu} \otimes (E_{jj}^{j})_{\mu} \otimes (E_{ij}^{i,j})_{\mu} \otimes (E_{ji}^{i,j})_{\mu},$$

$$+ \frac{1}{2} \sum_{i,j=4}^{5} (E_{ii}^{i})_{\mu} \otimes (E_{jj}^{j})_{\mu} \otimes (E_{ij}^{i,j})_{\mu} \otimes (E_{ji}^{i,j})_{\mu},$$

$$+ \frac{1}{2} (E_{55}^{i})_{\mu} \otimes (E_{11}^{i})_{\mu} \otimes (E_{11}^{j})_{\mu} \otimes (E_{11}^{j})_{\mu},$$

(14)

where $a_i$ is defined as

$$a_i := \begin{cases} 0 & (i \in \{2, 3\}) \\ 1 & (i \in \{4, 5\}) \end{cases},$$

(15)

Young diagrams $\alpha_i$ for $i \in \{1, 2, 3\}$ are defined as

$$\alpha_1 := \begin{array}{cccc} \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \end{array}, \quad \alpha_2 := \begin{array}{cccc} \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \end{array}, \quad \alpha_3 := \begin{array}{cccc} \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \end{array},$$

(16)

and standard tableaux $s_{j}^{\alpha_{i}}$ for $j \in \{1, \ldots, d_{\alpha_{i}}\}$ are defined in TABLE I. Then, $C$ is the Choi matrix of a unitary inversion comb as shown in the following Lemma. This Lemma immediately leads to Theorem 1.

**Lemma 3.** The matrix $C$ defined in Eq. (14) satisfies the quantum comb conditions (2)-(4) and the unitary inversion condition (5).

**Proof sketch.** The partial trace of $E_{ij}^\mu$ in the last system and the tensor product of $E_{ij}^\mu$ and the identity operator can be calculated using the relationships between standard tableaux. Using this fact, the quantum comb conditions (2)-(4) can be checked with a direct calculation. The unitary inversion condition (5) is shown to be equivalent to the following condition:

$$\text{Tr}(\mathcal{C}\Omega) = 1,$$

(17)

$$\Omega := \frac{1}{4} \sum_{\mu \in \mathcal{Y}^d} \sum_{i,j,k,l=1}^{d_{\mu}} [\pi_{\mu}]_{ikl}(E_{ijkl}^\mu)_{\mu} \otimes (E_{ijkl}^\mu)_{\mu},$$

(18)

where $\pi$ is a cyclic permutation defined as $\pi := (12345) \in \mathcal{S}_5$, $\mathcal{S}_5 \ni \sigma \mapsto \sigma_{\mu} \in \mathcal{L}(S_{\mu})$ is defined as Eq. (11), and $[\pi_{\mu}]_{ij} := \langle \mu, i|\pi_{\mu}|\mu, j\rangle$. The condition (17) can be checked with a direct calculation. See Supplemental Material [33] for the detail of the proof.

**SDP approach towards generalization for $d > 2$.**—We consider the problem to find deterministic exact $d$-dimensional unitary inversion protocols for general $d$. Similarly to Eq. (5), the unitary inversion condition for general $d$ and $n$ is given by

$$C \ast |U_d\rangle \langle U_d|_{\mathcal{P}^n} \ast = |U_d\rangle \langle U_d|_{\mathcal{P}^n},$$

(19)

where $\Omega_{d,n}$ is defined by

$$\Omega_{d,n} := \sum_{\mu \in \mathcal{Y}^d_{n+1}} \sum_{i,j,k,l=1}^{d_{\mu}} [\pi_{\mu}]_{ikl}(E_{ijkl}^\mu)_{\mu} \otimes (E_{ijkl}^\mu)_{\mu},$$

(21)

and standard tableaux $s_{j}^{\alpha_{i}}$ for $j \in \{1, \ldots, d_{\alpha_{i}}\}$ are defined in TABLE I. Then, $C$ is the Choi matrix of a quantum comb as shown in the following Lemma. This Lemma immediately leads to Theorem 1.
If the optimal value equals 1, the obtained optimal Choi matrix $C = C_{\text{opt}}$ corresponds to a quantum comb implementing a deterministic exact unitary inversion. If the optimal value is less than 1, it shows that there is no quantum comb implementing deterministic exact unitary inversion using $n$ calls of input unitary operation $U_d \in \text{SU}(d)$. Note that the SDP (22) is also used to analyze deterministic non-exact unitary inversion in Ref. [27].

However, the numerical calculation of the SDP (22) in Ref. [27] is limited to $n \leq 3$ for $d = 2$ and $n \leq 2$ for $d = 3$. We present the simplification of the SDP (22) as shown in Supplementary Material [33]. The main idea of the simplification is to utilize the $\text{SU}(d,n)$ symmetry of the operator $\Omega_{d,n}$ given by

$$\Omega_{d,n} \equiv \left[ U^{\otimes n+1}_d \otimes V^{\otimes n+1}_{PO^d} \right] = 0,$$  

(23)

for all $U,V \in \text{SU}(d)$. Due to this symmetry, the SDP (22) can be solved without loss of generality by imposing an additional constraint given by

$$[C, U^{\otimes n+1}_d \otimes V^{\otimes n+1}_{PO^d}] = 0,$$  

(24)

for all $U,V \in \text{SU}(d)$. The constraint (24) enables us to write down the Choi matrix $C$ with the basis $\{E_{ij}^{\mu}\}$ defined in Eq. (12) using a similar argument to derive Eq. (13) from the constraint (6), which reduces the number of variables of the SDP (22).

We calculate the simplified SDP in MATLAB [34] using the interpreters CVX [35, 36] and YALMIP [37–40] with the solvers SDPT3 [41] and SCS [42], and obtain the optimal values for $n \leq 5$ and $d \leq 6$. By estimating the analytical formula for the Choi matrix from the numerical result, we can derive the existence of deterministic exact unitary inversions analytically. In fact, the Choi matrix shown in Eq. (14) is derived from the numerical result for the case $d = 2$ and $n = 4$.

**Discussions.**—Once the Choi matrix $C$ of a quantum comb $\tilde{C}$ is obtained, we can write a quantum circuit implementing $\tilde{C}$ using isometry operations and the trace-out operation at the end [13] as shown in FIG. 2. The minimal dimension of the auxiliary system is given by the rank of $C$ [43], which is rank($C$) = 44 for the qubit unitary inversion comb given by Eq. (14). As shown in Supplemental Material [33], we can reduce the rank of the Choi matrix of a qubit unitary inversion comb to $14 \leq 2^4$ by giving up the $\text{SU}(2) \times \text{SU}(2)$ symmetry of the Choi matrix. Thus, we can implement a deterministic exact unitary inversion quantum comb using auxiliary 4 qubits.

We compare the performance of the deterministic exact unitary inversion with the previously known protocols. The optimal success probability of exact qubit unitary inversion using input unitaries in parallel is known to be $p = n/(n + 3)$ [21]. The success probability is improved using a “success-or-draw” protocol to $p = 1 - (2/3)^{\lfloor n/2 \rfloor}$.

To achieve $p \geq 99.9\%$, we need $n = 2997$ calls of $U_2$ (parallel) or $n = 36$ calls of $U_2$ (“success-or-draw”), while the deterministic exact protocol shown in this work achieves $p = 100\%$ using $n = 4$ calls of $U_2$.

As shown in Refs. [21, 27], any protocol using three 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 $U_2$ 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 $n \neq -1 \mod d$. The protocol shown in this Letter avoids this no-go theorem by removing the restriction that the protocols be clean. This means that the auxiliary state before the trace-out operation in FIG. 2 stores some information about $U_2$. Information of $U_2$ encoded in the auxiliary state might be used to another transformation of $U_2$. We leave this possibility as a future work.

**Conclusion.**—In this Letter, we showed the existence of deterministic exact unitary inversion protocol using 4 calls of input qubit unitary operation $U_2 \in \text{SU}(2)$ in sequence. We constructed the Choi matrix of the unitary inversion comb using the Young-Yamanouchi basis. We presented the SDP approach to seek deterministic exact unitary inversion for $d > 2$. We showed the simplification of the SDP using the $\text{SU}(d) \times \text{SU}(d)$ symmetry, which enables numerical calculation up to $n \leq 5$. Reference [13] presents the reduction of SDPs with $\text{SU}(d)$ 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 work 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 [46].
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Supplemental Material for: “Reversing unknown qubit-unitary operation, deterministically and exactly”

The unitary inversion condition

**Lemma 4.** For $\mathcal{P} = \mathcal{F} = \mathcal{I}_d = \mathcal{O}_d = \mathbb{C}^d$ and the Choi matrix $C \in \mathcal{L}(\mathcal{P} \otimes \mathcal{I}_n \otimes \mathcal{O}_n \otimes \mathcal{F})$ of a quantum comb $\tilde{\mathcal{C}}$, we show that

$$C \star |U_d\rangle\langle U_d|^{\otimes n} = |U_d^{-1}\rangle\langle U_d^{-1}|_{\mathcal{P}\mathcal{F}}$$  \hspace{1cm} (S1)

holds for all $U_d \in \text{SU}(d)$ if and only if

$$\text{Tr}(C \Omega_{d,n}) = 1$$  \hspace{1cm} (S2)

holds, where $\Omega_{d,n}$ is defined as

$$\Omega_{d,n} := \frac{1}{d^2} \int dU_d |U_d\rangle\langle U_d|^{\otimes n} \otimes |U_d\rangle\langle U_d|_{\mathcal{F}\mathcal{P}},$$  \hspace{1cm} (S3)

and $dU_d$ is the Haar measure on $\text{SU}(d)$. The operator $\Omega_{d,n}$ is expressed in the basis $\{E^\mu_n\}$ as

$$\Omega_{d,n} = \sum_{\mu \in \mathcal{V}_{n+1}^d} \sum_{i,j,k,l=1}^{d} \frac{[\pi^\mu_{ij}(E^\mu_{kl})^{\mathcal{F}\mathcal{P}}][\pi^\mu_{ij} \otimes (E^\mu_{ij})^{\mathcal{F}\mathcal{P}}]}{d^2 \pi^\mu_{ij}}.$$  \hspace{1cm} (S4)

where $\pi$ is a cyclic permutation defined as $\pi := (123 \cdots n+1) \in \mathcal{S}_{n+1}, \mathcal{S}_{n+1} \ni \sigma \mapsto \sigma \mu \in \mathcal{L}(\mathcal{S}_n)$ is defined as Eq. [11] of the main manuscript, and $[\pi^\mu_{ij}] := \langle \mu, i | \pi^\mu_{ij} | \mu, j \rangle$.

**Proof.** We introduce the channel fidelity [37] of two CPTP maps $\tilde{\Lambda}_1, \tilde{\Lambda}_2 : \mathcal{L}(\mathcal{P}) \to \mathcal{L}(\mathcal{F})$ given by

$$F_{ch}(\tilde{\Lambda}_1, \tilde{\Lambda}_2) := \mathcal{F}(J_{\tilde{\Lambda}_1/d}, J_{\tilde{\Lambda}_2/d}),$$  \hspace{1cm} (S5)

where $\mathcal{F}(\cdot, \cdot)$ is the fidelity of two quantum states given by $\mathcal{F}(\rho_1, \rho_2) := \left| \text{Tr}(\sqrt{\sqrt{\rho_1} \rho_2 \sqrt{\rho_1}}) \right|^2$, and the Choi matrix $J_{\tilde{\Lambda}}$ of a CPTP map $\tilde{\Lambda}$ is defined by $J_{\tilde{\Lambda}} := \sum_{ij} |i\rangle \langle j| \otimes \tilde{\Lambda}(|i\rangle \langle j|)$ using the computational basis $\{|i\rangle\}$. The channel fidelity $F_{ch}(\tilde{\Lambda}_1, \tilde{\Lambda}_2)$ satisfies the following property:

$$F_{ch}(\tilde{\Lambda}_1, \tilde{\Lambda}_2) \leq 1,$$  \hspace{1cm} (S6)

$$F_{ch}(\tilde{\Lambda}_1, \tilde{\Lambda}_2) = 1 \iff \tilde{\Lambda}_1 = \tilde{\Lambda}_2,$$  \hspace{1cm} (S7)

hold for all CPTP maps $\tilde{\Lambda}_1, \tilde{\Lambda}_2$. For $\tilde{\Lambda}_{U_d} := \tilde{\mathcal{C}} (U_d^{\otimes n})$, we define $f(U_d) := \mathcal{F}(\tilde{\Lambda}_{U_d}, \tilde{\Lambda}_{U_d^{-1}})$. Then, due to the properties [S6] and [S7], Eq. [S1] holds for all $U_d \in \text{SU}(d)$ if and only if

$$\int dU_d f(U_d) = 1$$  \hspace{1cm} (S8)

holds. The left hand side of this equation can be calculated as follows:

$$\int dU_d f(U_d) = \int dU_d F(C \star |U_d\rangle\langle U_d|^{\otimes n}, |U_d^{-1}\rangle\langle U_d^{-1}|_{\mathcal{P}\mathcal{F}})$$  \hspace{1cm} (S9)

$$= \int dU_d \text{Tr}(C \star |U_d\rangle\langle U_d|^{\otimes n} |U_d^{-1}\rangle\langle U_d^{-1}|_{\mathcal{P}\mathcal{F}})$$  \hspace{1cm} (S10)

$$= \int dU_d \text{Tr}(C |U_d\rangle\langle U_d|^{\otimes n})^{\mathcal{F}\mathcal{P}} \otimes |U_d^{-1}\rangle\langle U_d^{-1}|^{\mathcal{F}\mathcal{P}})$$  \hspace{1cm} (S11)

$$= \int dU_d \text{Tr}(C |U_d\rangle\langle U_d|^{\otimes n} \otimes |U_d\rangle\langle U_d|_{\mathcal{F}\mathcal{P}})$$  \hspace{1cm} (S12)

$$= \int dU_d \text{Tr}(C |U_d\rangle\langle U_d|^{\otimes n} \otimes |U_d\rangle\langle U_d|_{\mathcal{F}\mathcal{P}})$$  \hspace{1cm} (S13)

$$= \text{Tr}(C \Omega_{d,n}).$$  \hspace{1cm} (S14)
To evaluate the operator \( \Omega_{d,n} \), we permute the systems \( \mathcal{I}^n \mathcal{F} \) by applying the permutation \( \pi = (123\cdots n + 1) \) as
\[
[(P_\pi)_{\mathcal{I}^n \mathcal{F}} \otimes |\mathcal{P}\rangle \langle \mathcal{F}|_{\mathcal{I}^n \mathcal{F}}] \Omega_{d,n} [((P_\pi)_{\mathcal{I}^n \mathcal{F}} \otimes |\mathcal{P}\rangle \langle \mathcal{F}|_{\mathcal{I}^n \mathcal{F}}] = \frac{1}{d^2} \int dU_d |U_d\rangle \langle U_d|_{\mathcal{I}^n \mathcal{F}, \mathcal{P} \mathcal{O}^n}. \tag{S15}
\]
To calculate this quantity, we introduce the Gelfand-Zetlin basis \( \{|\mu,u\rangle \} \) of \( \mathcal{U}_\mu \) in Eq. (9) of the main manuscript. The set of vectors \( \{|\mu,u\rangle \mathcal{U}_\mu \otimes |\mu,i\rangle_{\mathcal{S}_\mu}\} \) forms the basis of \( \mathcal{C}^{\otimes n+1}_d \), which is called the Schur basis. The change of the basis from the computational basis to the Schur basis is called the quantum Schur transform \([48,51]\), denoted by \( U^{\text{Sch}} \). The matrix elements of \( U^{\text{Sch}} \) are real (see e.g., Section 4 of Ref. [51]), i.e., \( (U^{\text{Sch}})^* = U^{\text{Sch}} \). Therefore, the maximally entangled state between \( \mathcal{I}^n \mathcal{F} \) and \( \mathcal{P} \mathcal{O}^n \) in the computational basis is the same as that in the Schur basis, i.e.,
\[
\sum_{\mu \in \mathbb{Y}_{n+1}^d} \sum_{u=1}^{m_\mu} \sum_{i=1}^{d_\mu} \langle (|\mu,u\rangle \mathcal{U}_\mu \otimes |\mu,i\rangle_{\mathcal{S}_\mu})_{\mathcal{I}^n \mathcal{F}} \otimes (|\mu,u\rangle \mathcal{U}_\mu \otimes |\mu,i\rangle_{\mathcal{S}_\mu})_{\mathcal{P} \mathcal{O}^n} = \sum_{i_1,\cdots,i_{n+1}=1}^d |i_1 \cdots i_n\rangle_{\mathcal{I}^n \mathcal{F}} \otimes |i_1 \cdots i_n\rangle_{\mathcal{P} \mathcal{O}^n}. \tag{S16}
\]
Then, \(|U\rangle^{\otimes n+1}_{\mathcal{I}^n \mathcal{F}, \mathcal{P} \mathcal{O}^n} \) is given by
\[
|U\rangle^{\otimes n+1}_{\mathcal{I}^n \mathcal{F}, \mathcal{P} \mathcal{O}^n} = \sum_{i_1,\cdots,i_{n+1}=1}^d |i_1 \cdots i_n\rangle_{\mathcal{I}^n \mathcal{F}} \otimes U^{\otimes n+1} |i_1 \cdots i_n\rangle_{\mathcal{P} \mathcal{O}^n} \tag{S17}
\]
\[
= \sum_{\mu \in \mathbb{Y}_{n+1}^d} \sum_{u=1}^{m_\mu} \sum_{i=1}^{d_\mu} \langle (|\mu,u\rangle \mathcal{U}_\mu \otimes |\mu,i\rangle_{\mathcal{S}_\mu})_{\mathcal{I}^n \mathcal{F}} \otimes (U_{\mu} |\mu,u\rangle \mathcal{U}_\mu \otimes |\mu,i\rangle_{\mathcal{S}_\mu})_{\mathcal{P} \mathcal{O}^n}. \tag{S18}
\]
Thus, we obtain
\[
\int dU_d |U_d\rangle \langle U_d|_{\mathcal{I}^n \mathcal{F}, \mathcal{P} \mathcal{O}^n} = \sum_{\mu \in \mathbb{Y}_{n+1}^d} \sum_{i,j=1}^{d_\mu} \langle 1_{\mathcal{U}_\mu} \otimes |\mu,i\rangle \langle \mu,j|_{\mathcal{S}_\mu} \rangle_{\mathcal{I}^n \mathcal{F}} \otimes \langle 1_{\mathcal{U}_\mu} \otimes |\mu,i\rangle \langle \mu,j|_{\mathcal{S}_\mu} \rangle_{\mathcal{P} \mathcal{O}^n} \tag{S19}
\]
\[
= \sum_{\mu \in \mathbb{Y}_{n+1}^d} \sum_{i,j=1}^{d_\mu} \frac{(E_{ij}^\mu)_{\mathcal{I}^n \mathcal{F}} \otimes (E_{ij}^\mu)_{\mathcal{P} \mathcal{O}^n}}{m_\mu}. \tag{S20}
\]
Therefore, \( \Omega_{d,n} \) is given by
\[
\Omega_{d,n} = \sum_{\mu \in \mathbb{Y}_{n+1}^d} \sum_{i,j=1}^{d_\mu} \frac{(P_\pi E_{ij}^\mu P_\pi)_{\mathcal{I}^n \mathcal{F}} \otimes (E_{ij}^\mu)_{\mathcal{P} \mathcal{O}^n}}{d^2 m_\mu} \tag{S21}
\]
\[
= \sum_{\mu \in \mathbb{Y}_{n+1}^d} \sum_{i,j=1}^{d_\mu} \frac{[\pi_{\mu}]^*_{ij} (E_{ij}^\mu)_{\mathcal{I}^n \mathcal{F}} [\pi_{\mu}]_{ij} \otimes (E_{ij}^\mu)_{\mathcal{P} \mathcal{O}^n}}{d^2 m_\mu}. \tag{S22}
\]

\[\square\]

Formulas for the Young-Yamanouchi basis

In the main manuscript, the basis \( \{E_{ij}^\mu\} \) for the set of linear operators on \( \mathcal{C}^{\otimes n+1}_d \) commuting with \( U^{\otimes n+1} \) for all \( U \in \text{SU}(d) \) is introduced as
\[
(\mathcal{C}^{\otimes n+1}_d) = \bigoplus_{\mu \in \mathbb{Y}_{n+1}^d} \mathcal{U}_\mu \otimes \mathcal{S}_\mu, \tag{S23}
\]
\[
E_{ij}^\mu := 1_{\mathcal{U}_\mu} \otimes |\mu,i\rangle \langle \mu,j|_{\mathcal{S}_\mu}. \tag{S24}
\]
The superscript \( \mu \) runs in the set of Young diagrams with \( n+1 \) boxes and at most depth \( d \), denoted by \( \mathbb{Y}_{n+1}^d \), and subscripts \( i,j \) take values from 1 to \( d_\mu := \dim \mathcal{S}_\mu \) [see Eqs. (9)-(12) of the main manuscript for the detail]. Similarly,
we introduce the set of operators \( \{ E_{ij}^\mu \} \) for \( \alpha \in \mathbb{Y}^d \) and \( a, b = 1, \ldots, d_\alpha \), which forms the basis of the set of linear operators on \((\mathbb{C}^d)^{\otimes n}\) commuting with \( U^{\otimes n} \) for all \( U \in SU(d) \). Then, the following Lemmas hold.

**Lemma 5.** The basis \( \{ E_{ij}^\mu \} \) satisfies

\[
(E_{ij}^\mu)^* = E_{ji}^\mu, \tag{S25}
\]

\[
\text{Tr} E_{ij}^\mu = m_\mu \delta_{ij}, \tag{S26}
\]

\[
E_{ij}^\mu E_{kl}^\nu = \delta_{\mu\nu} \delta_{jk} E_{il}^\mu, \tag{S27}
\]

where \( X^* \) is the complex conjugate of \( X \) in the computational basis, \( m_\mu \) is defined as \( m_\mu := \dim U_\mu \) and \( \delta_{ij} \) is the Kronecker’s delta defined as \( \delta_{ij} = 1 \) and \( \delta_{ij} = 0 \) for \( i \neq j \).

**Lemma 6.** Let \( \alpha + \Box \) be the set of Young diagrams obtained by adding a box to \( \alpha \), and \( a_\mu \) be the index of the standard tableau \( s_\mu^\alpha \) obtained by adding a box \( \boxed{n+1} \) to a standard tableau \( s_\mu^\alpha \). Then, \( E_{ab}^\alpha \otimes 1_d \) can be written as

\[
E_{ab}^\alpha \otimes 1_d = \sum_{\mu \in \alpha + \Box} E_{a_\mu b_\mu}^\mu, \tag{S28}
\]

where \( 1_d \) is the identity operator on \( \mathbb{C}^d \).

**Lemma 7.** Let \( s_\mu^\alpha \) and \( s_\nu^\beta \) be the standard tableaux obtained by removing a box \( \boxed{n+1} \) from \( s_\mu^\alpha \) and \( s_\nu^\beta \), respectively. The partial trace of \( E_{ij}^\mu \) in the last system is given by

\[
\text{Tr}_{n+1} E_{ij}^\mu = \delta_{\alpha\beta} \frac{m_\mu}{m_\alpha} E_{ab}^\alpha. \tag{S29}
\]

**Proof of Lemma 5.** To show this Lemma, we introduce the Gelfand-Zetlin basis \( \{ |\mu, u\rangle \} \) of \( U_\mu \) in Eq. (S23). The set of vectors \( \{ |\mu, u\rangle \otimes |\mu, i\rangle_{S_\mu} \} \) forms the basis of \((\mathbb{C}^d)^{\otimes n+1}\), which is called the Schur basis. The change of the basis from the computational basis to the Schur basis is called the quantum Schur transform \[48–51\], denoted by \( U_{Sch} \). The matrix elements of \( U_{Sch} \) are real (see e.g., Section 4 of Ref. [51]), i.e., \( (U_{Sch})^* = U_{Sch} \). Therefore,

\[
E_{ij}^\mu = \sum_u |\mu, u\rangle \langle \mu, u|_U \otimes |\mu, i\rangle \langle \mu, j|_{S_\mu}
\]

is a real matrix in the computational basis, i.e., \( (E_{ij}^\mu)^* = E_{ij}^\mu \) holds. Equations (S26) and (S27) immediately come from the definition (S24).

**Proof of Lemma 6.** We show this Lemma using the similar discussion in Ref. [19], originally used to show the decomposition of quantum Schur transform into the series of Clebsch-Gordan transforms.

We review the definition of the Young-Yamanouchi basis. The symmetric group \( \mathfrak{S}_n \) can be regarded as a subgroup of \( \mathfrak{S}_{n+1} \) that leaves the last element fixed. Then, the irreducible representation space \( S_\mu \) of the symmetric group \( \mathfrak{S}_n \) decomposes into the irreducible representations of \( \mathfrak{S}_n \) when restricting to \( \mathfrak{S}_n \). We write the representation space of the restricted representation as \( S_\mu \downarrow \mathfrak{S}_n \). It is known that the decomposition of \( S_\mu \downarrow \mathfrak{S}_n \) is given by \[52\]

\[
S_\mu \downarrow \mathfrak{S}_n \cong \bigoplus_{\alpha \in \mu - \Box} S_\alpha. \tag{S31}
\]

The Young-Yamanouchi basis \( \{ |\mu, i\rangle \}_{i=1}^{d_\mu} \subset S_\mu \) is a subgroup-adapted basis, i.e., \( |\alpha, a\rangle \in S_\mu \) corresponds to the vector \( |\mu, a_\mu\rangle \in S_\alpha \) in the decomposition (S31). Here, \( a_\mu \) is the index of the standard tableau \( s_\mu^\alpha \) obtained by adding a box \( \boxed{n+1} \) to \( s_\alpha^\alpha \).

We show Lemma 6 by proving the following equality of two subspaces of \((\mathbb{C}^d)^{\otimes n+1}\):

\[
U_\alpha \otimes \text{span}\{|\alpha, a\rangle_{S_\alpha} + z|\alpha, b\rangle_{S_\alpha}\} \subset (\mathbb{C}^d)^{\otimes n+1} = \bigoplus_{\mu \in \alpha + \Box} U_\mu \otimes \text{span}\{|\mu, a_\mu\rangle_{S_\mu} + z|\mu, b_\mu\rangle_{S_\mu}\}, \tag{S32}
\]

where \( z \in \mathbb{C} \). If Eq. (S32) holds, by considering the projectors onto these subspaces, we obtain

\[
(E_{aa}^\alpha + z E_{ab}^\alpha + z^* E_{ba}^\alpha + z z^* E_{bb}^\alpha) \otimes 1_d = \sum_{\mu \in \alpha + \Box} E_{a_\mu a_\mu}^\mu + z E_{a_\mu b_\mu}^\mu + z^* E_{b_\mu a_\mu}^\mu + zz^* E_{b_\mu b_\mu}^\mu, \tag{S33}
\]
for all $z \in \mathbb{C}$. Therefore,

$$E_{ab}^\alpha \otimes 1_d = \sum_{\mu \in \alpha + \square} E_{a\mu,b\mu}^\mu$$  \hspace{1cm} (S34)

holds for all $\alpha \in \mathbb{Y}_n^d$ and $a, b \in \{1, \cdots, d \}$. The irreducible representation space $U_{\square}$ corresponding to the Young tableau $\mu = \square$ is $U_{\square} = \mathbb{C}^d$. For a Young tableau $\alpha \in \mathbb{Y}_n^d$, the space $U_{\alpha} \otimes U_{\square}$ can be decomposed into irreducible representations of $SU(d)$ as

$$U_{\alpha} \otimes U_{\square} \simeq \bigoplus_{\mu \in \alpha + \square} U_{\mu}.$$  \hspace{1cm} (S35)

Then, the space $(\mathbb{C}^d)^{\otimes n+1}$ decomposes as

$$(\mathbb{C}^d)^{\otimes n+1} = \bigoplus_{\alpha \in \mathbb{Y}_n^d} U_{\alpha} \otimes \mathbb{C}^d = \bigoplus_{\alpha \in \mathbb{Y}_n^d} (U_{\alpha} \otimes U_{\square}) \otimes \mathbb{C}^d \simeq \bigoplus_{\alpha \in \mathbb{Y}_n^d} \bigoplus_{\mu \in \alpha + \square} U_{\mu} \otimes \mathbb{C}^d \simeq \bigoplus_{\alpha \in \mathbb{Y}_n^d} \bigoplus_{\mu \in \alpha + \square} U_{\mu} \otimes U_{\alpha}.$$  \hspace{1cm} (S36)

In particular, the subspace $U_{\alpha} \otimes \text{span}\{|\alpha, a\rangle s_a + z|\alpha, b\rangle s_a\} \otimes \mathbb{C}^d$ of Eq. (S37) is given by

$$U_{\alpha} \otimes \text{span}\{|\alpha, a\rangle s_a + z|\alpha, b\rangle s_a\} \otimes \mathbb{C}^d \simeq \bigoplus_{\mu \in \alpha + \square} U_{\mu} \otimes \text{span}\{|\alpha, a\rangle s_a + z|\alpha, b\rangle s_a\}.$$  \hspace{1cm} (S38)

The subspace $\bigoplus_{\mu \in \alpha + \square} U_{\mu} \otimes \text{span}\{|\alpha, a\rangle s_a + z|\alpha, b\rangle s_a\}$ of Eq. (S38) can be regarded as the subspace of $U_{\mu} \otimes U_{\alpha} \otimes \mathbb{C}^d$ by the isomorphism

$$U_{\mu} \otimes \bigoplus_{\alpha \in \mu - \square} \mathbb{C}^{SU(d) \times \mathbb{S}_\alpha} \simeq \bigoplus_{\alpha \in \mu - \square} U_{\alpha} \otimes \mathbb{S}_\alpha.$$  \hspace{1cm} (S39)

Since the Young-Yamanouchi basis is a subgroup-adapted basis, the space $U_{\alpha} \otimes \text{span}\{|\alpha, a\rangle s_a + z|\alpha, b\rangle s_a\}$ corresponds to $U_{\mu} \otimes \text{span}\{|\mu, a\rangle s_a + z|\mu, b\rangle s_a\} \subset U_{\mu} \otimes \mathbb{S}_{\mu \downarrow s_a}$, where $a_\mu$ is the index of the standard tableau $s_{\mu_\alpha}$ obtained by adding a box $[n+1]$ to $s_{\alpha_\mu}$. Therefore, Eq. (S32) holds. $\square$

**Proof of Lemma 7.** This Lemma is shown in Ref. [53] (see Lemma 7 of Ref. [53]). Here, we present another proof based on Lemma 6 and the positivity of $E_{ii}^\mu + z E_{ij}^\mu + z^* E_{ji}^\mu + z z^* E_{jj}^\mu$ for all $z \in \mathbb{C}$.

First, $\text{Tr}_{n+1} E_{ij}^\mu$ satisfies $[\text{Tr}_{n+1} E_{ij}^\mu, U^{\otimes n}] = 0$ for all $U \in SU(d)$. Therefore, $\text{Tr}_{n+1} E_{ij}^\mu$ can be written as

$$\text{Tr}_{n+1} E_{ij}^\mu = \sum_{\beta \in \mathbb{Y}_n^d} \sum_{a,b=1}^{d_\beta} A_{ab}^\beta (\mu, i, j) E_{ab}^\beta,$$  \hspace{1cm} (S42)

using complex coefficients $A_{ab}^\beta (\mu, i, j) \in \mathbb{C}$. Since

$$E_{ii}^\mu + z E_{ij}^\mu + z^* E_{ji}^\mu + z z^* E_{jj}^\mu = 1_{U_{\mu}} \otimes (|\mu, i\rangle + z|\mu, j\rangle)(|\mu, i\rangle + z^* (\mu, j)|s_\mu \geq 0$$  \hspace{1cm} (S43)

holds for all $z \in \mathbb{C}$,

$$\sum_{\beta \in \mathbb{Y}_n^d} \sum_{a,b=1}^{d_\beta} |B_{ab}^\beta (\mu, i, j, z)| E_{ab}^\beta = \text{Tr}_{n+1} [E_{ii}^\mu + z E_{ij}^\mu + z^* E_{ji}^\mu + z z^* E_{jj}^\mu] \geq 0$$  \hspace{1cm} (S44)
holds, where the matrices \( B^\alpha(\mu, i, j, z) \) are defined by
\[
[B^\alpha(\mu, i, j, z)]_{ab} \defeq A_{ab}^\alpha(\mu, i, i) + zA_{ab}^\alpha(\mu, i, j) + z^*A_{ab}^\alpha(\mu, j, i) + zz^*A_{ab}^\alpha(\mu, j, j).
\] (S45)

Therefore, the matrices \( B^\alpha(\mu, i, j, z) \) are positive for all \( \beta \in \mathbb{Y}_n^\mu, \mu \in \mathbb{Y}_n^{\alpha+\square}, i, j \in \{1, \cdots, d_\mu\} \) and \( z \in \mathbb{C} \).

By taking the partial trace of the last system in Eq. (S34), we obtain
\[
\sum_{\mu \in \alpha+\square} \operatorname{Tr}_{\mu+1} E^\mu_{a,b} = dE^\alpha_{ab}.
\] (S46)

Therefore,
\[
\sum_{\mu \in \alpha+\square} B^\alpha(\mu, a, b, z) = d\delta_{\alpha\beta} X^\alpha(a, b, z)
\] (S47)
holds, where the matrix \( X^\alpha(a, b, z) \) is defined as
\[
[X^\alpha(a, b, z)]_{a'b'} \defeq \delta_{aa'}\delta_{bb'} + z\delta_{aa'}\delta_{ab'} + z^*\delta_{ba'}\delta_{bb'} + zz^*\delta_{ba'}\delta_{bb'}.
\] (S48)

Since \( B^\beta(\mu, a, b, z) \geq 0 \) holds for all \( \mu \in \alpha+\square \) and \( X^\alpha(a, b, z) \) is a one-dimensional projector,
\[
B^\beta(\mu, a, b, z) \propto \delta_{\alpha\beta} X^\alpha(a, b, z),
\] (S49)
i.e.,
\[
\operatorname{Tr}_{\mu+1} \left[ E^\mu_{a,b,a'} + zE^\mu_{a,b,a'} + z^*E^\mu_{b,a,b'} + zz^*E^\mu_{b,a,b'} \right] \propto E^\alpha_{aa} + zE^\alpha_{ab} + z^*E^\alpha_{ba} + zz^*E^\alpha_{bb}
\] (S50)
holds for all \( z \in \mathbb{C} \). Since the traces of the left and right hand sides are given by
\[
\operatorname{Tr}[E^\mu_{a,b,a'} + zE^\mu_{a,b,a'} + z^*E^\mu_{b,a,b'} + zz^*E^\mu_{b,a,b'}] = (1 + z^2)m_\mu,
\] (S51)
\[
\operatorname{Tr}[E^\alpha_{aa} + zE^\alpha_{ab} + z^*E^\alpha_{ba} + zz^*E^\alpha_{bb}] = (1 + z^2)m_\alpha,
\] (S52)
the proportional coefficient is determined as
\[
\operatorname{Tr}_{\mu+1} \left[ E^\mu_{a,b,a'} + zE^\mu_{a,b,a'} + z^*E^\mu_{b,a,b'} + zz^*E^\mu_{b,a,b'} \right] = \frac{m_\mu}{m_\alpha} [E^\alpha_{aa} + zE^\alpha_{ab} + z^*E^\alpha_{ba} + zz^*E^\alpha_{bb}].
\] (S53)

Therefore,
\[
\operatorname{Tr}_{\mu+1} E^\mu_{a,b} = \frac{m_\mu}{m_\alpha} E^\alpha_{ab}
\] (S54)
holds for all \( \alpha \in \mathbb{Y}_n^\mu, a, b \in \{1, \cdots, d_\alpha\} \) and \( \mu \in \alpha+\square \), which corresponds to the case \( \alpha = \beta \) in Lemma 4.

To complete the proof, we consider the case \( \alpha \neq \beta \), where \( s_\alpha^\mu \) and \( s_\beta^\mu \) be the standard tableaux obtained by removing a box \([n + 1]\) from \( s_\alpha^\mu \) and \( s_\beta^\mu \), respectively. Then, \( i \neq j \) holds. We fix \( i, j, \mu \) in the following argument. We consider the positive operator \( \operatorname{Tr}_{\mu+1} [E^\mu_{ii} + zE^\mu_{ij} + z^*E^\mu_{ji} + zz^*E^\mu_{jj}] \) to evaluate \( \operatorname{Tr}_{n+1} E^\mu_{ij} \). Due to Eq. (S34),
\[
\operatorname{Tr}_{n+1} E^\mu_{ii} = E^\alpha_{ii},
\] (S55)
\[
\operatorname{Tr}_{n+1} E^\mu_{jj} = E^\beta_{jj},
\] (S56)
hold. Defining \( F(\theta) \defeq \operatorname{Tr}_{n+1} [e^{i\theta}E^\mu_{ij} + e^{-i\theta}E^\mu_{ji}] \) for \( \theta \in \mathbb{R} \),
\[
E^\alpha_{aa} + |z|^2E^\beta_{bb} + |z|F(\theta) = \operatorname{Tr}_{n+1} [E^\mu_{ii} + zE^\mu_{ij} + z^*E^\mu_{ji} + zz^*E^\mu_{jj}] \geq 0
\] (S57)
holds for \( \theta \defeq \arg z \). Since \( |F(\theta), U^{\otimes n}| = 0 \) holds for all \( U \in \text{SU}(d) \), \( F(\theta) \) can be written as
\[
F(\theta) = \sum_{\gamma \in \mathbb{Y}_n^\mu} F^\gamma(\theta),
\] (S58)
\[
F^\gamma(\theta) \defeq \sum_{i, j=1}^{d_\gamma} f_{ij}^\gamma(\theta) E^\gamma_{ij},
\] (S59)
using complex coefficients \( f_{ij} \in \mathbb{C} \). In terms of \( F^\gamma(\theta) \), Eq. (S57) is written as

\[
F^\gamma(\theta) \geq \begin{cases} 
-\frac{1}{|z|^2} E_{aa}^\alpha & (\gamma = \alpha) \\
-|z| E_{bb}^\beta & (\gamma = \beta) \\
0 & (\text{otherwise})
\end{cases}
\] (S60)

By considering limits \( |z| \to \infty \) and \( |z| \to 0 \), we obtain \( F^\gamma(\theta) \geq 0 \) for all \( \gamma \in \mathbb{N}_n \), i.e., \( F(\theta) \geq 0 \). Since \( i \neq j \) holds, \( \text{Tr}[F(\theta)] = \text{Tr}[e^{i\theta} E_{ij}^\mu + e^{-i\theta} E_{ji}^\mu] = 0 \). Thus, \( F(\theta) = 0 \) holds, i.e.,

\[
\text{Tr}_{n+1}[e^{i\theta} E_{ij}^\mu + e^{-i\theta} E_{ji}^\mu] = 0
\] (S61)

holds for all \( \theta \in \mathbb{R} \). Therefore,

\[
\text{Tr}_{n+1} E_{ij}^\mu = 0.
\] (S62)

This completes the proof.

Proof of Lemma 3

The quantum comb condition for a matrix \( C \in \mathcal{L}(\mathcal{P} \otimes \mathcal{I}^4 \otimes \mathcal{O}^4 \otimes \mathcal{F}) \) is given by

\[
C \geq 0, \\
\text{Tr}_{\mathcal{I}} C_i = C_{i-1} \otimes 1_{\mathcal{O}_{i-1}}, \\
C_0 = 1,
\] (S63) (S64) (S65)
for $i \in \{1, \ldots, 5\}$, where $1_T$ is the identity operator on $\mathcal{H}$, $C_5 := C$, $C_{i-1} := \text{Tr}_{I_i O_{i-1}} C_i / d$, and $I_5, O_0$ are defined by $I_5 := F, O_0 := P$. These conditions can be checked with the following calculation using Lemmas 6 and 7:

\[
C = \frac{1}{2} (1_{U_{a_3}})_{1+F} \otimes (1_{U_{a_3}})_{p O^4} \otimes |\phi_1\rangle (S_{a_3})_{2+F} (S_{a_3})_{p O^4} \\
+ \frac{1}{2} (1_{U_{a_3}})_{1+F} \otimes (1_{U_{a_3}})_{p O^4} \otimes |\phi_2\rangle (S_{a_3})_{2+F} (S_{a_3})_{p O^4} \\
+ \frac{1}{2} (1_{U_{a_3}} \otimes |\alpha_3, 5\rangle (\alpha_3, 5|S_{a_3})_{1+F} \otimes (1_{U_{a_3}} \otimes |\alpha_1, 1\rangle (\alpha_1, 1|S_{a_3})_{p O^4} \\
+ 1_{U_{a_3}} \otimes |\alpha_2, 1\rangle (\alpha_2, 1|S_{a_3})_{p O^4} + |\alpha_2, 2\rangle (\alpha_2, 2|S_{a_3})_{p O^4} + 1_{U_{a_3}} \otimes |\alpha_3, 1\rangle (\alpha_3, 1|S_{a_3})_{p O^4}
\]

(S66)

\[
\geq 0,
\]

(S67)

\[
\text{Tr}_F C = \frac{1}{3} \sum_{i,j=2}^3 (E_{i,j}^2)_{1+F} \otimes (E_{7-1,7-j}^2)_{p O^4} + \sum_{i,j=4}^5 (E_{i,j}^2)_{1+F} \otimes (E_{8-1,8-j}^2 + E_{7-1,7-j}^2)_{p O^4} \\
+ (E_{i,j}^2)_{1+F} \otimes (E_{11}^2 + E_{11}^2 + E_{22}^2 + E_{11}^2)_{p O^4} \\
= \frac{1}{3} \sum_{i,j=2}^3 (E_{i,j}^2)_{1+F} \otimes (E_{11}^2 + E_{11}^2)_{p O^4} \otimes 1_{C_4} + \sum_{i,j=1}^2 (E_{i,j}^2)_{1+F} \otimes (E_{4-1,4-j}^2)_{p O^4} \otimes 1_{C_4} \\
+ \frac{1}{6} (E_{33}^2 + 3E_{22}^2)_{1+F} \otimes (E_{11}^2 + E_{11}^2)_{p O^4} \otimes 1_{C_4} \\
= C_4 \otimes 1_{C_4},
\]

(S68)

\[
\text{Tr}_{I_4} C_4 = \frac{1}{2} \sum_{i,j=1}^2 (E_{i,j}^2)_{1+F} \otimes (E_{11}^2)_{p O^4} + \frac{1}{2} (E_{22}^2)_{1+F} \otimes (E_{11}^2 + E_{11}^2)_{p O^4} \\
= \frac{1}{2} \sum_{i,j=1}^2 (E_{i,j}^2)_{1+F} \otimes (E_{3-1,3-j}^2)_{p O^4} \otimes 1_{C_3} + \frac{1}{2} (E_{22}^2)_{1+F} \otimes (E_{11}^2)_{p O^4} \otimes 1_{C_3} \\
= C_3 \otimes 1_{C_3},
\]

(S69)

\[
\text{Tr}_{I_4} C_3 = \frac{1}{3} (E_{i,j}^2)_{1+F} \otimes (E_{11}^2)_{p O^4} + (E_{22}^2)_{1+F} \otimes (E_{11}^2 + E_{11}^2)_{p O^4} \\
= (E_{i,j}^2)_{1+F} \otimes (E_{11}^2)_{p O^4} \otimes 1_{C_2} + \frac{1}{3} (E_{11}^2)_{1+F} \otimes (E_{11}^2)_{p O^4} \otimes 1_{C_2} \\
= C_2 \otimes 1_{C_2},
\]

(S70)

\[
\text{Tr}_{I_2} C_2 = \frac{1}{2} (E_{i,j}^2)_{1+F} \otimes (E_{11}^2)_{1+F} \otimes (E_{11}^2 + E_{11}^2)_{p O^4} \\
= \frac{1}{2} (E_{i,j}^2)_{1+F} \otimes (E_{11}^2)_{p O^4} \otimes 1_{C_1} \\
= C_1 \otimes 1_{C_1},
\]

(S71)

\[
\text{Tr}_{I_4} C_1 = (E_{i,j}^2)_{1+F} \otimes 1_{p},
\]

(S72)

where $|\phi_1\rangle \in S_{a_3} \otimes S_{a_2}$ and $|\phi_2\rangle \in S_{a_3} \otimes S_{a_2}$ are defined as

\[
|\phi_1\rangle := |\alpha_3, 2\rangle \otimes |\alpha_3, 5\rangle + |\alpha_3, 3\rangle \otimes |\alpha_3, 4\rangle - |\alpha_3, 4\rangle \otimes |\alpha_3, 3\rangle - |\alpha_3, 5\rangle \otimes |\alpha_3, 2\rangle,
\]

(S81)

\[
|\phi_2\rangle := |\alpha_3, 4\rangle \otimes |\alpha_2, 4\rangle + |\alpha_3, 5\rangle \otimes |\alpha_2, 3\rangle,
\]

(S82)
TABLE S1. Definition of standard tableaux $s_j^\mu$ for $\mu \in \{\alpha, \beta, \gamma, \delta, \epsilon\}$.

| $s_j^\mu$ | $j = 1$ | $j = 2$ | $j = 3$ | $j = 4$ | $j = 5$ |
|----------|--------|--------|--------|--------|--------|
| $i = 1$  | 1 2 3 4 5 | 1 2 3 4 5 | 1 2 3 4 5 | 1 2 3 4 5 | 1 2 3 4 5 |
| $i = 2$  | 1 2 3 4 5 | 1 2 3 4 5 | 1 2 3 4 5 | 1 2 3 4 5 | 1 2 3 4 5 |
| $i = 3$  | 1 2 3 4 5 | 1 2 3 4 5 | 1 2 3 4 5 | 1 2 3 4 5 | 1 2 3 4 5 |
| $i = 4$  | 1 2 3 4 5 | 1 2 3 4 5 | 1 2 3 4 5 | 1 2 3 4 5 | 1 2 3 4 5 |

$C_i$ for $i \in \{1, 2, 3, 4\}$ are defined as

$$C_4 := \frac{1}{3} \sum_{i,j=2}^3 (E_{i,j}^{81})_{I^4} \otimes (E_{4-i,4-j}^{83})_{PO^3} + \frac{2}{3} \sum_{i,j=1}^2 (E_{i,j}^{81})_{I^3} \otimes (E_{4-i,4-j}^{82})_{PO^2} + \frac{1}{6} (E_{33}^{82} + 3E_{22}^{84})_{I^4} \otimes (E_{11}^{81} + E_{22}^{82})_{PO^1},$$  

(S83)

$$C_3 := \frac{1}{2} \sum_{i,j=1}^2 (E_{i,j}^{81})_{I^3} \otimes (E_{4-i,4-j}^{82})_{PO^2} + \frac{1}{2} (E_{22}^{83})_{I^3} \otimes (E_{11}^{81})_{PO^2},$$  

(S84)

$$C_2 := (E_{11}^{81})_{I^2} \otimes (E_{11}^{81})_{PO^1} + \frac{1}{2} (E_{11}^{81})_{I^2} \otimes (E_{11}^{81})_{PO^1},$$  

(S85)

$$C_1 := \frac{1}{2} (E_{11}^{81})_{I^1} \otimes (E_{11}^{81})_{P}.$$  

(S86)

Young diagrams $\beta_i$, $\gamma_i$, $\delta_i$ and $\epsilon_i$ are defined as

$$\beta_1 = \begin{array}{c} \square \square \square \square \square \square \square \square \end{array}, \quad \beta_2 = \begin{array}{c} \square \square \square \square \square \square \square \square \end{array}, \quad \beta_3 = \begin{array}{c} \square \square \square \square \square \square \square \square \end{array}, \quad \gamma_1 = \begin{array}{c} \square \square \square \square \square \square \square \square \end{array}, \quad \gamma_2 = \begin{array}{c} \square \square \square \square \square \square \square \square \end{array}, \quad \delta_1 = \begin{array}{c} \square \square \square \square \square \square \square \square \end{array}, \quad \delta_2 = \begin{array}{c} \square \square \square \square \square \square \square \square \end{array}, \quad \epsilon_1 = \begin{array}{c} \square \square \square \square \square \square \square \square \end{array},$$  

(S87)

and standard tableaux $s_j^\mu$ for $\mu \in \{\alpha, \beta, \gamma, \delta, \epsilon\}$ and $j \in \{1, \ldots, d_\mu\}$ are defined in TABLE S1.

As shown in Lemma 4, the unitary inversion condition is given by $\text{Tr}(C\Omega) = 1$. Since the matrix representations of $\pi_\alpha$, and the values $m_\alpha$, are given by

$$\pi_{\alpha_1} = 1, \quad \pi_{\alpha_2} = \begin{pmatrix} -\frac{1}{4} & -\frac{\sqrt{3}}{12} & -\frac{\sqrt{3}}{12} & -\frac{\sqrt{10}}{4} \\ -\sqrt{\frac{5}{4}} & -1 & -\frac{\sqrt{2}}{12} & -\frac{\sqrt{10}}{4} \\ \frac{\sqrt{5}}{4} & -\frac{\sqrt{3}}{12} & -\frac{\sqrt{2}}{12} & -\frac{\sqrt{10}}{4} \\ 0 & \frac{\sqrt{3}}{6} & -\frac{1}{6} & -\frac{\sqrt{10}}{4} \\ 0 & 0 & \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}, \quad \pi_{\alpha_3} = \begin{pmatrix} -\frac{1}{3} & -\frac{\sqrt{3}}{4} & -\frac{\sqrt{3}}{4} & 0 & 0 \\ -\frac{\sqrt{3}}{4} & -\frac{1}{12} & -\sqrt{\frac{3}{2}} & -\frac{\sqrt{3}}{4} & -\frac{3}{4} \\ -\frac{\sqrt{3}}{4} & -\frac{1}{12} & -\sqrt{\frac{3}{2}} & -\frac{\sqrt{3}}{4} & -\frac{3}{4} \\ 0 & \frac{\sqrt{3}}{6} & -\frac{1}{6} & -\frac{\sqrt{3}}{4} & -\frac{3}{4} \\ 0 & \frac{\sqrt{3}}{6} & -\frac{1}{6} & -\frac{\sqrt{3}}{4} & -\frac{3}{4} \end{pmatrix},$$  

(S88)
the unitary inversion condition $\text{Tr}(C\Omega) = 1$ holds.

The simplified SDP to seek for deterministic exact $d$-dimensional unitary inversion for general $d$

**Theorem 8.** The maximum value of the SDP given by

$$\max \text{Tr}(C\Omega_{d,n})$$

s.t. $C$ is a quantum comb.

is the same as that of the following SDP:

$$\max \sum_{\mu \in \mathbb{Y}_{n+1}^d} \sum_{i,j,k,l=1}^{d_{\mu}} \frac{[\pi_{\mu}]_{ki}[\pi_{\mu}]_{lj} [C^\mu]_{ik,jl}}{d^2 m_\mu}$$

s.t. $C^{\mu\nu} \in \mathcal{L}(\mathbb{C}^{d_{\mu}} \otimes \mathbb{C}^{d_{\nu}}) \geq 0,$

$$\sum_{\alpha \in \gamma + \square} (X^\alpha_i \otimes 1_{d_\alpha})(C^\alpha_{\alpha_1}) m_{\beta_1}(X^\alpha_i \otimes 1_{d_\alpha})^\dagger = \sum_{\delta \in \beta - \square} (1_{d_\gamma} \otimes X^\delta_\beta)(C^\delta_{\beta_1}) m_{\delta_1}(1_{d_\gamma} \otimes X^\beta_\delta)^\dagger,$$

$$C^0_\emptyset = 1,$$

for all $i \in \{1, \cdots, n+1\}, \mu, \nu \in \mathbb{Y}_{n+1}^d, \gamma \in \mathbb{Y}_{i-1}^d,$$ and $\beta \in \mathbb{Y}_i^d,$ where $C^\alpha_{\alpha_1}$ for $\alpha, \beta \in \mathbb{Y}_i^d$ are defined by

$$C^\alpha_{\alpha_1} := C^{\alpha\beta}_{\alpha_1},$$

$$C^\alpha_{\alpha_1} := \frac{1}{d} \sum_{\mu \in \alpha + \square, \nu \in \beta + \square} (X^\alpha_\mu \otimes X^\beta_\nu)(C^\mu_{\alpha_1}) (X^\alpha_\mu \otimes X^\beta_\nu)^\dagger,$$

for $i \in \{1, \cdots, n+1\}, X^\alpha_\alpha$ for $\alpha \in \gamma + \square$ and $\gamma \in \mathbb{Y}_{i-1}^d$ are $d_\gamma \times d_\alpha$ matrices defined by

$$[X^\gamma_\alpha]_{c,a} := \delta_{c,a},$$

$c_\mu$ is the index of the standard tableau $s^\alpha_\emptyset$ obtained by adding a box $\square$ to the standard tableau $s^\alpha_\emptyset,$ and $\emptyset$ represents the Young tableau with zero boxes.

**Proof.** First, we show that the SDP (S90) can be solved without loss of generality by imposing an additional constraint given by

$$[C, U^{\otimes n+1}_{\mathbb{C}^2} \otimes V^{\otimes n+1}_{\mathbb{C}^2}] = 0,$$

for all $U, V \in \text{SU}(d).$ Suppose $C = C_{\text{opt}}$ achieves the maximal value of $\text{Tr}(C\Omega_{d,n})$ in the SDP (S90). Since the operator $\Omega_{d,n}$ satisfies

$$[\Omega_{d,n}, U^{\otimes n+1}_{\mathbb{C}^2} \otimes V^{\otimes n+1}_{\mathbb{C}^2}] = 0,$$

for all $U, V \in \text{SU}(d),$ the operator $C'_{\text{opt}}$ defined as

$$C'_{\text{opt}} := \int dU dV (U^{\otimes n+1}_{\mathbb{C}^2} \otimes V^{\otimes n+1}_{\mathbb{C}^2}) C_{\text{opt}}(U^{\otimes n+1}_{\mathbb{C}^2} \otimes V^{\otimes n+1}_{\mathbb{C}^2})^\dagger$$

satisfies

$$\text{Tr}(C'_{\text{opt}} \Omega_{d,n}) = \text{Tr}(C_{\text{opt}} \Omega_{d,n}),$$

where $dU$ and $dV$ are the Haar measure on $\text{SU}(d).$ When $C = C_{\text{opt}}$ satisfies the comb conditions given by

$$C \geq 0,$$

$$\text{Tr}_{l_i} C_i = C_{i-1} \otimes 1_{\mathbb{C}^{l_i}},$$

$$C_0 = 1,$$

$$C_{\alpha_1} = 6, \quad m_{\alpha_2} = 4, \quad m_{\alpha_3} = 2.$$
for \( i \in \{1, \cdots, n + 1\} \), where \( C_i \) is defined as \( C_{n+1} := C \) and \( C_{i-1} := \text{Tr}_{X_1 \cdots X_{i-1}} C_i / d \) (see Lemma 2 of the main manuscript), \( C_{\text{opt}}^{r} \) also satisfies the comb conditions. Thus, \( C = C_{\text{opt}}^{r} \) also achieves the maximal value of \( \text{Tr}(C \Omega_{d,n}) \) in the SDP (S90). Due to the property of the Haar measure, \( C_{\text{opt}}^{r} \) defined by Eq. (S97) satisfies

\[
[C_{\text{opt}}^{r}, U_{\Omega_{d,n}}^{\otimes n+1}] = 0,
\]

for all \( U, V \in SU(d) \). Therefore, the maximal value of the SDP (S90) can be searched within the set of operators \( C \) satisfying the \( SU(d) \times SU(d) \) symmetry (S95).

We consider operators \( C \in \mathcal{L}(\mathbb{F}) \) satisfying the \( SU(d) \times SU(d) \) symmetry (S95). The operator \( C_i \) defined as \( C_{n+1} := C \) and \( C_{i-1} := \text{Tr}_{X_1 \cdots X_{i-1}} C_i / d \) also satisfies the \( SU(d) \times SU(d) \) symmetry given by

\[
[C_i, U_{\Omega_{d,n}}^{\otimes i}] = 0, \quad \text{for all } U, V \in SU(d).
\]

Thus, \( C \) and \( C_i \) can be written as

\[
C = \sum_{\mu, \nu \in \mathbb{Y}_{n+1}^d} \sum_{i,j,k,l=1}^{d} \frac{C_{ijkl}^{\mu \nu}}{m_i m_j} (E_{ij}^{\mu})_{X \otimes (E_{kl}^{\nu})_{\Omega}}, \quad C_i = \sum_{\alpha, \beta \in \mathbb{Y}_{n+1}^d} \sum_{a,b=1}^{d} \sum_{c,d=1}^{d} \frac{C_{\alpha \beta abcd}^{\mu \nu}}{m_i m_j} (E_{ab}^{\alpha})_{X \otimes (E_{cd}^{\beta})_{\Omega}},
\]

using complex coefficients \( c_{ijkl}^{\mu \nu}, c_{\alpha \beta abcd}^{\mu \nu} \in \mathbb{C} \). We define \( C_{\mu \nu}^{C} \in \mathcal{L}(\mathbb{C}_{\mu \nu} \otimes \mathbb{C}_{\mu \nu}) \) and \( C_{i}^{\alpha \beta} \in \mathcal{L}(\mathbb{C}_{\alpha \beta} \otimes \mathbb{C}_{\alpha \beta}) \) for \( \mu, \nu \in \mathbb{Y}_{n+1}^d \), \( \alpha, \beta \in \mathbb{Y}_{n+1}^d \) by

\[
[C_{\mu \nu}]_{ik,jl} := c_{ijkl}^{\mu \nu}, \quad \quad [C_{i}^{\alpha \beta}]_{ac,bd} := c_{\alpha \beta abcd}^{\mu \nu}.
\]

From Lemma 5 and Eq. (S44), \( \text{Tr}(C \Omega_{d,n}) \) is given by

\[
\text{Tr}(C \Omega_{d,n}) = \frac{1}{d^2} \sum_{\mu, \nu, \mu' \in \mathbb{Y}_{n+1}^d} \sum_{i,j=1}^{d} \sum_{k,l=1}^{d} \sum_{\nu', \nu''}^{d} \text{Tr}(E_{ij}^{\mu} E_{k,l}^{\nu}) \text{Tr}(E_{i,j}^{\nu'} E_{i,\nu''}^{\nu''}) \frac{c_{ijkl}^{\mu \nu} c_{ijkl}^{\nu' \nu''}}{m_i^3},
\]

using complex coefficients \( c_{ijkl}^{\mu \nu}, c_{\alpha \beta abcd}^{\mu \nu} \in \mathbb{C} \). We define \( C_{\mu \nu}^{C} \in \mathcal{L}(\mathbb{C}_{\mu \nu} \otimes \mathbb{C}_{\mu \nu}) \) and \( C_{i}^{\alpha \beta} \in \mathcal{L}(\mathbb{C}_{\alpha \beta} \otimes \mathbb{C}_{\alpha \beta}) \) for \( \mu, \nu \in \mathbb{Y}_{n+1}^d \), \( \alpha, \beta \in \mathbb{Y}_{n+1}^d \) by

\[
[C_{\mu \nu}]_{ik,jl} := c_{ijkl}^{\mu \nu}, \quad \quad [C_{i}^{\alpha \beta}]_{ac,bd} := c_{\alpha \beta abcd}^{\mu \nu}.
\]

From Lemma 5 and Eq. (S44), \( \text{Tr}(C \Omega_{d,n}) \) is given by

\[
\frac{1}{d^2} \sum_{\mu, \nu, \mu' \in \mathbb{Y}_{n+1}^d} \sum_{i,j=1}^{d} \sum_{k,l=1}^{d} \sum_{\nu', \nu''}^{d} \text{Tr}(E_{ij}^{\mu} E_{k,l}^{\nu}) \text{Tr}(E_{i,j}^{\nu'} E_{i,\nu''}^{\nu''}) \frac{c_{ijkl}^{\mu \nu} c_{ijkl}^{\nu' \nu''}}{m_i^3},
\]

using complex coefficients \( c_{ijkl}^{\mu \nu}, c_{\alpha \beta abcd}^{\mu \nu} \in \mathbb{C} \). We define \( C_{\mu \nu}^{C} \in \mathcal{L}(\mathbb{C}_{\mu \nu} \otimes \mathbb{C}_{\mu \nu}) \) and \( C_{i}^{\alpha \beta} \in \mathcal{L}(\mathbb{C}_{\alpha \beta} \otimes \mathbb{C}_{\alpha \beta}) \) for \( \mu, \nu \in \mathbb{Y}_{n+1}^d \), \( \alpha, \beta \in \mathbb{Y}_{n+1}^d \) by

\[
[C_{\mu \nu}]_{ik,jl} := c_{ijkl}^{\mu \nu}, \quad \quad [C_{i}^{\alpha \beta}]_{ac,bd} := c_{\alpha \beta abcd}^{\mu \nu}.
\]

From Lemma 5 and Eq. (S44), \( \text{Tr}(C \Omega_{d,n}) \) is given by

\[
\frac{1}{d^2} \sum_{\mu, \nu, \mu' \in \mathbb{Y}_{n+1}^d} \sum_{i,j=1}^{d} \sum_{k,l=1}^{d} \sum_{\nu', \nu''}^{d} \text{Tr}(E_{ij}^{\mu} E_{k,l}^{\nu}) \text{Tr}(E_{i,j}^{\nu'} E_{i,\nu''}^{\nu''}) \frac{c_{ijkl}^{\mu \nu} c_{ijkl}^{\nu' \nu''}}{m_i^3},
\]

using complex coefficients \( c_{ijkl}^{\mu \nu}, c_{\alpha \beta abcd}^{\mu \nu} \in \mathbb{C} \). We define \( C_{\mu \nu}^{C} \in \mathcal{L}(\mathbb{C}_{\mu \nu} \otimes \mathbb{C}_{\mu \nu}) \) and \( C_{i}^{\alpha \beta} \in \mathcal{L}(\mathbb{C}_{\alpha \beta} \otimes \mathbb{C}_{\alpha \beta}) \) for \( \mu, \nu \in \mathbb{Y}_{n+1}^d \), \( \alpha, \beta \in \mathbb{Y}_{n+1}^d \) by

\[
[C_{\mu \nu}]_{ik,jl} := c_{ijkl}^{\mu \nu}, \quad \quad [C_{i}^{\alpha \beta}]_{ac,bd} := c_{\alpha \beta abcd}^{\mu \nu}.
\]

The quantum comb conditions (S99)-(S101) are written in terms of \( C_{\mu \nu}^{C} \) and \( C_{i}^{\alpha \beta} \) as follows. Since \( C \) is written as

\[
C = \sum_{\mu, \nu \in \mathbb{Y}_{n+1}^d} \sum_{i,j=1}^{d} \sum_{k,l=1}^{d} (I_{d_i}^{\mu})_{X \otimes (I_{d_j}^{\nu})_{\Omega}} \otimes \frac{c_{ijkl}^{\mu \nu}}{m_i m_j} |\mu, i, k, l, j, \nu \rangle \langle \nu, l|_{\Omega},
\]

the positivity of \( C \) [Eq. (S99)] is written as

\[
C_{\mu \nu}^{C} \geq 0
\]

for all \( \mu, \nu \in \mathbb{Y}_{n+1}^d \). From Lemma 7, \( \text{Tr}_{X} C_i \) and \( \text{Tr}_{X \cdots X_{i-1}} C_i \) are written as

\[
\text{Tr}_{X} C_i = \text{Tr}_{X} \left[ \sum \sum \sum \sum \frac{c_{\alpha \beta abcd}^{\mu \nu}}{m_i m_j} (E_{ab}^{\alpha})_{X} \otimes (E_{cd}^{\beta})_{\Omega} \right],
\]

using complex coefficients \( c_{ijkl}^{\mu \nu}, c_{\alpha \beta abcd}^{\mu \nu} \in \mathbb{C} \). We define \( C_{\mu \nu}^{C} \in \mathcal{L}(\mathbb{C}_{\mu \nu} \otimes \mathbb{C}_{\mu \nu}) \) and \( C_{i}^{\alpha \beta} \in \mathcal{L}(\mathbb{C}_{\alpha \beta} \otimes \mathbb{C}_{\alpha \beta}) \) for \( \mu, \nu \in \mathbb{Y}_{n+1}^d \), \( \alpha, \beta \in \mathbb{Y}_{n+1}^d \) by

\[
[C_{\mu \nu}]_{ik,jl} := c_{ijkl}^{\mu \nu}, \quad \quad [C_{i}^{\alpha \beta}]_{ac,bd} := c_{\alpha \beta abcd}^{\mu \nu}.
\]
where \( e_\mu \) is the index of the standard tableau \( s^\mu_\nu \) obtained by adding a box \( ] \) to the standard tableau \( s^\nu_\rho \). Then, \( C_{i-1} = \text{Tr}_{\mathcal{O}_{i-1}} C_i / d \) is written as

\[
C_{i-1} = \sum_{\gamma, \delta \in \mathcal{Y}_{d-1}, e, f = 1, g, h = 1} d_{\gamma} d_{\delta} C^{\gamma \delta}_{\mu \nu} (E_{\gamma \delta})_{\mu \nu} (E_{gh})_{\nu \mu} \phi_{\gamma \delta}^{-1} \phi_{\mu \nu}^{-1},
\]

(S116)

\[
c^{\gamma \delta}_{1-1, e f g h} := \frac{1}{d} \sum_{\alpha \in \gamma + \square, \beta \in \delta + \square} \sum_{a, b = 1, c, d = 1} d_{\alpha} d_{\beta} \delta_{a, \epsilon \mu} \delta_{b, \nu \mu} \delta_{c, g \beta} \delta_{d, h \beta} c^{\alpha \beta}_{a, b, c, d}.
\]

(S117)

In terms of the matrix representation (S107), Eq. (S117) is written as

\[
C^{\gamma \delta}_{1-1} = \frac{1}{d} \sum_{\alpha \in \gamma + \square, \beta \in \delta + \square} (X^\gamma_{\alpha} \otimes X^\delta_{\beta}) C^{\alpha \beta}_{\gamma \delta} (X^\gamma_{\alpha} \otimes X^\delta_{\beta})^\dagger,
\]

(S118)

where \( X^\gamma_{\alpha} \) is the \( d_{\gamma} \times d_{\alpha} \) matrix defined by

\[
[X^\gamma_{\alpha}]_{c, a} := \delta_{c, \gamma, a},
\]

(S119)

and \( c_\alpha \) is the index of the standard tableau \( c^{\alpha \beta}_{a} \) obtained by adding a box \( [ ] \) to \( c_{\gamma} \). From Lemma 6, \( C_{i-1} \otimes I_{\mathcal{O}_{i-1}} \) is written as

\[
C_{i-1} \otimes I_{\mathcal{O}_{i-1}} = \sum_{\gamma, \delta \in \mathcal{Y}_{d}, e, f = 1, g, h = 1} d_{\gamma} d_{\delta} C^{\gamma \delta}_{\mu \nu} (E_{\gamma \delta})_{\mu \nu} (E_{gh})_{\nu \mu} \phi_{\gamma \delta}^{-1} \phi_{\mu \nu}^{-1} \otimes I_{\mathcal{O}_{i-1}},
\]

(S120)

\[
= \sum_{\gamma, \delta \in \mathcal{Y}_{d}, e, f = 1, g, h = 1} d_{\gamma} d_{\delta} C^{\gamma \delta}_{\mu \nu} (E_{\gamma \delta})_{\mu \nu} (E_{gh})_{\nu \mu} \phi_{\gamma \delta}^{-1} \otimes I_{\mathcal{O}_{i-1}}.
\]

(S121)

Therefore, the condition (S100) is equivalent to the following equation:

\[
\sum_{\alpha \in \gamma + \square} \sum_{a, b = 1, c, d = 1} d_{\alpha} d_{\beta} \delta_{a, \epsilon \mu} \delta_{b, \nu \mu} \delta_{c, g \beta} \delta_{d, h \beta} c^{\alpha \beta}_{a, b, c, d} m_{\beta} = \sum_{\delta \in \beta - \square} \sum_{g, h = 1} d_{\delta} \frac{c^{\gamma \delta}_{1-1, e f g h} m_{\beta}}{m_{\delta}},
\]

(S122)

for all \( \gamma \in \mathcal{Y}_{d-1}, \beta \in \mathcal{Y}_{d}, e, f \in \{1, \ldots, d_{\gamma}\} \) and \( c, d \in \{1, \ldots, d_{\beta}\} \). In terms of the matrix representation (S107), this relation is written as

\[
\sum_{\alpha \in \gamma + \square} (X^\gamma_{\alpha} \otimes I_{d_{\beta}}) \frac{C^{\alpha \beta}_{\gamma \delta}}{m_{\beta}} (X^\delta_{\beta} \otimes I_{d_{\beta}})^\dagger = \sum_{\delta \in \beta - \square} (I_{d_{\gamma}} \otimes X^\delta_{\beta})^\dagger \frac{C^{\gamma \delta}_{1-1}}{m_{\delta}} (I_{d_{\gamma}} \otimes X^\delta_{\beta}),
\]

(S123)

for all \( \gamma \in \mathcal{Y}_{d-1}, \beta \in \mathcal{Y}_{d} \). Finally, since \( C_{0} = c^{0 \emptyset} \) holds, the condition (S101) is written as

\[
C^{0 \emptyset} = 1.
\]

(S124)

In conclusion, the optimal value of the SDP (S90) is the same as that of the following SDP:

\[
\max_{\mu \in \mathcal{Y}_{n+1}} \sum_{i, j, k, l = 1} d_{\mu} \frac{[\pi_{\mu}]_{ki} [\pi_{\mu}]_{ij} [C_{\mu \nu}]_{ji}}{d^{2} m_{\mu}}
\]

\[
\text{s.t.} \quad C^{\mu \nu} \in \mathcal{L}(C^{d_{\mu} \otimes d_{\nu}}) \geq 0,
\]

\[
\sum_{\alpha \in \gamma + \square} (X^\gamma_{\alpha} \otimes I_{d_{\beta}}) \frac{C^{\alpha \beta}_{\gamma \delta}}{m_{\beta}} (X^\delta_{\beta} \otimes I_{d_{\beta}})^\dagger = \sum_{\delta \in \beta - \square} (I_{d_{\gamma}} \otimes X^\delta_{\beta})^\dagger \frac{C^{\gamma \delta}_{1-1}}{m_{\delta}} (I_{d_{\gamma}} \otimes X^\delta_{\beta}),
\]

(S125)

for all \( i \in \{1, \ldots, n + 1\}, \mu, \nu \in \mathcal{Y}_{n+1}, \gamma \in \mathcal{Y}_{d-1}, \) and \( \beta \in \mathcal{Y}_{d} \).
Construction of the unitary inversion comb whose Choi matrix has rank 14

We consider the following Choi matrix \( C \in \mathcal{L}(\mathcal{P} \otimes \mathcal{I}^4 \otimes \mathcal{O}^4 \otimes \mathcal{F}) \):

\[
C = \frac{1}{2} \sum_{i,j=2}^{5} (-1)^{a_i + a_j} (E_{i,j}^{a_3})_{\mathcal{F}}^\dagger \otimes (E_{7-i,j-1}^{a_3})_{\mathcal{O}^3} + \frac{1}{2} \sum_{i,j=4}^{5} (E_{i,j}^{a_3})_{\mathcal{I}^4}^\dagger \otimes (E_{8-i,j-1}^{a_3})_{\mathcal{O}^4} + C',
\]

(S126)

where \( C' \in \mathcal{L}(\mathcal{P} \otimes \mathcal{I}^4 \otimes \mathcal{O}^4 \otimes \mathcal{F}) \) is a positive-semidefinite matrix satisfying

\[
\text{Tr}_\mathcal{F} C' = C'_4 \otimes I_{\mathcal{O}_4},
\]

(S127)

\[
\text{Tr}_\mathcal{I} C'_4 = C'_4 \otimes I_{\mathcal{O}_4},
\]

(S128)

\[
\text{Tr}_\mathcal{I} C'_3 = (E_{11}^{d_2})_{\mathcal{I}_2}^\dagger \otimes (E_{11}^{\gamma_1})_{\mathcal{O}_2},
\]

(S129)

for some matrices \( C'_4 \in \mathcal{L}(\mathcal{P} \otimes \mathcal{I}^4 \otimes \mathcal{O}^3) \) and \( C'_3 \in \mathcal{L}(\mathcal{P} \otimes \mathcal{I}^3 \otimes \mathcal{O}_2^2) \). Then, similarly to the proof of Lemma 3, we can show that the Choi matrix \( C \) defined above also satisfies Lemma 3. We construct the matrix \( C' \) satisfying the above conditions with as small a rank as possible. Due to the above conditions and the following inequality for any positive-semidefinite matrix \( A \in \mathcal{L}(\mathcal{A} \otimes \mathcal{B}) \) given by

\[
\text{rank}(A) \geq \frac{\text{rank}(\text{Tr}_A A)}{\text{dim} \mathcal{A}},
\]

(S130)

the rank of \( C' \) is lower bounded as

\[
\text{rank}(C') \geq \frac{\text{rank}(E_{11}^{d_2} \otimes E_{11}^{\gamma_1})}{2} = 2.
\]

(S131)

Since \( d_2 \) and \( \gamma_1 \) are given by

\[
d_2 = \begin{array}{|c|}
\hline
& \end{array}, \quad \gamma_1 = \begin{array}{|c|c|c|c|}
\hline
& & & \\
\hline
\end{array}
\]

(S132)

\((E_{11}^{d_2})_{\mathcal{I}_2}\) is the projector onto the antisymmetric subspace of \( \mathcal{I}_1 \otimes \mathcal{I}_2 \) and \((E_{11}^{\gamma_1})_{\mathcal{O}_2}\) is the projector onto the totally symmetric subspace of \( \mathcal{P} \otimes \mathcal{O}_1 \otimes \mathcal{O}_2 \). Therefore, \((E_{11}^{d_2})_{\mathcal{I}_2}\) and \((E_{11}^{\gamma_1})_{\mathcal{O}_2}\) are given by

\[
(E_{11}^{d_2})_{\mathcal{I}_2} = |\psi^\rangle \langle \psi |_{\mathcal{I}_1 \mathcal{I}_2},
\]

(S133)

\[
(E_{11}^{\gamma_1})_{\mathcal{O}_2} = \sum_{i=1}^{4} |\varphi_i \rangle \langle \varphi_i |_{\mathcal{P} \mathcal{O}_1 \mathcal{O}_2},
\]

(S134)

where \( |\psi^\rangle \in \mathcal{I}_1 \otimes \mathcal{I}_2 \) and \(|\varphi_i \rangle \in \mathcal{P} \otimes \mathcal{O}_1 \otimes \mathcal{O}_2 \) for \( i \in \{1, \ldots, 4\} \) are defined by

\[
|\psi^\rangle := \frac{|01\rangle - |10\rangle}{\sqrt{2}},
\]

(S135)

\[
|\varphi_1 \rangle := |000\rangle,
\]

(S136)

\[
|\varphi_2 \rangle := \frac{|100\rangle + |010\rangle + |001\rangle}{\sqrt{3}},
\]

(S137)

\[
|\varphi_3 \rangle := \frac{|110\rangle + |101\rangle + |011\rangle}{\sqrt{3}},
\]

(S138)

\[
|\varphi_4 \rangle := |111\rangle.
\]

(S139)

We define \( C' \) by

\[
C' := 4|\psi^\rangle \langle \psi |_{\mathcal{I}_1 \mathcal{I}_2} \otimes (|\varphi'_1 \rangle \langle \varphi'_1 | + |\varphi'_2 \rangle \langle \varphi'_2 |)_{\mathcal{P} \mathcal{O}_1 \mathcal{O}_2 \mathcal{I}_3} \otimes |\phi^+ \rangle \langle \phi^+ |_{\mathcal{O}_3 \mathcal{I}_4} \otimes |\phi^+ \rangle \langle \phi^+ |_{\mathcal{O}_4 \mathcal{F}},
\]

(S140)

where \(|\varphi'_i \rangle \in \mathcal{P} \otimes \mathcal{O}_1 \otimes \mathcal{O}_2 \otimes \mathcal{I}_3\) and \(|\phi^+ \rangle \in (\mathbb{C}^2)^{\otimes 2}\) are defined by

\[
|\varphi'_1 \rangle := |\varphi_1 \rangle_{\mathcal{P} \mathcal{O}_1 \mathcal{O}_2} \otimes |0\rangle_{\mathcal{I}_3} + |\varphi_2 \rangle_{\mathcal{P} \mathcal{O}_1 \mathcal{O}_2} \otimes |1\rangle_{\mathcal{I}_3},
\]

(S141)

\[
|\varphi'_2 \rangle := |\varphi_3 \rangle_{\mathcal{P} \mathcal{O}_1 \mathcal{O}_2} \otimes |0\rangle_{\mathcal{I}_3} + |\varphi_4 \rangle_{\mathcal{P} \mathcal{O}_1 \mathcal{O}_2} \otimes |1\rangle_{\mathcal{I}_3},
\]

(S142)

\[
|\phi^+ \rangle := \frac{|00\rangle + |11\rangle}{\sqrt{2}}.
\]

(S143)

Then, \( C' \) satisfies the conditions \( [\text{S127}], [\text{S129}] \), the rank of \( C' \) is \( \text{rank}(C') = 2 \) and the rank of \( C \) is \( \text{rank}(C) = 14 \).