One-to-One Correspondence Between Deterministic Port-Based Teleportation and Unitary Estimation

Satoshi Yoshida, Yuki Koizumi, Michał Studziński, Marco Túlio Quintino, and Mio Murao

***Abstract*—Port-based teleportation is a variant of quantum teleportation, where the receiver can choose one of the ports in his part of the entangled state shared with the sender, but cannot apply other recovery operations. We show that the optimal fidelity of deterministic port-based teleportation (dPBT) using $N = n + 1$ ports to teleport a d-dimensional state is equivalent to the optimal fidelity of d-dimensional unitary estimation using n calls of the input unitary operation. From any given dPBT, we can explicitly construct the corresponding unitary estimation protocol achieving the same optimal fidelity, and *vice versa*. Using the obtained one-to-one correspondence between dPBT and unitary estimation, we derive the asymptotic optimal fidelity of port-based teleportation given by $1 - O(d^4)N^{-2} \leq F \leq 1 - \Omega(d^4)N^{-2}$, which improves the previously known result given by $1 - O(d^5)N^{-2} \leq F \leq 1 - \Omega(d^2)N^{-2}$. We also show that the optimal fidelity of unitary estimation for the case $n \leq d - 1$ is $F = \frac{n+1}{d^2}$, and this fidelity is equal to the optimal fidelity of unitary inversion with $n \leq d - 1$ calls of the input unitary operation even if we allow indefinite causal order among the calls.**

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***Index Terms*—Quantum teleportation, unitary estimation, representation theory, higher-order quantum transformation.**

I. Introduction

QUANTUM teleportation [1] is one of the fundamental protocols in quantum information, which is widely used in quantum communication [2] and quantum computation [3], [4]. It also opens up a way to understand fundamental properties of quantum mechanics, such as quantum entanglement [5]. In the original protocol of quantum teleportation, Alice sends an unknown quantum state to Bob by using a shared entanglement with the Bell measurement on the unknown state and her share of the entangled state and classical communication. Depending on the outcome of Alice's measurement, Bob applies a Pauli operation on his part of the shared entangled state to recover her state.

Port-based teleportation (PBT) [6], [7] is a variant of the teleportation protocol, where Alice and Bob share an entangled $2N$-qudit state, and each of Alice and Bob possesses N qudits (called ports). Alice performs a joint measurement on an unknown state and Alice's N ports. Instead of applying a Pauli operation, Bob can only choose a port from N ports of the shared entanglement to recover Alice's state. Since Bob's recovery operation commutes with parallel calls of the same quantum operation applied to Bob's ports, we can use port-based teleportation to apply a quantum operation $\mathcal{E}$ to a quantum state prepared after the application of $\mathcal{E}$ in the following way. We first apply a quantum operation $\mathcal{E}$ in parallel to Bob's ports (storage) and use it for port-based teleportation of the quantum state ρ. As a result, Bob obtains the quantum state $\mathcal{E}(\rho)$ (retrieval). Such a task is called storage-and-retrieval [8], quantum learning [9], or universal programming [10], [11]. Beyond storage-and-retrieval, port-based teleportation has wide applications in quantum cryptography [12], Bell nonlocality [13], holography [14], [15], and higher-order quantum transformations [16], [17], [18], [19]. Port-based teleportation is also extended to the scenario where Alice's state is given by multi-qudit states (multi port-based teleportation) [20], [21] and continuous-variable states [22].

Since the no-programming theorem prohibits a deterministic and exact implementation of storage-and-retrieval [11], port-based teleportation is also impossible in a deterministic and exact way. This no-go theorem led researchers to consider probabilistic or approximate protocol [6], [7], [23], [24], [25], [26], [27], [28], [29], [30], [31], [32], [33], [34], [35], [36], [37]. The former is called probabilistic port-based teleportation

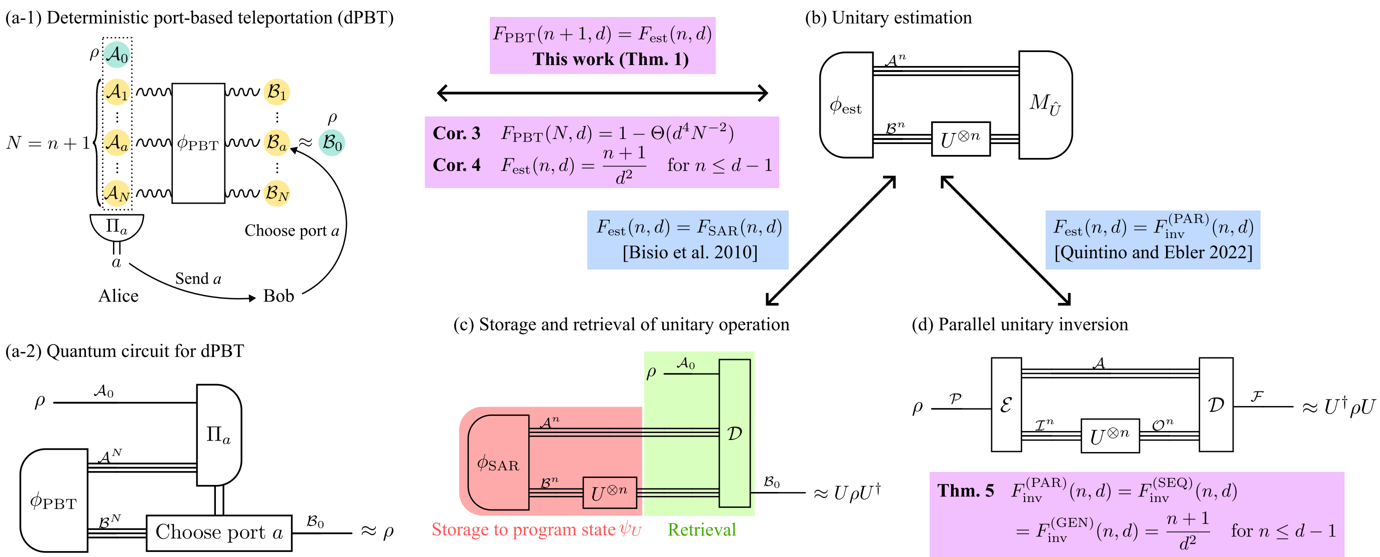

Fig. 1. This work shows the one-to-one correspondence between deterministic port-based teleportation (dPBT) and unitary estimation (see Thm. 1). Combining this result with [9] and [18], we also show the one-to-one correspondence with deterministic storage-and-retrieval (dSAR) of unitary operation and deterministic parallel unitary inversion. (a-1) In dPBT, Alice approximately teleports her unknown state ρ by sending the measurement outcome a of the joint measurement on the target state ρ and half of a shared $2N$-qudit entangled state ϕ_{PBT}. Bob chooses the port a of the other half to obtain a quantum state close to ρ. Its circuit description is shown in (a-2). By using the one-to-one correspondence, its asymptotic optimal fidelity is shown to be $F_{\mathrm{PBT}}(N,d)=1-\Theta(d^4N^{-2})$ (see Cor. 3). (b) In unitary estimation, n calls of unitary operator U are applied in parallel to the resource state ϕ_{est}, and the output state is measured in a positive operator-valued measure (POVM) measurement $\{M_{\hat{U}}\mathrm{d}\hat{U}\}_{\hat{U}}$ to obtain the estimated unitary $\hat{U}$. By using the one-to-one correspondence, its optimal fidelity is shown to be $F_{\mathrm{est}}(n,d)=\frac{n+1}{d^2}$ for $n\leq d-1$ (see Cor. 4). (c) In dSAR, n calls of U are applied into a resource state ρ_{SAR} to obtain a program state ψ_U. In a later moment, the action of U is retrieved by applying a quantum operation $\mathcal{D}$ on the joint system of the input state ρ and the program state ψ_U. (d) In deterministic parallel unitary inversion, an operation $\mathcal{E}$ is applied before n calls of an unknown unitary operator U, and an operation $\mathcal{D}$ is applied just after, in a way that the resulting composition is approximately U^{-1}. For $n\leq d-1$, the parallel protocol achieves the optimal fidelity even if we consider the most general protocol including the ones with indefinite causal order (see Thm. 5).

(pPBT), and the latter is called deterministic port-based teleportation (dPBT). The optimal success probability of pPBT is explicitly given in [7] and [25], and it is known to be utilized to achieve the optimal success probability of storage-and-retrieval of unitary operation [8]. On the other hand, less is known for the optimal fidelity of dPBT, and no closed formula is known except for the qubit case [6]. Its asymptotic form is shown in [28], but its lower and upper bounds do not coincide with each other. Also, dPBT is known not to provide the optimal fidelity of storage-and-retrieval of unitary operation [10], [18].

In this paper, we show a one-to-one correspondence of the dPBT with another widely explored task called the unitary estimation in the Bayesian framework [9], [10], [38], [39], [40], [41], [42], [43], [44], [45], [46], [47], [48], [49], [50]. We show that the optimal fidelity of d-dimensional unitary estimation using n calls of the input unitary operation is equivalent to that of dPBT using $N=n+1$ ports to teleport a d-dimensional state. Our proof is made in a constructive way, once the optimal protocol for dPBT is given, we can explicitly construct the corresponding unitary estimation protocol and *vice versa*. Combining our results with previously known the one-to-one correspondence between unitary estimation, deterministic storage-and-retrieval (dSAR) [9] and deterministic parallel unitary inversion [18], we then obtain a one-to-one correspondence between the four tasks (see Fig. 1). Note that this one-to-one correspondence does not imply that the optimal dPBT protocol provides the optimal fidelity of dSAR; rather, our result implies the opposite. If we use the dPBT protocol to perform the dSAR using n calls of the input unitary operation U, it provides the fidelity given by $F_{\mathrm{PBT}}(n,d)$, which is strictly smaller than $F_{\mathrm{SAR}}(n,d)=F_{\mathrm{PBT}}(n+1,d)$ from our one-to-one correspondence.

The one-to-one correspondence proved here allows us to translate previous results on the optimal fidelity of unitary estimation to that of dPBT and *vice versa*. This allows us to prove that the asymptotic fidelity of optimal dPBT is precisely $F_{\mathrm{PBT}}(N,d)=1-\Theta(d^4N^{-2})$, from a corresponding result for unitary estimation [10], [50]. This result improves upon the previous result [28] and gives a tight scaling with respect to d. Also, results from dPBT [26], allow us to show that the fidelity of unitary estimation is given by $\frac{n+1}{d^2}$ for $n\leq d-1$. Finally, we prove that the optimal fidelity of unitary inversion using n calls of the input unitary operation is given by that of unitary estimation for $n\leq d-1$ even when considering adaptive circuits or protocols without a definite causal order [51], [52], [53].

II. ONE-TO-ONE CORRESPONDENCE BETWEEN dPBT AND UNITARY ESTIMATION

In dPBT, Alice wants to teleport an arbitrary qudit state $\rho\in\mathcal{L}(\mathcal{A}_0)$ to Bob using a shared entangled $2N$-qudit state $\phi_{\mathrm{PBT}}\in\mathcal{L}(\mathcal{A}^N\otimes\mathcal{B}^N)$, where $\mathcal{L}(\mathcal{X})$ represents the set of linear operators on a Hilbert space $\mathcal{X}$, $\mathcal{A}^N$ and $\mathcal{B}^N$ are the joint Hilbert spaces defined by $\mathcal{A}^N=\bigotimes_{i=1}^N\mathcal{A}_i$ and $\mathcal{B}^N=\bigotimes_{i=1}^N\mathcal{B}_i$ for $\mathcal{A}_0\simeq\mathcal{A}_i\simeq\mathcal{B}_i\simeq\mathbb{C}^d$. Alice measures the quantum state ρ and half of the shared entangled state ϕ_{PBT} with a positive operator-valued measure (POVM) measurement $\{\Pi_a\}_{a=1}^N$, and sends the measurement outcome a to Bob. Bob chooses the port a from the other half of the shared entangled state ϕ_{PBT}, approximating Alice's state ρ. The quantum state Bob obtains is given by $\Lambda(\rho)$, where $\Lambda : \mathcal{L}(\mathcal{A}_0) \to \mathcal{L}(\mathcal{B}_0)$ is the teleportation channel [6], [54]

$$\Lambda(\rho) := \sum_{a=1}^{N} \mathrm{Tr}_{\mathcal{A}_0\mathcal{A}^N\overline{\mathcal{B}_a}}[(\Pi_a \otimes \mathbb{1}_{\mathcal{B}^N})(\rho \otimes \phi_{\mathrm{PBT}})], \tag{1}$$

with $\overline{\mathcal{B}_a} := \bigotimes_{i\neq a} \mathcal{B}_i$ and $\mathbb{1}$ being the identity operator. The performance of the dPBT protocol may be evaluated in terms of channel fidelity [55] between a quantum channel with map $\Lambda : \mathcal{L}(\mathbb{C}^d) \to \mathcal{L}(\mathbb{C}^d)$ and a unitary operator $U : \mathbb{C}^d \to \mathbb{C}^d$, quantity defined by

$$f(U, \Lambda) := \frac{1}{d^2} \sum_i |\mathrm{Tr}(K_i U^\dagger)|^2, \tag{2}$$

where $\{K_i\}_i$ is the set of Kraus operators of Λ satisfying $\Lambda(\rho) = \sum_i K_i \rho K_i^\dagger$ [56]. The performance of a dPBT protocol is then the fidelity between the teleportation channel of Eq. (1) and the identity channel represented by the identity operator $\mathbb{1}_d \in \mathcal{L}(\mathbb{C}^d)$, i.e,

$$F_{\mathrm{PBT}} := f(\mathbb{1}_d, \Lambda). \tag{3}$$

Unitary estimation is the task to obtain the classical description of the estimated unitary $\hat{U}$ of the input unitary operator $U \in \mathrm{SU}(d)$, which can be called n times. We use the Bayesian framework [38] to evaluate the performance of unitary estimation, and we assume a Haar-random prior distribution of the input unitary operator. The performance of an estimation protocol is given by its *average fidelity*

$$F_{\mathrm{est}}^{(\mathrm{ave})} := \int \mathrm{d}U \int \mathrm{d}\hat{U}\, p(\hat{U}|U) f(\hat{U}, \mathcal{U}), \tag{4}$$

where $p(\hat{U}|U)$ is the probability distribution of obtaining the estimator $\hat{U}$ given the input unitary operator U, $\mathrm{d}U$ and $\mathrm{d}\hat{U}$ are the Haar measures [57] on $\mathrm{SU}(d)$, f is the channel fidelity, and $\mathcal{U} : \mathcal{L}(\mathbb{C}^d) \to \mathcal{L}(\mathbb{C}^d)$ is the unitary operation defined by $\mathcal{U}(\cdot) := U(\cdot)U^\dagger$. The optimal fidelity is shown to be implementable by a parallel covariant protocol [9]. In the parallel covariant protocol [see Fig. 1 (b)], the n-fold unitary operator $U^{\otimes n}$ is applied to the resource state $\phi_{\mathrm{est}} \in \mathcal{L}(\mathcal{A}^n \otimes \mathcal{B}^n)$, and the POVM measurement $\left\{M_{\hat{U}} \mathrm{d}\hat{U}\right\}_{\hat{U}}$ is applied to obtain the estimated unitary $\hat{U}$, hence $p(\hat{U}|U) = \mathrm{tr}\left[M_{\hat{U}}\, (U^{\otimes n} \otimes \mathbb{1}_{\mathcal{A}^n})\phi_{\mathrm{est}}(U^{\otimes n} \otimes \mathbb{1}_{\mathcal{A}^n})^\dagger\right]$. Also, in the covariant protocol, the average-case fidelity coincides with the worst-case fidelity [38] $F_{\mathrm{est}}^{(\mathrm{wc})} := \inf_U \int \mathrm{d}\hat{U}\, p(\hat{U}|U) f(\hat{U}, \mathcal{U})$.

In the following, we present a one-to-one correspondence between dPBT and unitary estimation.

Theorem 1: The optimal fidelity of deterministic port-based teleportation (dPBT) using $N = n + 1$ ports to teleport a d-dimensional state [denoted by $F_{\mathrm{PBT}}(N, d)$] coincides with the optimal fidelity of unitary estimation using n calls of an input d-dimensional unitary operation [denoted by $F_{\mathrm{est}}(n, d)$], i.e.,

$$F_{\mathrm{PBT}}(n + 1, d) = F_{\mathrm{est}}(n, d) \tag{5}$$

holds. In addition, given any dPBT protocol using $N = n + 1$ ports, we can construct a unitary estimation protocol with n calls attaining the fidelity more than or equal to the fidelity of the dPBT, and *vice versa*.

Proof Sketch: We show this theorem by explicitly constructing a unitary estimation protocol from any given dPBT protocol and *vice versa* (see Fig. 2). We first convert any given dPBT and unitary estimation protocols into covariant protocol without decreasing the fidelity [9], [26], [30], [47], as shown in (a)→(b) and (c)→(d) of Fig. 2 (see Appendixes B and C for the details). The covariant protocol[1] are protocols with the resource states and the POVMs in specific forms that are covariant with respect to certain representations of the unitary group, see e.g., Def. 1 of [10]. The covariant dPBT and unitary estimation protocols are shown to be parametrized by non-negative weights $\vec{w} = \{w_\mu\}_\mu$ and $\vec{v} = \{v_\alpha\}_\alpha$ associated with irreducible representations of the unitary group $\mathrm{SU}(d)$, respectively, satisfying the normalization conditions given by

$$\sum_\mu w_\mu^2 = \sum_\alpha v_\alpha^2 = 1. \tag{6}$$

In addition, the corresponding fidelities are given by

$$F_{\mathrm{PBT}} = \vec{w}^{\mathsf{T}} M_{\mathrm{PBT}}(N, d)\vec{w}, \tag{7}$$

$$F_{\mathrm{est}} = \vec{v}^{\mathsf{T}} M_{\mathrm{est}}(n, d)\vec{v}, \tag{8}$$

using the teleportation matrix $M_{\mathrm{PBT}}(N, d)$ [26] and the estimation matrix $M_{\mathrm{est}}(n, d)$ [10], [43], [44], [47]. These two matrices are shown to be related by introducing a matrix $R(n, d)$ as shown below:

$$M_{\mathrm{PBT}}(N, d) = \frac{1}{d^2} R(N - 1, d)^{\mathsf{T}} R(N - 1, d), \tag{9}$$

$$M_{\mathrm{est}}(n, d) = \frac{1}{d^2} R(n, d) R^{\mathsf{T}}(n, d). \tag{10}$$

Then, we present an explicit recipe to convert between covariant protocols for dPBT with $N = n + 1$ calls and unitary estimation with n calls keeping the fidelity, given by multiplying $R(n, d)$ or $R(n, d)^{\mathsf{T}}$ to the weight vectors $\vec{w}$ or $\vec{v}$, respectively, as shown in (b) ↔ (d) of Fig. 2. A detailed proof of Thm. 1 is presented in Appendix D. □

III. One-to-One Correspondence Between Four Different Tasks

In [9], the optimal unitary estimation using n calls is shown to be equivalent to the optimal deterministic storage-and-retrieval (dSAR) protocol using n calls, and in [18], the optimal unitary estimation using n calls is shown to be equivalent to the optimal deterministic parallel unitary inversion protocol using n calls. Combining these with Thm. 1 proved in this work, we obtain the one-to-one correspondence among the optimal fidelity of these four tasks (see Fig. 1). For completeness, we now describe the task of dSAR and parallel unitary inversion.

The dSAR (see Fig. 1), also referred to as unitary learning, considers the problem of storing the usage of an arbitrary input unitary operation on some state in a way that the usage of this operation may be retrieved in a later moment. When the usage of the input operations is made in parallel, an

[1] A function f is called covariant with respect to the unitary representations U, V of the group G if and only if $f(U_g \cdot U_g^\dagger) = V_g f(\cdot) V_g^\dagger$ holds for all $g \in G$ [see, e.g., Eq. (1) in [58]].

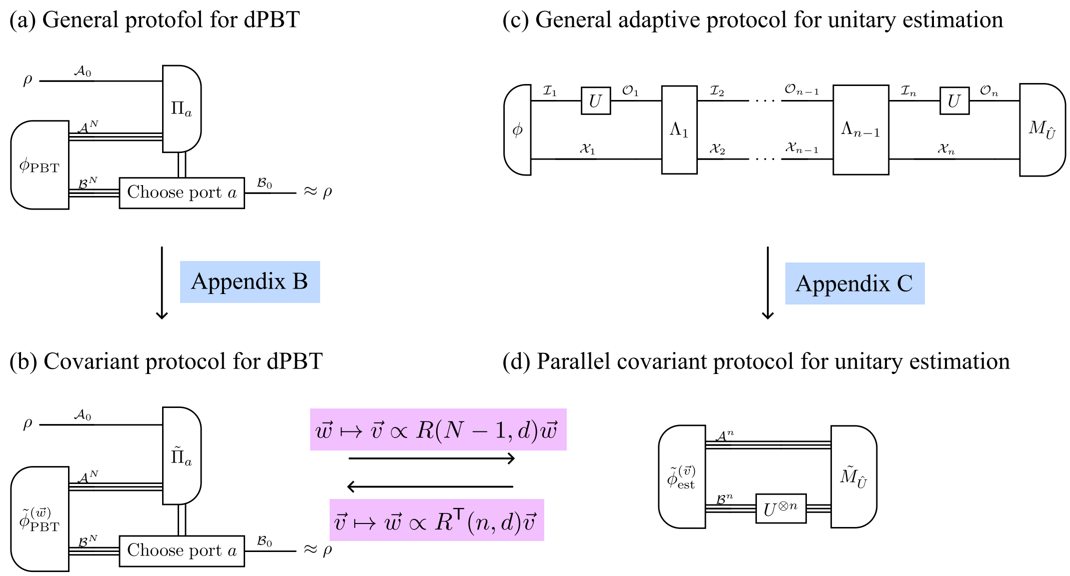

Fig. 2. Explicit construction of a unitary estimation protocol from any given dPBT protocol and *vice versa*. (a) General protocol for dPBT. (b) A covariant protocol for dPBT is constructed by using Eqs. (74), (76) and (78) to the general protocol (a) [26], [30] (see the details in Appendix B). (c) General adaptive protocol for unitary estimation. (d) A parallel covariant protocol for unitary estimation is constructed by using Eqs. (115), (119) and (120) to the general protocol (c) [9] (see the details in Appendix C). This work shows a transformation between the covariant protocols for dPBT and unitary estimation given in Eqs. (148) and (150). Combining this transformation with the constructions (a) → (b) and (c) → (d), we obtain a transformation between the sets of general protocols for unitary estimation and dPBT.

assumption which can be made without loss in performance [9], the task is described as follows. An arbitrary input unitary operator $U \in \mathrm{SU}(d)$ is called n times on a resource state $\phi_{\mathrm{SAR}} \in \mathcal{L}(\mathcal{A}\otimes\mathcal{I}^n)$, where $\mathcal{A}$ is an auxiliary space and the unitary operation $\mathcal{U}^{\otimes n}$ maps an input space $\mathcal{I}^n$ into an output space $\mathcal{O}^n$ to obtain a program state

$$\psi_U := \left(\mathbb{1}\otimes U^{\otimes n}\right)\phi_{\mathrm{SAR}}\left(\mathbb{1}\otimes U^{\otimes n}\right)^\dagger \in \mathcal{L}(\mathcal{A}\otimes\mathcal{O}^n). \tag{11}$$

Then, an arbitrary input state $\rho \in \mathcal{L}(\mathcal{P})$ is subjected to a quantum operation $\mathcal{D} : \mathcal{L}(\mathcal{P}\otimes\mathcal{A}\otimes\mathcal{O}^n) \to \mathcal{L}(\mathcal{F})$, often referred to as decoder [59], on the joint system of ρ and ψ_U to obtain the output state $\Lambda_U(\rho) := \mathcal{D}(\rho\otimes\psi_U) \in \mathcal{F}$, which we desired to be approximately the state $U\rho U^\dagger$. The performance of dSAR is evaluated by the average-case fidelity given by $F^{(\mathrm{ave})}_{\mathrm{SAR}} := \int \mathrm{d}U f(U,\Lambda_U)$, whose optimal value is always attainable by a covariant protocol, and respects [10] $F^{(\mathrm{ave})}_{\mathrm{SAR}} = 1 - \frac{1}{2}\|\Lambda_U - \mathcal{U}\|_\diamond$ for the covariant protocol, where $\|\cdot\|_\diamond$ is the diamond norm [60], [61]. Reference [9] shows that optimal dSAR protocol can always be implemented by using an estimation protocol, i.e., $F_{\mathrm{est}}(n,d) = F_{\mathrm{SAR}}(n,d)$ holds for optimal protocols. From our results, it implies that $F_{\mathrm{SAR}}(n,d) = F_{\mathrm{PBT}}(n+1,d)$.

In the task of transforming unitary operations, one is allowed to make n calls of unitary operation $\mathcal{U}(\cdot) = U(\cdot)U^\dagger : \mathcal{L}(\mathcal{I}_i) \to \mathcal{L}(\mathcal{O}_i)$, where $i \in \{1,\dots,n\}$, $U \in \mathrm{SU}(d)$ and we aim to design a quantum circuit which aims to output an operation $\mathcal{U}_g(\cdot) := g(U)\cdot g(U)^\dagger$, where $g : \mathrm{SU}(d) \to \mathrm{SU}(d)$. When the n calls of the input operation are made in parallel (see Fig. 1), the task consists in finding an encoder operation $\mathcal{E} : \mathcal{L}(\mathcal{P}) \to \mathcal{L}(\mathcal{A}\otimes\mathcal{I}^n)$, where $\mathcal{A}$ is an auxiliary space and $\mathcal{I}^n := \bigotimes_{i=1}^n \mathcal{I}_i$, and a decoder operation $\mathcal{D} : \mathcal{L}(\mathcal{A}\otimes\mathcal{O}^n) \to \mathcal{F}$, where $\mathcal{O}^n := \bigotimes_{i=1}^n \mathcal{O}_i$, such that the resulting output operation

$$\Lambda_U := \mathcal{D}\circ\left(\mathbb{1}_{\mathcal{A}}\otimes\mathcal{U}^{\otimes n}\right)\circ\mathcal{E}, \tag{12}$$

is approximately the operation $\mathcal{U}_g$, with $\mathbb{1}_{\mathcal{A}}$ here being the identity map in the auxiliary space. Similarly to dSAR, we evaluate the performance of a given protocol in terms of its average-case fidelity, $F^{(\mathrm{PAR})}_{\mathrm{g}} := \int \mathrm{d}U f(g(U),\Lambda_U)$.

Unitary estimation protocols can always be used to transform n calls of a unitary U into $g(U)$ with some fidelity $F^{(\mathrm{ave})}_{\mathrm{est}}$, for that one may simply estimate the unitary U as $\hat{U}$ and then to output $g(\hat{U})$. In [18], it is shown that if the target function $g : \mathrm{SU}(d) \to \mathrm{SU}(d)$ is antihomomorphic, i.e., $g(UV) = g(V)g(U)$ holds for all $U, V \in \mathrm{SU}(d)$, unitary estimation attains optimal performance for parallel unitary transformations. Since unitary inversion $g(U) = U^{-1}$ and unitary transposition $g(U) = U^T$ are antihomomorphisms, it follows from Thm. 1 that the optimal parallel unitary inversion and parallel unitary transposition with n calls is precisely $F_{\mathrm{PBT}}(n+1,d)$.

IV. Applications

Thm. 1 allows us to translate results on unitary estimation to results on dPBT, and *vice versa*. We now illustrate some of these applications. This section utilizes the big-O notation $O(\cdot)$, $\Omega(\cdot)$ and $\Theta(\cdot)$, defined as follows [62]:

$$f(x) = O(g(x)) \Leftrightarrow \limsup_{x\to\infty}\frac{|f(x)}{g(x)|} < \infty, \tag{13}$$

$$f(x) = \Omega(g(x)) \Leftrightarrow g(x) = O(f(x)), \tag{14}$$

$$f(x) = \Theta(g(x)) \Leftrightarrow f(x) = O(g(x)) \text{ and } f(x) = \Omega(g(x)). \tag{15}$$

Intuitively, $O(\cdot)$ represents a lower bound, $\Omega(\cdot)$ represents an upper bound, and $\Theta(\cdot)$ represents a tight bound.

Reference [10] shows a unitary estimation protocol asymptotically achieving $F_{\mathrm{est}}(n,d) \geq 1 - O(d^4)n^{-2}$. As shown in the following lemma, this lower bound is tight:

Lemma 2: The optimal fidelity of unitary estimation using n calls of an input d-dimensional unitary operation is upper bounded as

$$F_{\mathrm{est}}(n,d) \leq 1 - \Omega(d^4)n^{-2}. \tag{16}$$

Proof Sketch: Reference [50] shows a lower bound on the query complexity n to achieve a diamond-norm error ϵ for unitary estimation, given by $n = \Omega(d^2)/\epsilon$. The proof is based on constructing $\exp(\Omega(d^2))$ unitary channels that are ϵ-distant from each other and $O(\epsilon)$-close to the identity channel in terms of the diamond norm. We adapt their proof for the Bures distance [63] induced from the channel fidelity instead of the diamond norm to show this lemma. A detailed proof is presented in Appendix E. □

Thanks to Thm. 1, we have the following corollary.

Corollary 3: The asymptotic fidelity of optimal dPBT is given by

$$1 - O(d^4)N^{-2} \leq F_{\mathrm{PBT}}(N,d) \leq 1 - \Omega(d^4)N^{-2}. \tag{17}$$

Corollary 3 may be compared with previous results [28] which proved that

$$1 - O(d^5)N^{-2} \leq F_{\mathrm{PBT}}(N,d) \leq 1 - \Omega(d^2)N^{-2}. \tag{18}$$

In particular, we can explicitly construct the dPBT protocol whose fidelity scales with $1 - O(d^4)N^{-2}$ by combining the unitary estimation protocol in [10] with the obtained one-to-one correspondence, which improves over the protocol exhibiting the fidelity $1 - O(d^5)N^{-2}$ shown in [28]. This result also gives a partial answer to an open problem raised in [28] to determine $h(d) := \lim_{N\to\infty} N^2[1 - F_{\mathrm{PBT}}(N,d)]$, which is shown to be $h(d) = \Theta(d^4)$ by Cor. 3.

Reference [26] shows that, when $N \leq d$, optimal dPBT is given by $F_{\mathrm{PBT}}(N,d) = \frac{N}{d^2}$. Hence, from Thm. 1, we obtain the following corollary.

Corollary 4: When the number of the calls of the input unitary operation, denoted by n, satisfies $n \leq d-1$, the optimal fidelity of unitary estimation is given by

$$F_{\mathrm{est}}(n,d) = \frac{n+1}{d^2}. \tag{19}$$

Also, in Appendix F, we show that the optimal resource state for dPBT and unitary estimation are the same for the case $N = n+1 \leq d$. Hence, the optimal resource state is useful as a universal resource state for dPBT and unitary estimation.

V. Optimal Unitary Inversion for $n \leq d-1$

As previously mentioned, the task of transforming n calls of an arbitrary unitary operation into its inverse is attainable by an estimation strategy when only parallel uses of the input operation are allowed. However, already when $n = 2$ calls are allowed, the performance of sequential circuits for qubit unitary inversion outperforms parallel ones, and the performance of processes without a definite causal order [51], [52], [53] outperforms sequential ones [18]. Also, when $n = 4$ calls are allowed, there exists a sequential circuit which transforms an arbitrary qubit-unitary operation into its inverse operation with fidelity one [64], which was recently extended to an arbitrary dimension using $n = O(d^2)$ calls [65] (see also [66]).

In Appendix G, we show an upper bound of the fidelity of unitary inversion given by $\frac{n+1}{d^2}$ for $n \leq d-1$ even if we consider the most general protocols including the ones with indefinite causal order. Corollary 4 implies that this bound is achievable by an estimation-based strategy. More precisely, we prove the following theorem.

Theorem 5: When $n \leq d-1$, the optimal fidelity of d-dimensional unitary inversion with n calls of a unitary operation is given by

$$F_{\mathrm{inv}}^{(\mathrm{PAR})}(n,d) = F_{\mathrm{inv}}^{(\mathrm{SEQ})}(n,d) = F_{\mathrm{inv}}^{(\mathrm{GEN})}(n,d) = \frac{n+1}{d^2}, \tag{20}$$

where PAR, SEQ, and GEN refer to parallel, sequential, and general protocols including the ones with indefinite causal order, respectively.

VI. Conclusion

In this paper, we show the equivalence between the optimal fidelity of dPBT for $N = n+1$ and unitary estimation with n calls of the unitary operation by giving an explicit transformation between the optimal protocols. Combining this result with the previous results on the equivalence of the optimal fidelity between unitary estimation and dSAR [9], and also between parallel unitary inversion and unitary estimation [18], we obtain a one-to-one correspondence among four important quantum information tasks. Our correspondence result has the potential to accelerate the research on dPBT and unitary estimation since obtaining the optimal fidelity of dPBT in any setting, i.e., asymptotic or finite, can be immediately translated into that of unitary estimation, and *vice versa*. Here, we use this one-to-one correspondence to derive the asymptotically optimal dPBT protocol, a non-trivial result which improves the scaling of the fidelity derived in a previous work [28]. In a related topic, we prove that when only $n \leq d-1$ calls are available, deterministic unitary inversion can always be obtained by an estimation protocol, showing that sequential circuits and strategies without definite causal order are not useful in the regime of $n \leq d-1$ calls.

Our proof of the one-to-one correspondence is based on the covariant forms of dPBT and unitary estimation, which is shown to be optimal in terms of fidelity. On the other hand, [50] shows that a non-covariant adaptive protocol for unitary estimation with no auxiliary system achieves the asymptotically optimal performance in terms of the diamond-norm distance. Since the transformation from a general protocol to a covariant protocol may induce the increase of the resources other than the number of calls n, e.g., the number of required qudits or non-Clifford gates to run the protocols, and the amount of entanglement in the resource states, the corresponding dPBT protocol constructed by our methods may not be implemented efficiently for some other notions of efficiency. We leave it an open problem to construct a conversion between the fidelities of unitary estimation and dPBT in terms of resources other than the number of calls.

APPENDIX

Appendix A reviews mathematical tools based on the Young diagrams and the Schur-Weyl duality. Appendix B shows a construction of a covariant protocol for deterministic port-based teleportation (dPBT) from any given dPBT protocol, following [6], [26], and [30]. The teleportation fidelity of the obtained covariant protocol is also shown (see Lem. 10). Appendix C shows a construction of a parallel covariant protocol, for unitary estimation from any given adaptive protocol [9], [47]. The fidelity of the obtained covariant protocol is also shown (see Lem. 11). Appendix D proves Thm. 1, stating the one-to-one correspondence between dPBT and unitary estimation, by constructing a transformation between covariant protocols for dPBT and unitary estimation. Appendix E shows the asymptotically optimal fidelity of unitary estimation using the previous results from [10] and [50] (Lem. 2). Appendix F shows an optimal protocol for unitary estimation for $n \leq d-1$ corresponding to Cor. 4. Appendix G proves Thm. 5, stating that estimation-based protocol for unitary inversion is optimal for $n \leq d-1$ even when we consider indefinite causal order [51], [52], [53].

Appendix A Review of the Schur-Weyl Duality, Young Diagrams, and the Young-Yamanouchi Basis

This section reviews mathematical tools based on the Young diagrams and the Schur-Weyl duality. We suggest the standard textbooks, e.g. [68], [69], [70], for more detailed reviews.

A Young diagram is defined in association with a partition of n for a non-negative integer n. A partition of n is a non-decreasing sequence of positive integers $(\alpha_1, \ldots, \alpha_d)$ for any non-negative integer d with $\alpha_1 \geq \cdots \geq \alpha_d > 0$ which sums up to $\sum_{i=1}^d \alpha_i = n$. A partition of n can be represented as a Young diagram with n boxes, which has α_i boxes in the i-th row. For instance, $(2,1)$ can be represented as a Young diagram given by

$$\alpha = \ydiagram{2,1}. \tag{21}$$

We call d, the number of positive integers in the sequence associated with the Young diagram α, to be the depth of each Young diagram. We denote the set of Young diagrams with n boxes and at most depth d by $\mathbb{Y}_n^d$, i.e.,

$$\mathbb{Y}_n^d := \left\{(\alpha_1, \ldots, \alpha_{d'}) \mid {}^{0\leq d' \leq d, \alpha_1 \geq \cdots \geq \alpha_{d'} > 0,}_{\sum_{i=1}^{d'} \alpha_i = n}\right\}. \tag{22}$$

For a Young diagram α, we define the following two sets:

$$\begin{aligned}\alpha + \square := &\left\{(\alpha_1, \ldots, \alpha_i + 1, \ldots, \alpha_d) \;\middle|\; {}^{i\in\{1,\ldots,d\}}_{\text{s.t. } \alpha_{i-1} \geq \alpha_i + 1}\right\}\\ &\cup \{(\alpha_1, \ldots, \alpha_d, 1)\},\end{aligned}$$

$$\begin{aligned}&\alpha - \square\\ &:= \begin{cases}\left\{(\alpha_1, \ldots, \alpha_i - 1, \ldots, \alpha_d) \;\middle|\; {}^{i\in\{1,\ldots,d\}}_{\text{s.t. } \alpha_i - 1 \geq \alpha_{i+1}}\right\} & (\alpha_d > 1)\\ \left\{(\alpha_1, \ldots, \alpha_i - 1, \ldots, \alpha_d) \;\middle|\; {}^{i\in\{1,\ldots,d-1\}}_{\text{s.t. } \alpha_i - 1 \geq \alpha_{i+1}}\right\} & \\ \qquad \cup \{(\alpha_1, \ldots, \alpha_{d-1})\} & (\alpha_d = 1)\end{cases},\end{aligned} \tag{23}$$

where α_0 and α_{d+1} are taken to be $\alpha_0 = \infty$ and $\alpha_{d+1} = 0$, and $\alpha + \square (\alpha - \square)$ represents the set of Young diagrams adding a box to (removing a box from) α. For instance, for the Young diagram α given in Eq. (21), $\alpha + \square$ and $\alpha - \square$ are given by

$$\alpha + \square = \left\{\ydiagram{3,1}, \ \ydiagram{2,2}, \ \ydiagram{2,1,1}\right\}, \tag{24}$$

$$\alpha - \square = \left\{\ydiagram{1,1}, \ \ydiagram{2}\right\}. \tag{25}$$

For a Young diagram α with n boxes, we consider a sequence of Young diagrams given by

$$(\alpha^{(0)} = \emptyset, \alpha^{(1)}, \ldots, \alpha^{(n-1)}, \alpha^{(n)} = \alpha), \tag{26}$$

where $\emptyset$ is the Young diagram with zero boxes and $\alpha^{(i)}$ satisfies $\alpha^{(i+1)} \in \alpha^{(i)} + \square$. A sequence of Young diagrams can be represented by a standard Young tableau, which is given by filling i on the box of the Young diagram α that is added when we obtain $\alpha^{(i)}$ from $\alpha^{(i-1)}$. The Young diagram to be filled with numbers is called the frame of a corresponding standard tableau. For instance, a sequence

$$\left(\emptyset, \ \ydiagram{1}, \ \ydiagram{2}, \ \ydiagram{2,1}\right) \tag{27}$$

is represented by a standard tableau

$$\begin{ytableau} 1 & 2 \\ 3 \end{ytableau}, \tag{28}$$

with the frame

$$\ydiagram{2,1}. \tag{29}$$

The number of the standard tableaux with frame α, denoted by m_α, is given by the hook-length formula:

$$m_\alpha = \frac{n!}{\prod_{(i,j)\in\alpha} \mathrm{hook}_\lambda(i,j)}. \tag{30}$$

Here, (i,j) represents a box in the i-th row and the j-th column in the Young diagram α, $\mathrm{hook}_\lambda(i,j)$ is defined by

$$\mathrm{hook}_\lambda(i,j) := \alpha_i + \alpha'_j - i - j + 1, \tag{31}$$

and α_i and α'_j are the numbers of boxes in the i-th row and the j-th column of α, respectively. We denote the set of the standard tableaux with frame α by

$$\mathrm{STab}(\alpha) := \{s_1^\alpha, \ldots s_{m_\alpha}^\alpha\}, \tag{32}$$

where each standard tableau is indexed by $a \in \{1, \ldots, m_\alpha\}$ and the a-th standard tableau is denoted by s_a^α. For a Young diagrams α and a standard tableau s_a^α with frame α associated with a sequence (26), a standard tableau with frame $\mu \in \alpha + \square$ is referred to be obtained by adding a box $\boxed{n+1}$ to s_a^α, when its associated sequence is given by

$$(\alpha^{(0)} = \emptyset, \alpha^{(1)}, \ldots, \alpha^{(n-1)}, \alpha^{(n)} = \alpha, \alpha^{(n+1)} = \mu). \tag{33}$$

We denote the index of thus obtained standard tableau with frame μ by $a_\mu^\alpha \in \{1, \ldots, m_\mu\}$ so that the standard tableau itself is represented by $s_{a_\mu^\alpha}^\mu$. We also call s_a^α to be the standard tableau obtained by removing a box $\boxed{n+1}$ from $s^{\mu}_{a^{\alpha}_{\mu}}$. For instance, in the case of

$$\alpha = \ydiagram{2,1}, \quad s^{\alpha}_{a} = \begin{ytableau} 1 & 2 \\ 3 \end{ytableau}, \tag{34}$$

$$\alpha + \square = \left\{ \mu = \ydiagram{3,1}, \quad \nu = \ydiagram{2,2}, \quad \lambda = \ydiagram{2,1,1} \right\}, \tag{35}$$

the standard tableaux obtained by adding a box $\boxed{4}$ to s^{α}_{a} are given by

$$s^{\mu}_{a^{\alpha}_{\mu}} = \begin{ytableau} 1 & 2 & 4 \\ 3 \end{ytableau}, \quad s^{\nu}_{a^{\alpha}_{\nu}} = \begin{ytableau} 1 & 2 \\ 3 & 4 \end{ytableau}, \quad s^{\lambda}_{a^{\alpha}_{\lambda}} = \begin{ytableau} 1 & 2 \\ 3 \\ 4 \end{ytableau}. \tag{36}$$

We consider the following representations on $(\mathbb{C}^d)^{\otimes n}$ of the special unitary group $\mathrm{SU}(d)$ and the symmetric group $\mathfrak{S}_n$:

$$\mathrm{SU}(d) \ni U \mapsto U^{\otimes n} \in \mathcal{L}(\mathbb{C}^d)^{\otimes n}, \tag{37}$$

$$\mathfrak{S}_n \ni \sigma \mapsto V_\sigma \in \mathcal{L}(\mathbb{C}^d)^{\otimes n}, \tag{38}$$

where $\mathcal{L}(\mathcal{X})$ is the set of linear operators on a Hilbert space $\mathcal{X}$, and V_σ is a permutation operator defined as

$$V_\sigma |i_1 \cdots i_n\rangle := \left|i_{\sigma^{-1}(1)} \cdots i_{\sigma^{-1}(n)}\right\rangle \tag{39}$$

for the computational basis $\{|i\rangle\}_{i=1}^d$ of $\mathbb{C}^d$. Then, these representations are decomposed simultaneously as follows:

$$(\mathbb{C}^d)^{\otimes n} = \bigoplus_{\alpha \in \mathbb{Y}_n^d} \mathcal{U}_\alpha \otimes \mathcal{S}_\alpha, \tag{40}$$

$$U^{\otimes n} = \bigoplus_{\alpha \in \mathbb{Y}_n^d} U_\alpha \otimes \mathbb{1}_{\mathcal{S}_\alpha}, \tag{41}$$

$$V_\sigma = \bigoplus_{\alpha \in \mathbb{Y}_n^d} \mathbb{1}_{\mathcal{U}_\alpha} \otimes \sigma_\alpha, \tag{42}$$

where α runs in the set $\mathbb{Y}_n^d$ defined in Eq. (22), $\mathrm{SU}(d) \ni U \mapsto U_\alpha \in \mathcal{L}(\mathcal{U}_\alpha)$ is an irreducible representation of $\mathrm{SU}(d)$, and $\mathfrak{S}_n \ni \sigma \mapsto \sigma_\alpha \in \mathcal{L}(\mathcal{S}_\alpha)$ is an irreducible representation of $\mathfrak{S}_n$. This relation shows that any operator commuting with $U^{\otimes n}$ for all $U \in \mathrm{SU}(d)$ can be written as a linear combination of $\{V_\sigma\}_{\sigma \in \mathfrak{S}_n}$, which is called the Schur-Weyl duality. The orthogonal projector onto $\mathcal{U}_\alpha \otimes \mathcal{S}_\alpha$ is called the Young projector [21], denoted by P_α. The dimension of $\mathcal{U}_\alpha$, denoted by d_α, is given by the hook-content formula:

$$d_\alpha = \prod_{(i,j) \in \alpha} \frac{d + j - i}{\mathrm{hook}_\lambda(i,j)}. \tag{43}$$

The dimension of $\mathcal{S}_\alpha$ is given by m_α, which is the number of the standard tableaux with frame α given in Eq. (30). The dimension m_α satisfies the following Lemma.

Lemma 6: For any given Young diagram α with n boxes,

$$\sum_{\mu \in \alpha + \square} m_\mu = (n+1) m_\alpha \tag{44}$$

holds.

Proof: Since the irreducible representations α and $\mu \in \alpha + \square$ are related by

$$\mathrm{Ind}_{\mathfrak{S}_n}^{\mathfrak{S}_{n+1}} \mathcal{S}_\alpha = \bigoplus_{\mu \in \alpha + \square} \mathcal{S}_\mu, \tag{45}$$

where $\mathrm{Ind}_H^G \pi$ represents the induced representation for a finite group G, its subgroup H and a representation π of the group H. Then, we obtain

$$\sum_{\mu \in \alpha + \square} m_\mu = \dim \bigoplus_{\mu \in \alpha + \square} \mathcal{S}_\mu = \dim \mathrm{Ind}_{\mathfrak{S}_n}^{\mathfrak{S}_{n+1}} \mathcal{S}_\alpha \tag{46}$$

$$= \frac{|\mathfrak{S}_{n+1}|}{|\mathfrak{S}_n|} \dim \mathcal{S}_\alpha = (n+1) m_\alpha. \tag{47}$$

$\square$

Due to Schur's lemma, any operator commuting with $U^{\otimes n}$ can be written as a linear combination of the operators E^{α}_{ab} defined by [21]

$$E^{\alpha}_{ab} := \mathbb{1}_{\mathcal{U}_\alpha} \otimes |\alpha, a\rangle\langle \alpha, b|_{\mathcal{S}_\alpha}, \tag{48}$$

for $a, b \in \{1, \ldots, m_\alpha\}$, where $\{|\alpha, a\rangle\}$ is an orthonormal basis of $\mathcal{S}_\alpha$. In particular, we take the Young-Yamanouchi basis [71], [72] (or Young's orthogonal form [70]) of $\mathcal{S}_\alpha$. Each element in the Young-Yamanouchi basis $\{|\alpha, a\rangle\}$ is associated with the standard tableaux s^{α}_{a} in the set $\mathrm{STab}(\alpha)$ [see Eq. (32)]. The Young-Yamanouchi basis is a subgroup-adapted basis, i.e., the action of $\mathfrak{S}_n \subset \mathfrak{S}_{n+1}$ on the Young-Yamanouchi basis $\{|\mu, i\rangle\}$ for $\mu \in \mathbb{Y}_{n+1}^d$ is unitarily equivalent to the action of $\mathfrak{S}_n$ on the Young-Yamanouchi basis $\{|\alpha, a\rangle\}$ for $\alpha \in \mathbb{Y}_n^d$ as follows:

$$\langle \mu, i| \sigma_\mu |\mu, j\rangle = \delta_{\alpha,\beta} \langle \alpha, a| \sigma_\alpha |\beta, b\rangle \quad \forall \sigma \in \mathfrak{S}_n, \tag{49}$$

where s^{α}_{a} and s^{β}_{b} are the standard tableaux obtained by removing a box $\boxed{n+1}$ from s^{μ}_{i} and s^{μ}_{j}, respectively.

The basis $\{E^{\mu}_{ij}\}$ satisfies the following Lemmas (see, e.g., [21], [64] for the proofs):

Lemma 7: The basis $\{E^{\mu}_{ij}\}$ satisfies

$$(E^{\mu}_{ij})^* = E^{\mu}_{ij}, \tag{50}$$

$$\mathrm{Tr}\, E^{\mu}_{ij} = d_\mu \delta_{i,j}, \tag{51}$$

$$E^{\mu}_{ij} E^{\nu}_{kl} = \delta_{\mu,\nu} \delta_{j,k} E^{\mu}_{il}, \tag{52}$$

where X^* is the complex conjugate of X in the computational basis and $\delta_{i,j}$ is the Kronecker delta defined as $\delta_{i,i} = 1$ and $\delta_{i,j} = 0$ for $i \neq j$.

Lemma 8: Let a^{α}_{μ} be the index of a standard tableau $s^{\mu}_{a^{\alpha}_{\mu}}$ obtained by adding a box $\boxed{n+1}$ to a standard tableau s^{α}_{a} for $\alpha \in \mathbb{Y}_n^d$ and $\mu \in \alpha + \square$. Then, $E^{\alpha}_{ab} \otimes \mathbb{1}_d$ can be written as

$$E^{\alpha}_{ab} \otimes \mathbb{1}_d = \sum_{\mu \in \alpha + \square} E^{\mu}_{a^{\alpha}_{\mu} b^{\alpha}_{\mu}}, \tag{53}$$

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

Lemma 9: Let s^{α}_{a} and s^{β}_{b} be the standard tableaux obtained by removing a box $\boxed{n+1}$ from s^{μ}_{i} and s^{μ}_{j}, respectively, for $\mu, \nu \in \mathbb{Y}_{n+1}^d$. The partial trace of E^{μ}_{ij} in the last system is given by

$$\mathrm{Tr}_{n+1} E^{\mu}_{ij} = \delta_{\alpha\beta} \frac{d_\mu}{d_\alpha} E^{\alpha}_{ab}. \tag{54}$$

Appendix B Covariant Protocol for dPBT

This section shows that any dPBT protocol can be converted into a canonical form of the protocol, which we call the covariant protocol, without decreasing the teleportation fidelity, following [6], [26], and [30] (see Eqs. (74), (76) and (78) and Figs. 2 (a) and (b)). The teleportation fidelity of the covariant protocol is shown in Lem. 10, which is shown in [26] and [30].

We consider a general protocol for dPBT given by Eq. (1) of the main text. We take an eigendecomposition of the resource state ϕ_{PBT} given by[2]

$$\phi_{\mathrm{PBT}} = \sum_k |\phi^{(k)}\rangle\langle\phi^{(k)}|, \tag{55}$$

$$\left|\phi^{(k)}\right\rangle = (O^{(k)}_{\mathcal{A}^N} \otimes \mathbb{1}_{\mathcal{B}^N}) \bigotimes_{a=1}^{N} \left|\phi^+\right\rangle_{\mathcal{A}_a\mathcal{B}_a}, \tag{56}$$

where $O^{(k)}$ is a linear operator on $\mathcal{A}^N$ satisfying the normalization condition $\sum_k \mathrm{Tr}[O^{(k)\dagger}O^{(k)}] = d^N$, and $\left|\phi^+\right\rangle$ is the maximally entangled state defined by $\left|\phi^+\right\rangle := \frac{1}{\sqrt{d}}\sum_{i=1}^d |ii\rangle$ using the computational basis $\{|i\rangle\}_{i=1}^d$ of $\mathbb{C}^d$. Using this expression, the teleportation fidelity (3) is written by

$$\begin{aligned} &f(\mathbb{1}_d, \Lambda) \\ &= \frac{1}{d^2}\sum_{a=1}^N \sum_k \mathrm{Tr}[(O^{(k)}_{\mathcal{A}^N} \otimes \mathbb{1}_{\mathcal{A}_0})\sigma_a (O^{(k)}_{\mathcal{A}^N} \otimes \mathbb{1}_{\mathcal{A}_0})^\dagger \Pi_a] \quad (57)\\ &= \frac{1}{d^2}\sum_{a=1}^N \mathrm{Tr}(\tilde{\Pi}_a\sigma_a), \quad (58)\end{aligned}$$

where σ_a and $\tilde{\Pi}_a$ are defined by

$$\sigma_a := \frac{1}{d^{N-1}}\left(\mathbb{1}_{\overline{\mathcal{A}_a}} \otimes |\phi^+\rangle\langle\phi^+|_{\mathcal{A}_a\mathcal{A}_0}\right), \tag{59}$$

$$\tilde{\Pi}_a := \sum_k (O^{(k)}_{\mathcal{A}^N} \otimes \mathbb{1}_{\mathcal{A}_0})^\dagger \Pi_a (O^{(k)}_{\mathcal{A}^N} \otimes \mathbb{1}_{\mathcal{A}_0}), \tag{60}$$

and $\overline{\mathcal{A}_a}$ is defined by $\overline{\mathcal{A}_a} := \bigotimes_{i\neq a}\mathcal{A}_i$. The set of operators $\{\tilde{\Pi}_a\}_{a=1}^N$ defined in Eq. (60) corresponds to the set of operators $\{\Pi_a\}_{a=1}^N$ satisfying $\Pi_a \geq 0$ and $\sum_a \Pi_a = \mathbb{1}$ if and only if

$$\tilde{\Pi}_a \geq 0, \quad \sum_a \tilde{\Pi}_a = X_{\mathcal{A}^N} \otimes \mathbb{1}_{\mathcal{A}_0}, \tag{61}$$

where X is defined by

$$X := \sum_k O^{(k)\dagger}O^{(k)}. \tag{62}$$

Therefore, the optimal channel fidelity for a resource state given by Eqs. (55) and (56) is written as the following semidefinite programming (SDP):

$$\begin{aligned} &\max \frac{1}{d^2}\sum_{a=1}^N \mathrm{Tr}(\tilde{\Pi}_a\sigma_a), \\ &\text{s.t. } \tilde{\Pi}_a \geq 0, \quad \sum_a \tilde{\Pi}_a = X_{\mathcal{A}^N} \otimes \mathbb{1}_{\mathcal{A}_0}, \quad \mathrm{Tr}(X) = d^N. \end{aligned} \tag{63}$$

Since the operator σ_a satisfies the unitary group symmetry and symmetric group covariance given by

$$[U^{\otimes N}_{\mathcal{A}^N} \otimes U^*_{\mathcal{A}_0}, \sigma_a] = 0 \quad \forall U \in \mathrm{SU}(d), \tag{64}$$

$$[(V_\pi)_{\mathcal{A}^N} \otimes \mathbb{1}_{\mathcal{A}_0}]\sigma_a[(V_\pi)_{\mathcal{A}^N} \otimes \mathbb{1}_{\mathcal{A}_0}]^\dagger = \sigma_{\pi(a)} \quad \forall \pi \in \mathfrak{S}_N, \tag{65}$$

where V_π is the permutation operator defined in Appendix A and $*$ denotes the complex conjugate in the computational basis, we obtain

$$\max \frac{1}{d^2}\sum_{a=1}^N \mathrm{Tr}(\tilde{\Pi}_a\sigma_a) = \max \frac{1}{d^2}\sum_{a=1}^N \mathrm{Tr}(\tilde{\Pi}'_a\sigma_a), \tag{66}$$

where $\tilde{\Pi}'_a$ is $\mathrm{SU}(d) \times \mathfrak{S}_N$-twirled operator defined by

$$\begin{aligned}\tilde{\Pi}'_a := \frac{1}{N!}\sum_{\pi\in\mathfrak{S}_N}\int_{\mathrm{SU}(d)} \mathrm{d}U[(U^{\otimes N}V_\pi)_{\mathcal{A}^N} \otimes U^*_{\mathcal{A}_0}] \\ \times \Pi_{\pi^{-1}(a)}[(U^{\otimes N}V_\pi)_{\mathcal{A}^N} \otimes U^*_{\mathcal{A}_0}]^\dagger. \end{aligned} \tag{67}$$

The set of operators $\{\tilde{\Pi}'_a\}_a$ satisfies $\tilde{\Pi}'_a \geq 0$ and $\sum_{a=1}^N \tilde{\Pi}'_a = X'_{\mathcal{A}^N} \otimes \mathbb{1}_{\mathcal{A}_0}$ for the operator X' defined by

$$X' := \frac{1}{N!}\sum_{\pi\in\mathfrak{S}_N}\int_{\mathrm{SU}(d)} \mathrm{d}U(U^{\otimes N}V_\pi)X(U^{\otimes N}V_\pi)^\dagger, \tag{68}$$

satisfying the unitary group and symmetric group symmetry given by

$$[U^{\otimes N}, X'] = 0 \quad \forall U \in \mathrm{SU}(d), \tag{69}$$

$$[V_\pi, X'] = 0 \quad \forall \pi \in \mathfrak{S}_N. \tag{70}$$

Therefore, X' can be written as

$$X' = d^N \sum_\mu \frac{w_\mu^2}{d_\mu m_\mu}P_\mu, \tag{71}$$

where w_μ is defined by

$$w_\mu := \sqrt{\frac{\mathrm{Tr}(X'P_\mu)}{d^N}} = \sqrt{\frac{\mathrm{Tr}(XP_\mu)}{d^N}}, \tag{72}$$

and P_μ is the Young projector (see Appendix A). Since the operator X can be written by the resource state ϕ_{PBT} as

$$X = d^N[\mathrm{Tr}_{\mathcal{A}^N}(\phi^*_{\mathrm{PBT}})]_{\mathcal{B}^N\to\mathcal{A}^N}, \tag{73}$$

where the subscript $\mathcal{B}^N \to \mathcal{A}^N$ represents a relabelling the space from $\mathcal{B}^N$ to $\mathcal{A}^N$, we obtain

$$w_\mu = \sqrt{\mathrm{Tr}[\phi^*_{\mathrm{PBT}}[(P_\mu)_{\mathcal{A}^N} \otimes \mathbb{1}_{\mathcal{B}^N}]]}. \tag{74}$$

Thus, the solution of the SDP (63) is upper bounded by the following SDP:

$$\begin{aligned} &\max \frac{1}{d^2}\sum_{a=1}^N \mathrm{Tr}(\tilde{\Pi}_a\sigma_a), \\ &\text{s.t. } \tilde{\Pi}_a \geq 0, \sum_a \tilde{\Pi}_a = X'_{\mathcal{A}^N} \otimes \mathbb{1}_{\mathcal{A}_0}, \mathrm{Tr}(X') = d^N, X' \text{ is given by Eq.(71)}. \end{aligned} \tag{75}$$

which corresponds to the SDP (63) for a pure resource state given by

$$\left|\tilde{\phi}^{(\vec{w})}_{\mathrm{PBT}}\right\rangle := (O^{(\vec{w})}_{\mathcal{A}^N} \otimes \mathbb{1}_{\mathcal{B}^N}) \bigotimes_{a=1}^N \left|\phi^+\right\rangle_{\mathcal{A}_a\mathcal{B}_a}, \tag{76}$$

$$O^{(\vec{w})}_{\mathcal{A}^N} := \sqrt{d^N}\sum_{\mu\in\mathbb{Y}_N^d} \frac{w_\mu}{\sqrt{d_\mu m_\mu}}P_\mu. \tag{77}$$

[2] We consider a slightly more general setting where the resource state is a mixed state than a usual setting where the resource state is a pure state. This extra argument is given to explicitly provide a covariant protocol corresponding to any given dPBT protocol.

Reference [30] shows that the SDP (75) gives the optimal value when the POVM is given by the square-root measurement (or the pretty good measurement) [73], [74], [75] for the state ensemble $\{(1/N, \sigma_a)\}_{a=1}^N$:

$$\Pi_a = \sigma^{-1/2}\sigma_a\sigma^{-1/2}, \tag{78}$$

$$\sigma := \sum_a \sigma_a. \tag{79}$$

We call the dPBT protocol with the resource state given in (76) and the POVM given in (78) the covariant protocol since they are covariant with respect to representations of the symmetric group $\mathfrak{S}_N$ and the unitary group $\mathrm{SU}(d)$ as follows:

$$(U_{\mathcal{A}^N}^{\otimes N} \otimes U_{\mathcal{B}^N}^{*\otimes N})\left|\tilde{\phi}_{\mathrm{PBT}}^{(\vec{w})}\right\rangle = \left|\tilde{\phi}_{\mathrm{PBT}}^{(\vec{w})}\right\rangle \quad \forall U \in \mathrm{SU}(d), \tag{80}$$

$$[(V_\pi)_{\mathcal{A}^N} \otimes (V_\pi)_{\mathcal{B}^N}]\left|\tilde{\phi}_{\mathrm{PBT}}^{(\vec{w})}\right\rangle = \left|\tilde{\phi}_{\mathrm{PBT}}^{(\vec{w})}\right\rangle \quad \forall \pi \in \mathfrak{S}_N, \tag{81}$$

$$(U_{\mathcal{A}^N}^{\otimes N} \otimes U_{\mathcal{A}_0}^{*})\Pi_a(U_{\mathcal{A}^N}^{\otimes N} \otimes U_{\mathcal{A}_0}^{*})^\dagger = \Pi_a \quad \forall U \in \mathrm{SU}(d), \tag{82}$$

$$[(V_\pi)_{\mathcal{A}^N} \otimes \mathbb{1}_{\mathcal{A}_0}]\Pi_a[(V_\pi)_{\mathcal{A}^N} \otimes \mathbb{1}_{\mathcal{A}_0}]^\dagger = \Pi_{\pi(a)} \quad \forall \pi \in \mathfrak{S}_N, \tag{83}$$

which can be shown using Eqs. (64), (65), and (77).

In conclusion, any dPBT protocol can be converted into a covariant protocol using the resource state defined in Eqs. (74) and (76) and the square-root measurement defined in Eq. (78) without decreasing the teleportation fidelity [see Fig. 2 (b)]. The teleportation fidelity for the obtained covariant protocol is given by the following Lemma.

Lemma 10: [26], [30] The fidelity of d-dimensional dPBT for N ports is given by

$$F_{\mathrm{PBT}}(N, d) = \vec{w}^\top M_{\mathrm{PBT}}(N, d)\vec{w}, \tag{84}$$

using a vector $\vec{w} = (w_\mu)_{\mu \in \mathbb{Y}_N^d}$ satisfying $w_\mu \geq 0$ for all $\mu \in \mathbb{Y}_N^d$ and $\sum_{\mu \in \mathbb{Y}_n^d} w_\mu^2 = 1$. The $|\mathbb{Y}_N^d| \times |\mathbb{Y}_N^d|$ matrix $M_{\mathrm{PBT}}(N, d)$ defined by

$$(M_{\mathrm{PBT}}(N, d))_{\mu\nu} = \frac{1}{d^2}\#[(\mu - \square) \cap (\nu - \square)], \tag{85}$$

where $\mu - \square$ and $\nu - \square$ are defined in Eq. (23), and $\#(\mathbb{X})$ is the cardinality of a set $\mathbb{X}$. In particular, the optimal fidelity of dPBT is given by

$$F_{\mathrm{PBT}}(N, d) = \max_{\|\vec{w}\|=1} \vec{w}^\top M_{\mathrm{PBT}}(N, d)\vec{w}, \tag{86}$$

which equals to the maximal eigenvalue of $M_{\mathrm{PBT}}(N, d)$.

Proof: See the details in [30]. □

Appendix C Parallel Covariant Protocol for Unitary Estimation

This section shows that any general adaptive protocol for unitary estimation can be converted into a canonical form of the protocol, which we call the parallel covariant protocol [9], [47] without decreasing the fidelity [see Eqs. (115), (119) and (120) and Figs. 2 (c) and (d)]. The fidelity of the parallel covariant protocol is shown in Lem. 11.

Reference [9] shows that the optimal fidelity of dSAR can be achieved by a covariant parallel "measure-and-prepare" protocol. We show a similar construction to convert any unitary estimation protocol into a covariant parallel protocol. This construction is based on the Choi representation of quantum operations and quantum supermaps [76], [77], [78].

We briefly review the Choi representation. We consider a quantum operation $\Lambda : \mathcal{L}(\mathcal{I}) \to \mathcal{L}(\mathcal{O})$, where $\mathcal{I}$ and $\mathcal{O}$ are the Hilbert spaces corresponding to the input and output systems, and $\mathcal{L}(\mathcal{X})$ is the set of linear operators on a linear space $\mathcal{X}$. The Choi matrix $J_\Lambda \in \mathcal{L}(\mathcal{I} \otimes \mathcal{O})$ is defined by

$$J_\Lambda := \sum_{i,j} |i\rangle\langle j|_{\mathcal{I}} \otimes \Lambda(|i\rangle\langle j|)_{\mathcal{O}}, \tag{87}$$

where $\{|i\rangle\}_i$ is the computational basis of $\mathcal{I}$, and the subscripts $\mathcal{I}$ and $\mathcal{O}$ represent the Hilbert spaces where each term is defined. The Choi matrix of the unitary operation $\mathcal{U}(\cdot) = U(\cdot)U^\dagger$ is given by $J_{\mathcal{U}} = |U\rangle\rangle\langle\langle U|$, where $|U\rangle\rangle$ is the dual ket defined by

$$|U\rangle\rangle := \sum_i |i\rangle \otimes U|i\rangle. \tag{88}$$

In the Choi representation, the composition of a quantum operation Λ with a quantum state ρ and that of quantum operations Λ_1, Λ_2 are represented in a unified way using a link product $*$ as

$$\Lambda(\rho) = J_\Lambda * \rho, \tag{89}$$

$$J_{\Lambda_2 \circ \Lambda_1} = J_{\Lambda_1} * J_{\Lambda_2}, \tag{90}$$

where the link product $*$ for $A \in \mathcal{L}(\mathcal{X} \otimes \mathcal{Y})$ and $B \in \mathcal{L}(\mathcal{Y} \otimes \mathcal{Z})$ is defined as [78]

$$A * B := \mathrm{Tr}_{\mathcal{Y}}[(A^{\top_{\mathcal{Y}}} \otimes \mathbb{1}_{\mathcal{Z}})(\mathbb{1}_{\mathcal{X}} \otimes B)], \tag{91}$$

and $A^{\top_{\mathcal{Y}}}$ is the partial transpose of A over the subspace $\mathcal{Y}$.

The most general protocol for the unitary estimation within the quantum circuit framework is given by [9], [78]

$$p(\hat{U}|U) = \mathrm{Tr}\Big[M_{\hat{U}}(\mathcal{U}_{\mathcal{I}_n \to \mathcal{O}_n} \otimes \mathbb{1}_{\mathcal{X}_n}) \circ \Lambda_{n-1} \circ \cdots \circ \Lambda_1 \circ (\mathcal{U}_{\mathcal{I}_1 \to \mathcal{O}_1} \otimes \mathbb{1}_{\mathcal{X}_1}) \circ \phi\Big], \tag{92}$$

where $\mathcal{I}_i$ and $\mathcal{O}_i$ for $i \in \{1, \ldots, n\}$ are Hilbert spaces defined by $\mathcal{I}_i \simeq \mathcal{O}_i \simeq \mathbb{C}^d$, $\mathcal{X}_i$ for $i \in \{1, \ldots, n\}$ are auxiliary Hilbert spaces, Λ_i are completely positive and trace preserving (CPTP) maps whose input and output spaces are given by $\Lambda_i : \mathcal{L}(\mathcal{O}_i \otimes \mathcal{X}_i) \to \mathcal{L}(\mathcal{I}_{i+1} \otimes \mathcal{X}_{i+1})$, ϕ is a quantum state on the Hilbert space $\mathcal{I}_1 \otimes \mathcal{X}_1$, and $\{M_{\hat{U}} \mathrm{d}\hat{U}\}_{\hat{U}}$ is a POVM on the Hilbert space $\mathcal{O}_n \otimes \mathcal{X}_n$ [see Fig. 2 (c)]. In the Choi representation, Eq. (92) can be written as

$$p(\hat{U}|U) = T_{\hat{U}} * [J_{\mathcal{U}}^{\otimes n}]_{\mathcal{I}^n\mathcal{O}^n}, \tag{93}$$

where $\{T_{\hat{U}} \mathrm{d}\hat{U}\}_{\hat{U}}$ is called a quantum tester [79], [80], [81], [82] defined by

$$T_{\hat{U}} := \phi * J_{\Lambda_1} * \cdots * J_{\Lambda_{n-1}} * M_{\hat{U}}^\top \in \mathcal{L}(\mathcal{I}^n \otimes \mathcal{O}^n), \tag{94}$$

and $\mathcal{I}^n$ and $\mathcal{O}^n$ are the joint Hilbert spaces defined by $\mathcal{I}^n := \bigotimes_{i=1}^n \mathcal{I}_i$ and $\mathcal{O}^n := \bigotimes_{i=1}^n \mathcal{O}_i$, respectively. The quantum tester satisfies the positivity and normalization conditions given by [79], [80], [81], [82]

$$T_{\hat{U}} \geq 0, \quad \mathrm{Tr}\left[\int \mathrm{d}\hat{U} T_{\hat{U}}\right] = d^n. \tag{95}$$

In terms of the quantum tester $\{T_{\hat{U}} \mathrm{d}\hat{U}\}_{\hat{U}}$, the average-case fidelity of unitary estimation is given by

$$F_{\mathrm{est}}^{(\mathrm{ave})} = \frac{1}{d^2} \int \mathrm{d}U \int \mathrm{d}\hat{U} T_{\hat{U}} * J_{\mathcal{U}}^{\otimes n} |\mathrm{Tr}(\hat{U}^\dagger U)|^2. \tag{96}$$

Since

$$(V_{\mathcal{I}^n}^{\otimes n} \otimes W_{\mathcal{O}^n}^{\otimes n}) T_{\hat{U}} (V_{\mathcal{I}^n}^{\otimes n} \otimes W_{\mathcal{O}^n}^{\otimes n})^\dagger * J_{\mathcal{U}}^{\otimes n} = T_{\hat{U}} * J_{\mathcal{W}^\mathsf{T} \circ \mathcal{U} \circ \mathcal{V}}^{\otimes n} \quad \forall V, W \in \mathrm{SU}(d) \tag{97}$$

holds, we obtain

$$F_{\mathrm{est}}^{(\mathrm{ave})} = \frac{1}{d^2} \int \mathrm{d}U \int \mathrm{d}\hat{U} T'_{\hat{U}} * J_{\mathcal{U}}^{\otimes n} |\mathrm{Tr}(\hat{U}^\dagger U)|^2, \tag{98}$$

where $T'_{\hat{U}}$ is a SU(d)-twirled operator given by

$$T'_{\hat{U}} := \int \mathrm{d}V \int \mathrm{d}W (V_{\mathcal{I}^n}^{\otimes n} \otimes W_{\mathcal{O}^n}^{\otimes n}) T_{W^\mathsf{T} \hat{U} V} (V_{\mathcal{I}^n}^{\otimes n} \otimes W_{\mathcal{O}^n}^{\otimes n})^\dagger. \tag{99}$$

Therefore, the average-case fidelity of the original adaptive protocol can be achieved by any protocol having the probability distribution given by

$$\tilde{p}(\hat{U}|U) := T'_{\hat{U}} * J_{\mathcal{U}}^{\otimes n}. \tag{100}$$

We show that a parallel protocol can implement the probability distribution (100) using an argument shown in [79], [80], and [82]. Defining T' by

$$\begin{aligned} T' &:= \int \mathrm{d}\hat{U} T'_{\hat{U}} \quad &(101)\\ &= \int \mathrm{d}\hat{U} \int \mathrm{d}V \int \mathrm{d}W (V_{\mathcal{I}^n}^{\otimes n} \otimes W_{\mathcal{O}^n}^{\otimes n}) T_{\hat{U}} (V_{\mathcal{I}^n}^{\otimes n} \otimes W_{\mathcal{O}^n}^{\otimes n})^\dagger, \quad &(102) \end{aligned}$$

the operator T' satisfies the following SU(d) symmetry:

$$[V_{\mathcal{I}^n}^{\otimes n} \otimes W_{\mathcal{O}^n}^{\otimes n}, T'] = 0 \quad \forall V, W \in \mathrm{SU}(d). \tag{103}$$

From Eq. (95), T' satisfies the following positivity and normalization conditions:

$$T' \geq 0, \quad \mathrm{Tr}(T') = d^n. \tag{104}$$

We define a quantum state $|\phi'_{\mathrm{est}}\rangle$ and a POVM $\{M'_{\hat{U}} \mathrm{d}U\}$ by [79], [80], and [82]

$$\begin{aligned} |\phi'_{\mathrm{est}}\rangle &:= \sqrt{T'}^\mathsf{T} |\mathbb{1}\rangle\rangle_{\mathcal{I}^n \mathcal{O}^n}, \quad &(105)\\ M'_{\hat{U}} &:= (T'^{-1/2} T'_{\hat{U}} T'^{-1/2})^\mathsf{T}, \quad &(106) \end{aligned}$$

where the normalization condition of $|\phi'_{\mathrm{est}}\rangle$ can be checked as follows:

$$\begin{aligned} &\mathrm{Tr}[|\phi'_{\mathrm{est}}\rangle\langle\phi'_{\mathrm{est}}|]\\ &= T' * |\mathbb{1}\rangle\rangle\langle\langle\mathbb{1}|_{\mathcal{I}^n \mathcal{O}^n} \quad &(107)\\ &= \int \mathrm{d}\hat{U} \int \mathrm{d}V \int \mathrm{d}W (V_{\mathcal{I}^n}^{\otimes n} \otimes W_{\mathcal{O}^n}^{\otimes n})\\ &\qquad \times T_{W^\mathsf{T} \hat{U} V} (V_{\mathcal{I}^n}^{\otimes n} \otimes W_{\mathcal{O}^n}^{\otimes n})^\dagger * |\mathbb{1}\rangle\rangle\langle\langle\mathbb{1}| \quad &(108)\\ &= \int \mathrm{d}\hat{U} \int \mathrm{d}V \int \mathrm{d}W p(W^\mathsf{T} \hat{U} V | W^\mathsf{T} V) \quad &(109)\\ &= 1. \quad &(110) \end{aligned}$$

The probability distribution given in Eq. (100) can be implemented by measuring the quantum state $(\mathbb{1}_{\mathcal{I}^n} \otimes U_{\mathcal{O}^n}^{\otimes n}) |\phi'_{\mathrm{est}}\rangle$ with the POVM $\{M'_{\hat{U}} \mathrm{d}\hat{U}\}_{\hat{U}}$ since

$$\begin{aligned} &\mathrm{Tr}[M'_{\hat{U}} (\mathbb{1}_{\mathcal{I}^n} \otimes U_{\mathcal{O}^n}^{\otimes n}) |\phi'_{\mathrm{est}}\rangle\langle\phi'_{\mathrm{est}}| (\mathbb{1}_{\mathcal{I}^n} \otimes U_{\mathcal{O}^n}^{\otimes n})^\dagger]\\ &= \mathrm{Tr}\Big[(T'^{-1/2} T'_{\hat{U}} T'^{-1/2})^\mathsf{T} (\mathbb{1}_{\mathcal{I}^n} \otimes U_{\mathcal{O}^n}^{\otimes n}) \sqrt{T'}^\mathsf{T}\\ &\qquad \times |\mathbb{1}\rangle\rangle\langle\langle\mathbb{1}|_{\mathcal{I}^n \mathcal{O}^n} \sqrt{T'}^\mathsf{T} (\mathbb{1}_{\mathcal{I}^n} \otimes U_{\mathcal{O}^n}^{\otimes n})^\dagger\Big] \quad &(111)\\ &= \mathrm{Tr}[T'^\mathsf{T}_{\hat{U}} (\mathbb{1}_{\mathcal{I}^n} \otimes U_{\mathcal{O}^n}^{\otimes n}) |\mathbb{1}\rangle\rangle\langle\langle\mathbb{1}|_{\mathcal{I}^n \mathcal{O}^n} (\mathbb{1}_{\mathcal{I}^n} \otimes U_{\mathcal{O}^n}^{\otimes n})^\dagger] \quad &(112)\\ &= T'_{\hat{U}} * J_{\mathcal{U}}^{\otimes n} \quad &(113) \end{aligned}$$

holds, where we use Eq. (103) in Eq. (112).

Due to the unitary group symmetry (103), $\sqrt{T'}^\mathsf{T}$ can be written as

$$\sqrt{T'}^\mathsf{T} = \bigoplus_{\alpha, \beta \in \mathbb{Y}_n^d} \mathbb{1}_{\mathcal{U}_{\alpha,1}} \otimes \mathbb{1}_{\mathcal{U}_{\beta,2}} \otimes \left(\sqrt{X_{\alpha\beta}}\right)_{\mathcal{S}_{\alpha,1} \mathcal{S}_{\beta,2}}, \tag{114}$$

where $(\mathcal{U}_{\alpha,1}, \mathcal{S}_{\alpha,1}), (\mathcal{U}_{\beta,2}, \mathcal{S}_{\beta,2})$ are the Hilbert spaces given by the decomposition (40) for $\mathcal{O}^n$ and $\mathcal{I}^n$, respectively, and $X_{\alpha\beta}$ is a positive semidefinite matrix. Therefore, $|\phi'_{\mathrm{est}}\rangle$ can be written as

$$|\phi'_{\mathrm{est}}\rangle = \left|\tilde{\phi}_{\mathrm{est}}^{(\vec{v})}\right\rangle := \bigoplus_{\alpha \in \mathbb{Y}_n^d} \frac{v_\alpha}{\sqrt{d_\alpha}} |W_\alpha\rangle\rangle, \tag{115}$$

$$|W_\alpha\rangle\rangle := \sum_{s=1}^{d_\alpha} |\alpha, s\rangle_{\mathcal{U}_{\alpha,1}} \otimes |\alpha, s\rangle_{\mathcal{U}_{\alpha,2}} \otimes |\mathrm{arb}\rangle_{\mathcal{S}_{\alpha,1} \mathcal{S}_{\alpha,2}}, \tag{116}$$

where v_α and $|\mathrm{arb}\rangle$ are given by

$$v_\alpha := \sqrt{d_\alpha \sum_{i,j=1}^{m_\alpha} \langle \alpha, i| \otimes \langle \alpha, i| X_{\alpha\alpha} |\alpha, j\rangle \otimes |\alpha, j\rangle}, \tag{117}$$

$$|\mathrm{arb}\rangle := \frac{\sqrt{d_\alpha}}{v_\alpha} \sqrt{X_{\alpha\alpha}} \sum_{i=1}^{m_\alpha} |\alpha, i\rangle_{\mathcal{S}_{\alpha,1}} \otimes |\alpha, i\rangle_{\mathcal{S}_{\alpha,2}}. \tag{118}$$

As shown in Lem. 11, $|\mathrm{arb}\rangle$ does not affect the fidelity of unitary estimation, so it can be chosen arbitrarily. The coefficient v_α is given from T as

$$v_\alpha = \sqrt{\mathrm{Tr}[T |\mathbb{1}\rangle\rangle\langle\langle\mathbb{1}|_{\mathcal{I}^n \mathcal{O}^n} (P_\alpha)_{\mathcal{I}^n} \otimes (P_\alpha)_{\mathcal{O}^n}]}, \tag{119}$$

where P_α is the Young projector (see Appendix A). The optimal POVM for the probe state (115) is given by the covariant form [47]:

$$\begin{aligned} M_{\hat{U}} &:= |\eta_{\hat{U}}\rangle\langle\eta_{\hat{U}}|, \quad &(120)\\ |\eta_{\hat{U}}\rangle &:= \bigoplus_{\alpha \in \mathbb{Y}_n^d} [(\hat{U}_\alpha)_{\mathcal{U}_{\alpha,1}} \otimes \mathbb{1}_{\mathcal{S}_{\alpha,1} \mathcal{U}_{\alpha,2} \mathcal{S}_{\alpha,2}}] \sqrt{d_\alpha} |W_\alpha\rangle\rangle, \quad &(121) \end{aligned}$$

where $\hat{U}_\alpha$ is the irreducible representation α of $\hat{U}$. By relabelling the Hilbert spaces $\mathcal{I}^n$ and $\mathcal{O}^n$ as $\mathcal{A}^n$ and $\mathcal{B}^n$, respectively, the obtained protocol is given as Fig. 2 (d). We call the unitary estimation protocol with the probe state given in (115) and the POVM given in (120) the parallel covariant protocol since they are covariant with respect to representations of the unitary group SU(d) as follows:

$$(V_{\mathcal{A}^n}^{\otimes n} \otimes V_{\mathcal{B}^n}^{*\otimes n}) \left|\tilde{\phi}_{\text{est}}^{(\vec{v})}\right\rangle = \left|\tilde{\phi}_{\text{est}}^{(\vec{v})}\right\rangle \quad \forall V \in \mathrm{SU}(d), \tag{122}$$

$$(V_{\mathcal{A}^n}^{\otimes n} \otimes W_{\mathcal{B}^n}^{\otimes n}) M_{\hat{U}} (V_{\mathcal{A}^n}^{\otimes n} \otimes W_{\mathcal{B}^n}^{\otimes n})^\dagger = M_{V\hat{U}W^\mathsf{T}} \quad \forall V, W \in \mathrm{SU}(d). \tag{123}$$

In conclusion, any given protocol for unitary estimation can be converted into a parallel covariant protocol for the probe state given by Eqs. (115) and (119) and the covariant POVM given in Eq. (120). Note that this construction can also be applied to the case when the original unitary estimation protocol is given by an indefinite causal order protocol [51], [52], [53]. The average-case fidelity of the parallel covariant protocol for unitary estimation is given as the following Lemma.

Lemma 11 [10]: The fidelity of the parallel covariant protocol using the probe state (115) and the POVM (120) for d-dimensional unitary estimation using n calls is given by

$$F_{\text{est}}(n,d) = \vec{v}^\mathsf{T} M_{\text{est}}(n,d) \vec{v}, \tag{124}$$

using a vector $\vec{v} = (v_\alpha)_{\alpha \in \mathbb{Y}_n^d}$ satisfying $v_\alpha \geq 0$ for all $\alpha \in \mathbb{Y}_n^d$ and $\sum_{\alpha \in \mathbb{Y}_n^d} v_\alpha^2 = 1$. The $|\mathbb{Y}_n^d| \times |\mathbb{Y}_n^d|$ matrix $M_{\text{est}}(n,d)$ is defined by

$$(M_{\text{est}}(n,d))_{\alpha\beta} = \frac{1}{d^2} \#[(\alpha + \square) \cap (\beta + \square) \cap \mathbb{Y}_{n+1}^d], \tag{125}$$

where $\alpha + \square$ and $\beta + \square$ are defined in Eq. (23). In particular, the optimal fidelity of unitary estimation is given by

$$F_{\text{est}}(n,d) = \max_{\|\vec{v}\|=1} \vec{v}^\mathsf{T} M_{\text{est}}(n,d) \vec{v}, \tag{126}$$

which equals to the maximal eigenvalue of $M_{\text{est}}(n,d)$.

Proof: [3] From Eq. (115) and (121), the probability distribution of obtaining the estimator $\hat{U}$ is

$$\begin{aligned} &p(\hat{U}|U) \\ &= \mathrm{Tr}[M_{\hat{U}} (U^{\otimes n} \otimes \mathbb{1}_d^{\otimes n}) |\tilde{\phi}_{\text{est}}^{(\vec{v})}\rangle\langle\tilde{\phi}_{\text{est}}^{(\vec{v})}| (U^{\otimes n} \otimes \mathbb{1}_d^{\otimes n})^\dagger] \quad (127) \\ &= \Bigg| \sum_{\alpha \in \mathbb{Y}_n^d} v_\alpha \langle\!\langle W_\alpha | [(\hat{U}_\alpha)_{\mathcal{U}_{\alpha,1}} \otimes \mathbb{1}_{\mathcal{S}_{\alpha,1}} \otimes \mathbb{1}_{\mathcal{U}_{\alpha,2}} \otimes \mathbb{1}_{\mathcal{S}_{\alpha,2}}]^\dagger \\ &\qquad \times [(U_\alpha)_{\mathcal{U}_{\alpha,1}} \otimes \mathbb{1}_{\mathcal{S}_{\alpha,1}} \otimes \mathbb{1}_{\mathcal{U}_{\alpha,2}} \otimes \mathbb{1}_{\mathcal{S}_{\alpha,2}}] | W_\alpha \rangle\!\rangle \Bigg|^2 \quad (128) \\ &= \left| \sum_{\alpha \in \mathbb{Y}_n^d} v_\alpha \sum_{s=1}^{d_\alpha} \langle \alpha, s | \hat{U}_\alpha^\dagger U_\alpha | \alpha, s \rangle \right|^2 \quad (129) \\ &= \left| \sum_{\alpha \in \mathbb{Y}_n^d} v_\alpha \chi^\alpha(\hat{U}^\dagger U) \right|^2, \quad (130) \end{aligned}$$

where $\chi^\alpha(U)$ is the character of the irreducible representation α defined by $\chi^\alpha(U) := \mathrm{Tr}(U_\alpha)$. The fidelity is given by

$$\begin{aligned} &F_{\text{est}}(n,d) \\ &= \int \mathrm{d}U \int \mathrm{d}\hat{U} \frac{1}{d^2} \left|\mathrm{Tr}(\hat{U}^\dagger U)\right|^2 \left| \sum_{\alpha \in \mathbb{Y}_n^d} v_\alpha \chi^\alpha(\hat{U}^\dagger U) \right|^2 \quad (131) \\ &= \frac{1}{d^2} \int \mathrm{d}U \int \mathrm{d}\hat{U} \left| \chi(\hat{U}^\dagger U) \sum_{\alpha \in \mathbb{Y}_n^d} v_\alpha \chi^\alpha(\hat{U}^\dagger U) \right|^2, \quad (132) \end{aligned}$$

where χ is defined by $\chi(U) := \mathrm{Tr}(U)$, which corresponds to the character of the irreducible representation $\square$. Since the characters satisfy the following properties:

$$\chi(V)\chi^\alpha(V) = \sum_{\mu \in \alpha + \square \cap \mathbb{Y}_{n+1}^d} \chi^\mu(V) \quad \forall V \in \mathrm{SU}(d), \tag{133}$$

$$\int \mathrm{d}V \chi^\mu(V) \chi^{\nu,*}(V) = \delta_{\mu,\nu} \quad \forall \mu, \nu \in \mathbb{Y}_n^d, \tag{134}$$

the average-case fidelity is given by

$$\begin{aligned} &F_{\text{est}}(n,d) \\ &= \frac{1}{d^2} \int \mathrm{d}U \int \mathrm{d}\hat{U} \left| \sum_{\alpha \in \mathbb{Y}_n^d} v_\alpha \sum_{\mu \in \alpha + \square} \chi^\alpha(\hat{U}^\dagger U) \right|^2 \quad (135) \\ &= \frac{1}{d^2} \int \mathrm{d}U \int \mathrm{d}\hat{U} \sum_{\alpha,\beta \in \mathbb{Y}_n^d} v_\alpha v_\beta \\ &\qquad \times \sum_{\mu \in \alpha + \square} \sum_{\nu \in \beta + \square} \chi^\alpha(\hat{U}^\dagger U) \chi^{\beta,*}(\hat{U}^\dagger U) \quad (136) \\ &= \frac{1}{d^2} \int \mathrm{d}U \left[\sum\nolimits_{\alpha,\beta \in \mathbb{Y}_n^d} v_\alpha v_\beta \sum_{\mu \in \alpha + \square} \sum_{\nu \in \beta + \square} \delta_{\mu,\nu} \right] \quad (137) \\ &= \frac{1}{d^2} \left[\sum\nolimits_{\alpha,\beta \in \mathbb{Y}_n^d} v_\alpha v_\beta \sum_{\mu \in \alpha + \square} \sum_{\nu \in \beta + \square} \delta_{\mu,\nu} \right]. \quad (138) \end{aligned}$$

The third equality follows from the invariance of the Haar measure given by $\mathrm{d}\hat{U} = \mathrm{d}(\hat{U}^\dagger U)$ [57]. The fourth equality arises from the normality of the Haar measure, i.e., $\int \mathrm{d}U = 1$, which explicitly demonstrates that average-case fidelity coincides with the worst-case fidelity for the covariant protocol. Rearranging this equation, the fidelity $F_{\text{est}}(n,d)$ is expressed with the estimation matrix $M_{\text{est}}(n,d)$ defined in Eq. (125) as

$$F_{\text{est}}(n,d) = \vec{v}^\mathsf{T} M_{\text{est}}(n,d) \vec{v}, \tag{139}$$

where $\vec{v}$ is a unit vector supported by $\mathbb{Y}_n^d$. $\square$

Appendix D Proof of Thm. 1: One-to-One Correspondence Between dPBT and Unitary Estimation

In this section, we prove the main theorem of this paper.

Proof of Thm. 1: We prove this Theorem by constructing a transformation between covariant protocols for dPBT using $N = n + 1$ ports and unitary estimation using n calls of the input unitary operation, which does not decrease the fidelity. Since the covariant protocol is shown to achieve the optimal fidelity for dPBT [26], [30], the transformation from dPBT to unitary estimation shows

$$F_{\text{PBT}}(n+1,d) \leq F_{\text{est}}(n,d). \tag{140}$$

Similarly, since the parallel covariant protocol is shown to achieve the optimal fidelity for unitary estimation [9], [47], the transformation from unitary estimation to dPBT shows

$$F_{\text{est}}(n,d) \leq F_{\text{PBT}}(n+1,d). \tag{141}$$

[3] The proof presented in [10] contains small inconsistencies; hence, for completeness, we present a full proof here.

Therefore, we obtain

$$F_{\rm PBT}(n+1,d) = F_{\rm est}(n,d). \tag{142}$$

In addition, since an explicit construction of the covariant protocols for dPBT and unitary estimation from any given protocol are shown in Appendixes B and C, this transformation shows a transformation between any given dPBT protocol and unitary estimation protocol. Below, we show the transformation between the covariant protocols for dPBT and unitary estimation.

As shown in Lemmas 10 and 11, the fidelity of the covariant dPBT and untiary estimation protocols are given by

$$F_{\rm PBT}(N,d) = \vec{w}^{\mathsf{T}} M_{\rm PBT}(N,d)\vec{w}, \tag{143}$$
$$F_{\rm est}(n,d) = \vec{v}^{\mathsf{T}} M_{\rm est}(n,d)\vec{v}. \tag{144}$$

Reference [26] shows that the matrix $M_{\rm PBT}(n+1,d)$ in Eq. (85) can be written as

$$M_{\rm PBT}(n+1,d) = \frac{1}{d^2} R^{\mathsf{T}}(n,d)R(n,d), \tag{145}$$

where $R(n,d)$ is a $|\mathbb{Y}_n^d| \times |\mathbb{Y}_{n+1}^d|$ matrix defined by

$$(R(n,d))_{\alpha,\mu} = \begin{cases} 1 & (\mu \in \alpha + \square) \\ 0 & (\text{otherwise}) \end{cases} \quad \forall \alpha \in \mathbb{Y}_n^d, \mu \in \mathbb{Y}_{n+1}^d. \tag{146}$$

From Eq. (125), the matrix $M_{\rm est}(n,d)$ can also be written as

$$M_{\rm est}(n,d) = \frac{1}{d^2} R(n,d)R^{\mathsf{T}}(n,d). \tag{147}$$

Thus, from a given covariant protocol for dPBT parametrized by $\vec{w}$, one can obtain a parallel covariant protocol for unitary estimation parametrized by

$$\vec{v} := \frac{R(n,d)\vec{w}}{\|R(n,d)\vec{w}\|} \tag{148}$$

without decreasing the fidelity since

$$\frac{\vec{v}^{\mathsf{T}} M_{\rm est}(n,d)\vec{v}}{\vec{w}^{\mathsf{T}} M_{\rm PBT}(N,d)\vec{w}} = \frac{\vec{w}^{\mathsf{T}} R^{\mathsf{T}}(n,d)R(n,d)R^{\mathsf{T}}(n,d)R(n,d)\vec{w}}{\vec{w}^{\mathsf{T}} R^{\mathsf{T}}(n,d)R(n,d)\vec{w}\ \vec{w}^{\mathsf{T}} R^{\mathsf{T}}(n,d)R(n,d)\vec{w}} \geq 1 \tag{149}$$

holds, where we use $\vec{w}\vec{w}^{\mathsf{T}} \leq \mathbb{1}$. Similarly, from a given parallel covariant protocol for unitary estimation parametrized by $\vec{v}$, one can obtain a covariant protocol for dPBT parametrized by

$$\vec{w} := \frac{R^{\mathsf{T}}(n,d)\vec{v}}{\|R^{\mathsf{T}}(n,d)\vec{v}\|} \tag{150}$$

without decreasing the fidelity since

$$\frac{\vec{w}^{\mathsf{T}} M_{\rm PBT}(N,d)\vec{w}}{\vec{v}^{\mathsf{T}} M_{\rm est}(n,d)\vec{v}} = \frac{\vec{v}^{\mathsf{T}} R(n,d)R^{\mathsf{T}}(n,d)R(n,d)R^{\mathsf{T}}(n,d)\vec{v}}{\vec{v}^{\mathsf{T}} R(n,d)R^{\mathsf{T}}(n,d)\vec{v}\vec{v}^{\mathsf{T}} R(n,d)R^{\mathsf{T}}(n,d)\vec{v}} \geq 1 \tag{151}$$

holds, where we use $\vec{v}\vec{v}^{\mathsf{T}} \leq \mathbb{1}$. □

Appendix E Proof of Lem. 2: Asymptotically Optimal Fidelity of Unitary Estimation

Reference [10] shows a unitary estimation protocol achieving the fidelity given by

$$F_{\rm est}(n,d) \geq 1 - O(d^4)n^{-2}. \tag{152}$$

This section shows that this scaling is tight, as shown below:

Theorem 12: Suppose there exists a sequence of protocols, for $d \in \{2,\ldots\}$, $\epsilon < \frac{1}{200}$ and an unknown unitary operator $U \in \mathrm{SU}(d)$, using $n_{d,\epsilon}$ calls of $U, U^\dagger, cU := |0\rangle\langle 0|\otimes \mathbb{1}_d + |1\rangle\langle 1| \otimes U, cU^\dagger := |0\rangle\langle 0| \otimes \mathbb{1}_d + |1\rangle\langle 1| \otimes U^\dagger$ to obtain the estimator $\hat{U}$ satisfying $f(\hat{U},\mathcal{U}) > 1-\epsilon^2$ with probability $\mathrm{Prob}[f(\hat{U},\mathcal{U}) > 1-\epsilon^2] \geq \frac{2}{3}$. Then, $n_{d,\epsilon}$ must satisfy $n_{d,\epsilon} \geq \Omega(d^2)/\epsilon$.

Proof of Lem. 2: If unitary estimation achieves the average-case channel fidelity $F_{\rm est}(n,d) = 1-\frac{1}{3}\epsilon^2$ using n calls of the input unitary operator $U \in \mathrm{SU}(d)$, the probability of obtaining the estimator $\hat{U}$ satisfying $f(\hat{U},\mathcal{U}) > 1-\epsilon^2$ should be $\geq \frac{2}{3}$ since

$$F_{\rm est}(n,d) \leq 1 - \mathrm{Prob}[f(\hat{U},\mathcal{U}) \leq 1-\epsilon^2]\epsilon^2 \tag{153}$$
$$= 1 - [1 - \mathrm{Prob}[f(\hat{U},\mathcal{U}) > 1-\epsilon^2]]\epsilon^2 \tag{154}$$

holds. Then, from Thm. 12, we obtain $n \geq \Omega(d^2)/\epsilon$, i.e., $\epsilon \geq \Omega(d^2)/n$. Therefore, we have the following upper bound on the fidelity of unitary estimation:

$$F_{\rm est}(n,d) = 1 - \frac{1}{3}\epsilon^2 \leq 1 - \Omega(d^4)n^{-2}. \tag{155}$$

□

Reference [50] shows a lower bound on the diamond-norm error of unitary estimation, which is given as follows:

Proposition 13 (Theorem 1.2 in *[50]*): Suppose there exists a sequence of protocols, for $d \in \{2,\ldots\}, \epsilon < \frac{1}{8}$ and an unknown unitary operator $U \in \mathrm{SU}(d)$, using $n_{d,\epsilon}$ calls of $U, U^\dagger, cU := |0\rangle\langle 0| \otimes \mathbb{1}_d + |1\rangle\langle 1| \otimes U, cU^\dagger := |0\rangle\langle 0| \otimes \mathbb{1}_d + |1\rangle\langle 1| \otimes U^\dagger$ to obtain the estimator $\hat{U}$ satisfying $\|\hat{\mathcal{U}}-\mathcal{U}\|_\diamond < \epsilon$ with probability $\mathrm{Prob}[\|\hat{\mathcal{U}}-\mathcal{U}\|_\diamond < \epsilon] \geq \frac{2}{3}$. Then, $n_{d,\epsilon}$ must satisfy $n_{d,\epsilon} \geq \Omega(d^2)/\epsilon$.

To extend Proposition 13 for the worst-case fidelity as shown in Thm. 12, we first review the proof shown in [50]. It first shows a lower bound on the query complexity of unitary estimation with a constant error given by $\Omega(d^2)$. The proof of this lower bound uses the reduction of unitary estimation to the discrimination task among the set of unitaries $\mathcal{N}_d$ in which the different unitary operator has a constant distance. The construction of such a set is shown in Proposition 15, and the lower bound of the query complexity of the discrimination task is shown in Proposition 16. Then, we consider the unitary estimation with the error ϵ. Since the error ϵ on $U \in \mathrm{SU}(d)$ can be translated to a constant error on $U^{1/\alpha}$ for $\alpha = \Theta(\epsilon)$, the unitary estimation with the error ϵ can be translated to the estimation of $R \in \mathrm{SU}(d)$ with a constant error using R^α. To uniquely define R^α for $\alpha \in [-1,1]$, we restrict R to be a Hermitian unitary (Definition 14). It is shown that any protocol using n calls of R^α can be simulated by using $\Theta(\alpha n)$ calls of cR (Lem. 17). By combining this result with the lower bound on the query complexity of unitary estimation with a constant error, we obtain $\Theta(\alpha n) = \Omega(d^2)$, i.e., $n = \Theta(d^2/\epsilon)$.

Definition 14 (Definition 4.4 in [50]): A unitary $R \in \mathrm{SU}(d)$ is called a reflection if $R^2 = \mathbb{1}_d$ holds. For a reflection $R \in \mathrm{SU}(d)$ and $\alpha \in [-1, 1]$, we define

$$R^\alpha := \frac{1}{2}(\mathbb{1}_d + R) + e^{-i\pi\alpha}\frac{1}{2}(\mathbb{1}_d - R). \tag{156}$$

Proposition 15 (Proposition 4.1 in *[50]*): There exists a sequence of sets of reflections $\mathcal{N}_d = \{U_x\}_{x=1}^{N_d} \subset \mathrm{SU}(d)$ for $d \in \{2, \ldots\}$ with $N_d \geq \exp(d^2/64)$ such that

$$\|\mathcal{U}_x - \mathcal{U}_y\|_\diamond \geq \frac{1}{4} \quad \forall x \neq y. \tag{157}$$

Proposition 16 (Proposition 4.2 + Lemma 4.3 in *[50]*): Let $\mathcal{N}_d = \{U_x\}_{x=1}^{N_d} \subset \mathrm{SU}(d)$ be a set of unitary operators defined for $d \in \{2, \ldots\}$. Suppose there exists a sequence of protocols for $d \in \{2, \ldots\}$ using n_d queries of the input unitary operator U_x for unknown $x \in \{1, \ldots, N_d\}$ to obtain the estimator $\hat{x}$ with the success probability

$$\frac{1}{N_d}\sum_{x=1}^{N_d} \mathrm{Prob}[\hat{x} = x|x] \geq \exp(-cn_d) \tag{158}$$

for $d \geq 100/c' \geq 1$ and $N_d \geq \exp(c'd^2)$ for some constants $c, c' > 0$. Then, n_d should satisfy

$$n_d \geq c''d^2 \tag{159}$$

for some constant c'' that depends only on c and c'.

Lemma 17 (Lemma 4.5 in [50]): For a reflection $R \in \mathrm{SU}(d)$ and $U := R^\alpha$, let $C \in \mathrm{SU}(D)$ be a unitary operator implemented by a quantum circuit using n queries to U or $U^\dagger$. Then, there exists a unitary operator $C_R \in \mathrm{SU}(2^n D)$ implemented by a quantum circuit with n auxiliary qubits using $50 + 100\alpha n$ queries to cR such that

$$C_R(|\psi\rangle \otimes |0\rangle^{\otimes n}) = \nu\left|\widetilde{\mathrm{out}}\right\rangle + \left|\Phi^\perp\right\rangle, \tag{160}$$

where $\left|\widetilde{\mathrm{out}}\right\rangle$ is a normalized vector satisfying

$$\left\|\left|\widetilde{\mathrm{out}}\right\rangle - C\,|\psi\rangle\right\|_2 \leq \exp(-99\alpha\pi n - 20), \tag{161}$$

for the 2-norm $\|\cdot\|_2$ defined by $\|\,|\psi\rangle\,\|_2 := \sqrt{\langle\psi\rangle}$, $\nu \in \mathbb{C}$ is a complex number satisfying

$$|\nu| \geq 0.99\exp(-\alpha\pi n/2), \tag{162}$$

and $\left|\Phi^\perp\right\rangle$ satisfies $(\mathbb{1}_D \otimes \langle 0|^{\otimes n})\left|\Phi^\perp\right\rangle = 0$.

We extend Proposition 15 for the case of channel fidelity. To this end, we define the Bures distance [63] $d_B(U, V)$ between two unitary operators $U, V \in \mathrm{SU}(d)$ by

$$d_B(U, V) := \sqrt{1 - f(U, \mathcal{V})}, \tag{163}$$

which satisfies the following properties:

$$d_B(U, W) \leq d_B(U, V) + d_B(V, W), \tag{164}$$

$$d_B(U, V) = d_B(AUB, AVB) \quad \forall A, B \in \mathrm{SU}(d), \tag{165}$$

$$d_B(U, V) \geq \frac{1}{\sqrt{2d}}\min_{\phi\in\mathrm{U}(1)}\|U - \phi V\|_{\mathrm{tr}}, \tag{166}$$

where U(1) is the set of complex numbers with a unit norm, $\|\cdot\|_{\mathrm{tr}}$ is the trace norm defined by

$$\|\rho\|_{\mathrm{tr}} := \mathrm{Tr}\,\sqrt{\rho^\dagger\rho}. \tag{167}$$

The inequality (166) is shown below. First, the Bures distance $d_B(U, V)$ is given by

$$d_B(U, V) = \frac{1}{\sqrt{2d}}\min_{\phi\in\mathrm{U}(1)}\|U - \phi V\|_{\mathrm{F}}, \tag{168}$$

where $\|\cdot\|_{\mathrm{F}}$ is the Frobenius norm defined by

$$\|\rho\|_{\mathrm{F}} := \sqrt{\mathrm{Tr}(\rho^\dagger\rho)}. \tag{169}$$

Then, the inequality (166) holds since

$$\|\rho\|_{\mathrm{F}} = \sqrt{\sum_{i=1}^d \lambda_i^2} \geq \sqrt{\frac{1}{d}\left(\sum_{i=1}^d \lambda_i\right)^2} = \frac{\|\rho\|_{\mathrm{tr}}}{\sqrt{d}}, \tag{170}$$

where $\lambda_i \geq 0$ are singular values of ρ. Then, we show the following Proposition:

Proposition 18: There exists a sequence of sets of reflections $\mathcal{N}_d = \{U_x\}_{x=1}^{N_d} \subset \mathrm{SU}(d)$ for $d \in \{2, \ldots\}$ with $N_d \geq \exp(d^2/288)$ such that

$$d_B(U_x, U_y) \geq \frac{1}{100} \quad \forall x \neq y. \tag{171}$$

Proof: We construct the sequence of the sets $\mathcal{N}_d$ similarly to the proof of Proposition 15 in [50]. For $d \in \{2, 3\}$, $\mathcal{N}_d$ defined by

$$\mathcal{N}_d := \{\mathbb{1}_d, X_2 \oplus \mathbb{1}_{d-2}\} \tag{172}$$

satisfies the properties shown in Proposition 18, where X_2 is a Pauli X matrix defined by $X_2 := |+\rangle\langle+| - |-\rangle\langle-|$ for $|\pm\rangle := (|0\rangle \pm |1\rangle)/\sqrt{2}$. We construct $\mathcal{N}_d$ for $d \geq 4$ as shown below. We define r and b by

$$r := \left\lfloor\frac{d-1}{3}\right\rfloor \geq d/6, \quad b := d - 2r \geq r \quad \forall d \geq 4. \tag{173}$$

There exists a sequence of sets of $2r$-dimensional density operators $\mathcal{D}_r = \{\rho_x\}_{x=1}^{N_d}$, where $D_r \geq \exp(r^2/8)$ and ρ_x has rank r, exactly half of the eigenvalues are $1/r$ and the other half are zero, and

$$\|\rho_x - \rho_y\|_{\mathrm{tr}} \geq \frac{1}{4} \quad \forall x \neq y \tag{174}$$

as shown in Lemma 8 of [83]. Defining the set of reflections

$$\mathcal{N}_d := \{U_x := V_x \oplus \mathbb{1}_b := (2r\rho_x - \mathbb{1}_{2r}) \oplus \mathbb{1}_b\}_{x=1}^{N_d}, \tag{175}$$

$\mathcal{N}_d$ satisfies the properties shown in Proposition 18 as shown below. The number of elements in $\mathcal{N}_d$ satisfies

$$N_d \geq \exp(r^2/8) \geq \exp(d^2/288) \quad \forall d \geq 4. \tag{176}$$

The Bures distance between two different elements $U_x, U_y \in \mathcal{N}_d$ is given by

$$\begin{aligned} &d_B(U_x, U_y)\\ &\geq \frac{1}{\sqrt{2d}}\min_{\phi\in\mathrm{U}(1)}\|U_x - \phi U_y\|_{\mathrm{tr}} &(177)\\ &= \frac{1}{\sqrt{2d}}\min_{\phi\in\mathrm{U}(1)}\|(V_x - \phi V_y) \oplus (1-\phi)\mathbb{1}_b\|_{\mathrm{tr}} &(178)\end{aligned}$$

$$\geq \frac{1}{\sqrt{2}d} \min_{\phi\in\mathrm{U}(1)} \max\{\|\phi\mathbb{1}_{2r} - V_y^\dagger V_x\|_{\mathrm{tr}}, \|(1-\phi)\mathbb{1}_b\|_{\mathrm{tr}}\} \tag{179}$$

$$\geq \frac{1}{\sqrt{2}d} \min_{\phi\in\mathrm{U}(1)} \max\{\|\mathbb{1}_{2r} - V_y^\dagger V_x\|_{\mathrm{tr}} - \|(\phi-1)\mathbb{1}_{2r}\|_{\mathrm{tr}}, \|(1-\phi)\mathbb{1}_b\|_{\mathrm{tr}}\} \tag{180}$$

$$= \frac{1}{\sqrt{2}d} \min_{\phi\in\mathrm{U}(1)} \max\{\|\mathbb{1}_{2r} - V_y^\dagger V_x\|_{\mathrm{tr}} - 2r|\phi-1|, b|\phi-1|\} \tag{181}$$

$$\geq \frac{1}{\sqrt{2}d}\frac{b}{2r+b}\|\mathbb{1}_{2r} - V_y^\dagger V_x\|_{\mathrm{tr}} \tag{182}$$

$$= \frac{1}{\sqrt{2}d}\frac{b}{2r+b}\|V_y - V_x\|_{\mathrm{tr}} \tag{183}$$

$$= \frac{2r}{\sqrt{2}d}\frac{b}{2r+b}\|\rho_y - \rho_x\|_{\mathrm{tr}} \tag{184}$$

$$\geq \frac{r}{2\sqrt{2}d}\frac{b}{2r+b} \tag{185}$$

$$\geq \frac{1}{36\sqrt{2}} \tag{186}$$

$$\geq \frac{1}{100}. \tag{187}$$

□

Proof of Thm. 12: We show Thm. 12 following a similar argument for the proof of Proposition 13 shown in [50]. The proof shown here is almost the same as shown in [50], but we put a proof here for completeness.

Suppose there exists a quantum circuit $\mathcal{A}$ using $n_{d,\epsilon}$ queries to the oracles cU and c$U^\dagger$ to obtain the estimator $\hat{U}$ satisfying $f(\hat{U},\mathcal{U}) > 1-\epsilon^2$, i.e., $d_B(\hat{U},U) < \epsilon$ for $\epsilon < 1/200$. If U is given by $U = R^\alpha$ for $\alpha = \lfloor\frac{1}{200\epsilon}\rfloor^{-1}$, we can obtain the estimator $\hat{R} := \hat{U}^{1/\alpha}$ satisfying $d_B(\hat{R},R) < 1/200$ with probability $\geq \frac{2}{3}$ since

$$d_B(\hat{R},R) = d_B(\hat{U}^{1/\alpha}, U^{1/\alpha}) \tag{188}$$

$$\leq \sum_{p=1}^{1/\alpha} d_B(\hat{U}^p U^{1/\alpha-p}, \hat{U}^{p-1}U^{1/\alpha-p+1}) \tag{189}$$

$$= \frac{1}{\alpha}d_B(\hat{U},U) < \frac{\epsilon}{\alpha} \leq \frac{1}{200} \tag{190}$$

holds.

Next, we show that the quantum circuit $\mathcal{A}$ can be simulated with a black-box access to cc$R$. Suppose a quantum circuit $\mathcal{A}$ consists of a unitary operator $C \in \mathrm{SU}(D)$ followed by a quantum measurement $\mathcal{M}$ [56]. Using Lem. 17, we obtain a unitary operator C_R using $n'_{d,\epsilon} = 50 + 100\alpha n_{d,\epsilon}$ queries to cc$R$ satisfying Eq. (160). We define a quantum circuit $\mathcal{A}_R$, which first measures the output state of auxiliary qubits in the computational basis. If the measurement outcome is $(0,\ldots,0)$, we perform the measurement $\mathcal{M}$ on the target system and declare failure otherwise. From Eq. (162), the postselection probability is given by

$$|\nu|^2 \geq 0.99^2\exp(-\alpha\pi n_{d,\epsilon}). \tag{191}$$

We denote the probability distribution of the measurement outcome of $\mathcal{A}$ and $\mathcal{A}_R$ conditioned on the postselection by $\mathbf{a}$ and a_R, respectively. Then, from Eq. (161), the total variation distance $\mathrm{dist}_{\mathrm{TV}}(a,a_R)$ of $\mathbf{a}$ and a_R is given by [84]

$$\begin{aligned}\mathrm{dist}_{\mathrm{TV}}(a,a_R) &\leq 4\left\|\,|\widetilde{\mathrm{out}}\rangle - C|\psi\rangle\right\|_2 \\ &\leq 4\exp(-99\alpha\pi n_{d,\epsilon} - 20).\end{aligned} \tag{192}$$

Thus, the success probability for $\mathcal{A}_R$ to obtain the estimator $\hat{R}$ satisfying $d_B(\hat{R},R) < 1/200$ is given by

$$\begin{aligned}&\mathrm{Prob}_{\mathcal{A}_R}[d_B(\hat{R},R) < 1/200] \\ &= \mathrm{Prob}_{\mathcal{A}_R}[\text{post selection}] \\ &\quad\times \mathrm{Prob}_{\mathcal{A}_R}[d_B(\hat{R},R) < 1/200|\text{post selection}] \quad (193)\\ &\geq 0.99^2\exp(-\alpha\pi n_{d,\epsilon}) \\ &\quad\times\left[\mathrm{Prob}_{\mathcal{A}}[d_B(\hat{R},R) < 1/200] - \mathrm{dist}_{\mathrm{TV}}(a,a_R)\right] \quad (194)\\ &\geq 0.99^2\exp(-\alpha\pi n_{d,\epsilon}) \\ &\quad\times\left[\frac{2}{3} - 4\exp(-99\alpha\pi n_{d,\epsilon} - 20)\right] \quad (195)\\ &\geq \frac{1}{2}\exp(-\alpha\pi n_{d,\epsilon}). \quad (196)\end{aligned}$$

If we have a promise that R is taken from a set $\mathcal{N} \subset \mathrm{SU}(d)$, we can discriminate an element cc$R$ in cc$\mathcal{N} := \{\mathrm{cc}R|R\in\mathcal{N}\} \subset \mathrm{SU}(4d)$ with probability $\geq \frac{1}{2}\exp(-\alpha\pi n_{d,\epsilon}) \geq \exp(\delta_2 - \delta_1 n'_{d,\epsilon})$ using $n'_{d,\epsilon} = 50 + 100\alpha n_{d,\epsilon}$ queries to cc$R$ for constants $\delta_1 \geq 0$ and $\delta_2 \in \mathbb{R}$ that do not depend on d and ϵ. From Proposition 16, we obtain

$$n'_{d,\epsilon} = \Omega(d^2), \tag{197}$$

i.e.,

$$n_{d,\epsilon} = \frac{n'_{d,\epsilon} - 50}{100\alpha} \geq \Omega(d^2)/\epsilon \tag{198}$$

holds. □

Appendix F Proof of Cor. 4: Optimal Unitary Estimation Protocol for $n \leq d-1$

In this section, we explicitly construct the optimal unitary estimation protocol for $n \leq d-1$ shown in Cor. 4. To this end, we apply the transformation shown in Appendix D to the optimal covariant dPBT protocol shown in [6] and [26].

The optimal deterministic port-based teleportation using N ports to teleport a d-dimensional state for the case of $N \leq d$ is constructed in [26], which shows the following fidelity:

$$F_{\mathrm{PBT}}(N,d) = \frac{N}{d^2}, \tag{199}$$

where the optimal resource state is the covariant state (76) parametrized by $\vec{w}$ given as

$$w_\mu = \frac{m_\mu}{\sqrt{N!}}, \tag{200}$$

where m_μ is the multiplicity of the irreducible representation μ of the unitary group (see Appendix A). By using the one-to-one correspondence between the unitary estimation and PBT shown in Thm. 1, we obtain the optimal unitary estimation with the covariant probe state (115) parametrized by $\vec{v}$ given as

$$v_\alpha \propto \sum_\mu (R(n,d))_{\alpha,\mu} w_\mu \tag{201}$$

$$\propto \sum_{\mu\in\alpha+\square} m_\mu \tag{202}$$
$$= N m_\alpha, \tag{203}$$

where we used Lem. 6. Since $\sum_{\alpha\in\mathbb{Y}_n^d} m_\alpha^2 = n! = (N-1)!$ holds for $n \le d-1$, we obtain

$$v_\alpha = \frac{m_\alpha}{\sqrt{n!}}. \tag{204}$$

The optimal fidelity of the unitary estimation is given by

$$F_{\mathrm{est}}(d,n) = F_{\mathrm{PBT}}(d, N = n+1) = \frac{n+1}{d^2}. \tag{205}$$

Appendix G Proof of Thm. 5: Optimality of Parallel Unitary Inversion for $n \le d-1$

In this section, we show Thm. 5, stating that parallel protocol achieves the optimal fidelity of unitary inversion among the most general transformation of quantum operations including the ones with indefinite causal order. To this end, we first review the framework of quantum supermaps representing the transformation of quantum operations. Then, we show the proof of Thm. 5.

The quantum supermap [59], [78] is given as a linear map $\mathcal{C} : \bigotimes_{i=1}^n [\mathcal{L}(\mathcal{I}_i) \to \mathcal{L}(\mathcal{O}_i)] \to [\mathcal{L}(\mathcal{P}) \to \mathcal{L}(\mathcal{F})]$, where $\mathcal{I}_i$ and $\mathcal{O}_i$ are the Hilbert spaces representing the input and output systems of the i-th input quantum operation, $\mathcal{P}$ and $\mathcal{F}$ are the Hilbert spaces representing the input and output systems of the output quantum operation. Since the quantum supermaps should preserve the completely positive (CP) and trace-preserving (TP) maps, it satisfies the completely CP preserving (CCPP) condition [16], [85] given by

$$(\mathcal{C}\otimes I)(\Lambda) \text{is CP} \quad \forall \text{CP maps } \Lambda, \tag{206}$$

and TP preserving (TPP) condition [16], [85] given by

$$\mathcal{C}(\Lambda) \text{is TP} \quad \forall \text{ TP maps } \Lambda. \tag{207}$$

There exist quantum supermaps satisfying both the CCPP and TPP conditions but not implementable within the quantum circuit framework [78], [86], called quantum supermaps with indefinite causal order [51], [52], [53]. The most general quantum supermap including the one with indefinite causal order can be represented by the Choi matrix [78] $C \in \mathcal{L}(\mathcal{P}\otimes\mathcal{I}^n\otimes\mathcal{O}^n\otimes\mathcal{F})$ satisfying $C \ge 0$, $L_{\mathrm{GEN}}(C) = 0$ and $\mathrm{Tr}(C) = d^n$, where L_{GEN} is a linear map corresponding to the TPP condition, and $\mathcal{I}^n$ and $\mathcal{O}^n$ are the joint Hilbert spaces defined by $\mathcal{I}^n := \bigotimes_{i=1}^n \mathcal{I}_i$ and $\mathcal{O}^n := \bigotimes_{i=1}^n \mathcal{O}_i$, respectively.

Using the framework of the quantum supermap, we show Thm. 5.

Proof of Thm. 5: Since the optimal fidelity of parallel unitary inversion is the same as that of unitary estimation [18], we obtain

$$F_{\mathrm{inv}}^{(\mathrm{PAR})}(n,d) = \frac{n+1}{d^2} \tag{208}$$

for $n \le d-1$ from Cor. 4. We conclude the proof of Thm. 5 by showing an upper bound on the optimal fidelity for indefinite causal order protocol. To this end, we introduce a semidefinite programming (SDP) to obtain the optimal fidelity of unitary inversion. The optimal fidelity of deterministic unitary inversion using general protocols is given by the following SDP [18]:

$$\begin{aligned} &\max \mathrm{Tr}(C\Omega)\\ \text{s.t. } &\mathcal{L}(\mathcal{P}\otimes\mathcal{I}^n\otimes\mathcal{O}^n\otimes\mathcal{F}) \ni C \ge 0,\\ &L_{\mathrm{GEN}}(C) = 0,\\ &\mathrm{Tr}(C) = d^n. \end{aligned} \tag{209}$$

where $\Omega \in \mathcal{L}(\mathcal{P}\otimes\mathcal{I}^n\otimes\mathcal{O}^n\otimes\mathcal{F})$ is a positive operator called the performance operator. The performance operator Ω is given by

$$\Omega := \frac{1}{d^2}\int \mathrm{d}U_d |U_d\rangle\rangle\langle\langle U_d|^{\otimes n}_{\mathcal{I}^n\mathcal{O}^n} \otimes |U_d\rangle\rangle\langle\langle U_d|_{\mathcal{F}\mathcal{P}}, \tag{210}$$

where $\mathrm{d}U_d$ is the Haar measure on $\mathrm{SU}(d)$, $|U_d\rangle\rangle$ is the dual vector of $U_d \in \mathrm{SU}(d)$ given in Eq. (88), and the subscripts $\mathcal{I}^n\mathcal{O}^n$ and $\mathcal{P}\mathcal{F}$ represent the Hilbert spaces where the corresponding operators act. As shown in [18] and [64], the performance operator Ω satisfies the unitary group symmetry given by

$$[\Omega, U_{\mathcal{I}^n\mathcal{F}}^{\otimes n+1} \otimes V_{\mathcal{O}^n\mathcal{P}}^{\otimes n+1}] = 0 \quad \forall U, V \in \mathrm{SU}(d). \tag{211}$$

Thus, it can be represented by a linear combination of $\{(E_{ij}^\mu)_{\mathcal{I}^n\mathcal{F}} \otimes (E_{kl}^\nu)_{\mathcal{O}^n\mathcal{P}}\}_{\mu,\nu\in\mathbb{Y}_{n+1}^d, i,j\in\{1,\ldots,m_\mu\}, k,l\in\{1,\ldots,m_\nu\}}$ using the operator E_{ij}^μ defined in Eq. (48), as follows [18], [64][4]:

$$\Omega = \frac{1}{d^2}\sum_{\mu\in\mathbb{Y}_{n+1}^d}\sum_{i,j=1}^{m_\mu} \frac{(E_{ij}^\mu)_{\mathcal{I}^n\mathcal{F}} \otimes (E_{ij}^\mu)_{\mathcal{O}^n\mathcal{P}}}{d_\mu}. \tag{212}$$

In addition, the performance operator Ω satisfies the symmetric group symmetry given by

$$[\Omega, (V_\sigma)_{\mathcal{I}^n} \otimes (V_\sigma)_{\mathcal{O}^n} \otimes \mathbb{1}_{\mathcal{P}\mathcal{F}}] = 0 \quad \forall \sigma \in \mathfrak{S}_n, \tag{213}$$

where V_σ is the representation of the symmetric group defined in Eq. (39). The dual problem of the SDP (209) is given by [81]

$$\begin{aligned} &\min \lambda\\ \text{s.t. } &W \in \mathcal{L}(\mathcal{P}\otimes\mathcal{I}^n\otimes\mathcal{O}^n)\\ &\Omega \le \lambda(W\otimes\mathbb{1}_{\mathcal{F}}),\\ &\mathrm{Tr}_{\mathcal{O}_i} W = \mathrm{Tr}_{\mathcal{I}_i\mathcal{O}_i} W \otimes \frac{\mathbb{1}_{\mathcal{I}_i}}{d} \quad \forall i \in \{1,\ldots,n\},\\ &\mathrm{Tr}\, W = d^n, \end{aligned} \tag{214}$$

and any feasible solution of the dual problem (214) gives an upper bound of the optimal fidelity of deterministic unitary inversion using general protocols.

We construct a feasible solution of the dual SDP (214) with

$$\lambda = \frac{n+1}{d^2}, \tag{215}$$

which shows that the optimal fidelity of unitary inversion using general protocols is bounded by

$$F_{\mathrm{inv}}^{(\mathrm{GEN})}(n,d) \le \frac{n+1}{d^2}. \tag{216}$$

[4]Note that [64] defines d_μ and m_μ in the opposite notation.

Since $F_{\mathrm{inv}}^{(\mathrm{PAR})}(n,d) \leq F_{\mathrm{inv}}^{(\mathrm{SEQ})}(n,d) \leq F_{\mathrm{inv}}^{(\mathrm{GEN})}(n,d)$ hold, we obtain

$$\frac{n+1}{d^2} = F_{\mathrm{inv}}^{(\mathrm{PAR})}(n,d) \leq F_{\mathrm{inv}}^{(\mathrm{SEQ})}(n,d) \leq F_{\mathrm{inv}}^{(\mathrm{GEN})}(n,d) \leq \frac{n+1}{d^2}, \tag{217}$$

i.e., $F_{\mathrm{inv}}^{(\mathrm{PAR})}(n,d) = F_{\mathrm{inv}}^{(\mathrm{SEQ})}(n,d) = F_{\mathrm{inv}}^{(\mathrm{GEN})}(n,d) = \frac{n+1}{d^2}$ holds. Due to the unitary group and symmetric group symmetries (211) and (213) of the performance operator Ω, the constraints in the dual SDP (214) is invariant under the twirling operations given by

$$W \mapsto \int \mathrm{d}U \int \mathrm{d}V (U_{\mathcal{I}^n}^{\otimes n} \otimes V_{\mathcal{O}^n\mathcal{P}}^{\otimes n+1}) W (U_{\mathcal{I}^n}^{\otimes n} \otimes V_{\mathcal{O}^n\mathcal{P}}^{\otimes n+1})^\dagger, \tag{218}$$

$$W \mapsto \frac{1}{n!} \sum_{\sigma\in\mathfrak{S}_n} [(V_\sigma)_{\mathcal{I}^n} \otimes (V_\sigma)_{\mathcal{O}^n} \otimes \mathbb{1}_{\mathcal{P}}] \times W[(V_\sigma)_{\mathcal{I}^n} \otimes (V_\sigma)_{\mathcal{O}^n} \otimes \mathbb{1}_{\mathcal{P}}]^\dagger. \tag{219}$$

Thus, without loss of generality, we can assume that W satisfies the unitary group and symmetric group symmetries given by

$$[W, U_{\mathcal{I}^n}^{\otimes n} \otimes V_{\mathcal{O}^n\mathcal{P}}^{\otimes n+1}] = 0 \quad \forall U, V \in \mathrm{SU}(d), \tag{220}$$

$$[W, (V_\sigma)_{\mathcal{I}^n} \otimes (V_\sigma)_{\mathcal{O}^n} \otimes \mathbb{1}_{\mathcal{P}}] = 0 \quad \forall \sigma \in \mathfrak{S}_n. \tag{221}$$

We assume the following ansatz on W:

$$W = \sum_{\alpha\in\mathbb{Y}_n^d} \sum_{\mu\in\alpha+\square} w_{\alpha\mu} \sum_{a,b=1}^{m_\alpha} (E_{ab}^\alpha)_{\mathcal{I}^n} \otimes (E_{a_\mu^\alpha b_\mu^\alpha}^\mu)_{\mathcal{O}^n\mathcal{P}}, \tag{222}$$

where $w_{\alpha\mu} \geq 0$. Note that the operator $(E_{a_\mu^\alpha b_\mu^\alpha}^\mu)_{\mathcal{O}^n\mathcal{P}}$ is well-defined for all $\mu \in \alpha+\square$ since $\alpha+\square \subset \mathbb{Y}_{n+1}^d$ holds for all $\alpha \in \mathbb{Y}_n^d$ when $n \leq d-1$. The ansatz (222) satisfies the unitary group symmetry (220) by definition of the operators E_{ab}^α. The ansatz (222) also satisfies the symmetric group symmetry (221) since

$$\begin{aligned}
&[(V_\sigma)_{\mathcal{I}^n} \otimes (V_\sigma)_{\mathcal{O}^n} \otimes \mathbb{1}_{\mathcal{P}}] W [(V_\sigma)_{\mathcal{I}^n} \otimes (V_\sigma)_{\mathcal{O}^n} \otimes \mathbb{1}_{\mathcal{P}}]^\dagger \\
&= \sum_{\alpha\in\mathbb{Y}_n^d} \sum_{\mu\in\alpha+\square} w_{\alpha\mu} (\mathbb{1}_{\mathcal{U}_\alpha})_{\mathcal{I}^n} \otimes (\mathbb{1}_{\mathcal{U}_\mu})_{\mathcal{O}^n\mathcal{P}} \\
&\quad \otimes (\sigma_\alpha|\alpha,a\rangle\langle\alpha,b|\sigma_\alpha^\dagger)_{\mathcal{S}_\alpha} \otimes (\sigma_\mu|\mu,a_\mu^\alpha\rangle\langle\mu,b_\mu^\alpha|\sigma_\mu^\dagger)_{\mathcal{S}_\mu} && (223)\\
&= \sum_{\alpha\in\mathbb{Y}_n^d} \sum_{\mu\in\alpha+\square} w_{\alpha\mu} \sum_{a,b=1}^{m_\alpha} (\mathbb{1}_{\mathcal{U}_\alpha})_{\mathcal{I}^n} \otimes (\mathbb{1}_{\mathcal{U}_\mu})_{\mathcal{O}^n\mathcal{P}} \\
&\quad \otimes (|\alpha,a\rangle\langle\alpha,b|)_{\mathcal{S}_\alpha} \otimes (|\mu,a_\mu^\alpha\rangle\langle\mu,b_\mu^\alpha|)_{\mathcal{S}_\mu} && (224)\\
&= W && (225)
\end{aligned}$$

holds, where we use the equality

$$\sum_{a=1}^{m_\alpha} \sigma_\alpha |\alpha,a\rangle \otimes \sigma_\mu |\mu,a_\mu^\alpha\rangle = \sum_{a=1}^{m_\alpha} \sigma_\alpha |\alpha,a\rangle \otimes \sigma_\mu^* |\mu,a_\mu^\alpha\rangle \tag{226}$$

$$= \sum_{a=1}^{m_\alpha} |\alpha,a\rangle \otimes |\mu,a_\mu^\alpha\rangle, \tag{227}$$

which is derived from the fact that σ_μ is a real matrix in the Young-Yamanouchi basis[5] and the action of $\sigma \in \mathfrak{S}_n$ on $|\mu,a_\mu^\alpha\rangle$ is unitarily equivalent to the action of σ on $|\alpha,a\rangle$ as shown in Eq. (49). Due to the permutation symmetry (221), the constraints of the dual SDP (214) hold if

$$\Omega \leq \lambda (W \otimes \mathbb{1}_{\mathcal{F}}), \tag{228}$$

$$\mathrm{Tr}_{\mathcal{O}_n} W = \mathrm{Tr}_{\mathcal{I}_n\mathcal{O}_n} W \otimes \frac{\mathbb{1}_{\mathcal{I}_n}}{d}, \tag{229}$$

$$\mathrm{Tr}\, W = d^n. \tag{230}$$

The right-hand side of the inequality (228) is given by

$$\begin{aligned}
&\lambda(W \otimes \mathbb{1}_{\mathcal{F}}) \\
&= \lambda \sum_{\alpha\in\mathbb{Y}_n^d} \sum_{\mu,\nu\in\alpha+\square} w_{\alpha\mu} \sum_{a,b=1}^{m_\alpha} (E_{a_\nu^\alpha b_\nu^\alpha}^\nu)_{\mathcal{I}^n\mathcal{F}} \otimes (E_{a_\mu^\alpha b_\mu^\alpha}^\mu)_{\mathcal{O}^n\mathcal{P}} && (231)\\
&\geq \lambda \sum_{\alpha\in\mathbb{Y}_n^d} \sum_{\mu\in\alpha+\square} w_{\alpha\mu} \sum_{a,b=1}^{m_\alpha} (E_{a_\mu^\alpha b_\mu^\alpha}^\mu)_{\mathcal{I}^n\mathcal{F}} \otimes (E_{a_\mu^\alpha b_\mu^\alpha}^\mu)_{\mathcal{O}^n\mathcal{P}} && (232)\\
&= \lambda \sum_{\mu\in\mathbb{Y}_{n+1}^d} \sum_{\alpha\in\mu-\square} w_{\alpha\mu} \sum_{a,b=1}^{m_\alpha} (E_{a_\mu^\alpha b_\mu^\alpha}^\mu)_{\mathcal{I}^n\mathcal{F}} \otimes (E_{a_\mu^\alpha b_\mu^\alpha}^\mu)_{\mathcal{O}^n\mathcal{P}} && (233)\\
&= \lambda \sum_{\mu\in\mathbb{Y}_{n+1}^d} \sum_{\alpha\in\mu-\square} m_\alpha w_{\alpha\mu} (\mathbb{1}_{\mathcal{U}_\mu})_{\mathcal{I}^n\mathcal{F}} \otimes (\mathbb{1}_{\mathcal{U}_\mu})_{\mathcal{O}^n\mathcal{P}} \\
&\quad \otimes |\phi_{\alpha,\mu}\rangle\langle\phi_{\alpha,\mu}|_{\mathcal{S}_\mu\mathcal{S}_\mu}, && (234)
\end{aligned}$$

where $|\phi_{\alpha,\mu}\rangle \in \mathcal{S}_\mu \otimes \mathcal{S}_\mu$ is defined by

$$|\phi_{\alpha,\mu}\rangle := \frac{1}{\sqrt{m_\alpha}} \sum_{a=1}^{m_\alpha} |\mu,a_\mu\rangle_{\mathcal{S}_\mu} \otimes |\mu,a_\mu\rangle_{\mathcal{S}_\mu}. \tag{235}$$

On the other hand, the left-hand side of the inequality (228) is given by

$$\begin{aligned}
\Omega &= \frac{1}{d^2} \sum_{\mu\in\mathbb{Y}_{n+1}^d} \sum_{i,j=1}^{m_\mu} \frac{(E_{ij}^\mu)_{\mathcal{I}^n\mathcal{F}} \otimes (E_{ij}^\mu)_{\mathcal{O}^n\mathcal{P}}}{d_\mu} && (236)\\
&= \frac{1}{d^2} \sum_{\mu\in\mathbb{Y}_{n+1}^d} \frac{1}{d_\mu} (\mathbb{1}_{\mathcal{U}_\mu})_{\mathcal{I}^n\mathcal{F}} \otimes (\mathbb{1}_{\mathcal{U}_\mu})_{\mathcal{O}^n\mathcal{P}} \otimes |\phi_\mu\rangle\langle\phi_\mu|_{\mathcal{S}_\mu\mathcal{S}_\mu}, && (237)
\end{aligned}$$

where $|\phi_\mu\rangle \in \mathcal{S}_\mu \otimes \mathcal{S}_\mu$ is defined by

$$|\phi_\mu\rangle := \frac{1}{\sqrt{m_\mu}} \sum_{i=1}^{m_\mu} |\mu,i\rangle_{\mathcal{S}_\mu} \otimes |\mu,i\rangle_{\mathcal{S}_\mu}. \tag{238}$$

Since $|\phi_\mu\rangle = \sum_{\alpha\in\mu-\square} c_{\alpha,\mu} |\phi_{\alpha,\mu}\rangle$ and $\sum_{\alpha\in\mu-\square} |c_{\alpha,\mu}|^2 = 1$ holds for $c_{\alpha,\mu} := \sqrt{m_\alpha/m_\mu}$, we have the following inequality:

$$\sum_{\alpha\in\mu-\square} |\phi_{\alpha,\mu}\rangle\langle\phi_{\alpha,\mu}| \geq |\phi_\mu\rangle\langle\phi_\mu|. \tag{239}$$

Therefore, by taking $w_{\alpha\mu}$ as

$$w_{\alpha\mu} = \frac{m_\mu}{(n+1)m_\alpha d_\mu}, \tag{240}$$

and λ as in Eq. (215), we obtain the inequality (228) as shown below:

$$\begin{aligned}
&\lambda(W \otimes \mathbb{1}_{\mathcal{F}}) \\
&\geq \frac{1}{d^2} \sum_{\mu\in\mathbb{Y}_{n+1}^d} \frac{m_\mu}{d_\mu} \sum_{\alpha\in\mu-\square} (\mathbb{1}_{\mathcal{U}_\mu})_{\mathcal{I}^n\mathcal{F}} \otimes (\mathbb{1}_{\mathcal{U}_\mu})_{\mathcal{O}^n\mathcal{P}} \\
&\quad \otimes |\phi_{\alpha,\mu}\rangle\langle\phi_{\alpha,\mu}|_{\mathcal{S}_\mu\mathcal{S}_\mu} && (241)
\end{aligned}$$

[5] See, e.g., [70].

$$\geq \frac{1}{d^2}\sum_{\mu\in\mathbb{Y}^d_{n+1}}\frac{1}{d_\mu}(\mathbb{1}_{\mathcal{U}_\mu})_{\mathcal{I}^n\mathcal{F}}\otimes(\mathbb{1}_{\mathcal{U}_\mu})_{\mathcal{O}^n\mathcal{P}}\otimes|\phi_\mu\rangle\langle\phi_\mu|_{\mathcal{S}_\mu\mathcal{S}_\mu} \tag{242}$$

$$= \Omega. \tag{243}$$

The constraint (229) is confirmed as follows. By defining $\tau := (n, n+1) \in \mathfrak{S}_{n+1}$, $\operatorname{Tr}_{\mathcal{O}_n} W$ is given by

$$\operatorname{Tr}_{\mathcal{O}_n} W$$
$$= [\operatorname{Tr}_{\mathcal{P}}[(\mathbb{1}_{\mathcal{I}^n}\otimes(V_\tau)_{\mathcal{O}^n\mathcal{P}})W(\mathbb{1}_{\mathcal{I}^n}\otimes(V_\tau)_{\mathcal{O}^n\mathcal{P}})^\dagger]]_{\mathcal{O}_n\to\mathcal{P}}, \tag{244}$$

where subscript $\mathcal{O}_n \to \mathcal{P}$ represents the relabelling of the Hilbert spaces. This is further calculated as

$$\operatorname{Tr}_{\mathcal{O}_n} W$$
$$= \frac{1}{n+1}\sum_{\alpha\in\mathbb{Y}^d_n}\sum_{\mu\in\alpha+\square}\frac{m_\mu}{m_\alpha d_\mu}\sum_{a,b=1}^{m_\alpha}(E^\alpha_{ab})_{\mathcal{I}^n} \otimes [\operatorname{Tr}_{\mathcal{P}}[V_\tau(E^\mu_{a_\mu b_\mu})V_\tau^\dagger]_{\mathcal{O}^n\mathcal{P}}]_{\mathcal{O}_n\to\mathcal{P}} \tag{245}$$

$$= \frac{1}{n+1}\sum_{\alpha\in\mathbb{Y}^d_n}\sum_{\mu\in\alpha+\square}\frac{m_\mu}{m_\alpha d_\mu}\sum_{a,b=1}^{m_\alpha}\sum_{i,j=1}^{m_\mu}(E^\alpha_{ab})_{\mathcal{I}^n} \otimes [\tau_\mu]_{ia_\mu}[\tau_\mu^\dagger]_{b_\mu j}[\operatorname{Tr}_{\mathcal{P}}(E^\mu_{ij})_{\mathcal{O}^n\mathcal{P}}]_{\mathcal{O}_n\to\mathcal{P}} \tag{246}$$

$$= \frac{1}{n+1}\sum_{\alpha\in\mathbb{Y}^d_n}\sum_{\mu\in\alpha+\square}\frac{m_\mu}{m_\alpha}\sum_{a,b=1}^{m_\alpha}\sum_{i,j=1}^{m_\mu}(E^\alpha_{ab})_{\mathcal{I}^n} \otimes \sum_{\beta\in\mu-\square}\sum_{c,d=1}^{d_\beta}[\tau_\mu]_{c^\beta_\mu a^\alpha_\mu}[\tau^\dagger_\mu]_{b^\alpha_\mu d^\beta_\mu}\frac{(E^\beta_{cd})_{\mathcal{O}^{n-1}\mathcal{P}}}{d_\beta} \tag{247}$$

$$= \sum_{\alpha,\beta\in\mathbb{Y}^d_n}\sum_{a,b=1}^{m_\alpha}\sum_{c,d=1}^{d_\beta}A^{\alpha\beta}_{abcd}(E^\alpha_{ab})_{\mathcal{I}^n}\otimes(E^\beta_{cd})_{\mathcal{O}^{n-1}\mathcal{P}}, \tag{248}$$

where $[\tau_\mu]_{ij} := \langle\mu, i|\tau_\mu|\mu, j\rangle$, a^α_μ represents the index of the standard tableaux $s^\mu_{a^\alpha_\mu}$ obtained by adding a box $\boxed{n+1}$ to the standard tableaux s^α_a, and the coefficient $A^{\alpha\beta}_{abcd}$ is defined by

$$A^{\alpha\beta}_{abcd} := \frac{1}{n+1}\sum_{\mu\in(\alpha+\square)\cap(\beta+\square)}\frac{m_\mu}{m_\alpha}[\tau_\mu]_{c^\beta_\mu a^\alpha_\mu}[\tau^\dagger_\mu]_{b^\alpha_\mu d^\beta_\mu}. \tag{249}$$

To proceed with the calculation, we show the following Lemma for the coefficient $A^{\alpha\beta}_{abcd}$:

Lemma 19: When $n \leq d-1$ holds, coefficient $A^{\alpha\beta}_{abcd}$ defined by Eq. (249) is given by

$$A^{\alpha\beta}_{abcd} = \frac{1}{n}\sum_{\lambda\in(\alpha-\square)\cap(\beta-\square)}\sum_{p,q=1}^{m_\lambda}\frac{m_\beta}{m_\lambda}\delta_{a,p^\lambda_\alpha}\delta_{b,q^\lambda_\alpha}\delta_{c,p^\lambda_\beta}\delta_{d,q^\lambda_\beta}. \tag{250}$$

We prove Lem. 19 in the end of this section. Using this relation, $\operatorname{Tr}_{\mathcal{O}_n} W$ is further calculated as

$$\operatorname{Tr}_{\mathcal{O}_n} W$$
$$= \frac{1}{n}\sum_{\alpha,\beta\in\mathbb{Y}^d_n}\sum_{\lambda\in(\alpha-\square)\cap(\beta-\square)}\sum_{p,q=1}^{m_\lambda}\frac{m_\beta}{m_\lambda}\left(E^\alpha_{p^\lambda_\alpha q^\lambda_\alpha}\right)_{\mathcal{I}^n} \otimes \frac{\left(E^\beta_{p^\lambda_\beta q^\lambda_\beta}\right)_{\mathcal{O}^{n-1}\mathcal{P}}}{d_\beta} \tag{251}$$

$$= \frac{1}{n}\sum_{\lambda\in\mathbb{Y}^d_{n-1}}\sum_{\beta\in\lambda+\square}\frac{m_\beta}{m_\lambda d_\beta}\sum_{p,q=1}^{m_\lambda}\sum_{\alpha\in\lambda+\square}\left(E^\alpha_{p^\lambda_\alpha q^\lambda_\alpha}\right)_{\mathcal{I}^n} \otimes\left(E^\beta_{p^\lambda_\beta q^\lambda_\beta}\right)_{\mathcal{O}^{n-1}\mathcal{P}} \tag{252}$$

$$= \frac{1}{n}\sum_{\lambda\in\mathbb{Y}^d_{n-1}}\sum_{\beta\in\lambda+\square}\frac{m_\beta}{m_\lambda d_\beta}\sum_{p,q=1}^{m_\lambda}\sum_{\alpha\in\lambda+\square}\left(E^\lambda_{pq}\right)_{\mathcal{I}^{n-1}} \otimes\left(E^\beta_{p^\lambda_\beta q^\lambda_\beta}\right)_{\mathcal{O}^{n-1}\mathcal{P}}\otimes\mathbb{1}_{\mathcal{I}_n}. \tag{253}$$

Thus, the constraint (229) holds.

The constraint (230) is satisfied since

$$\operatorname{Tr} W = \frac{1}{n+1}\sum_{\alpha\in\mathbb{Y}^d_n}\sum_{\mu\in\alpha+\square}m_\mu d_\alpha \tag{254}$$

$$= \sum_{\alpha\in\mathbb{Y}^d_n}m_\alpha d_\alpha \tag{255}$$

$$= \dim\bigoplus_{\alpha\in\mathbb{Y}^d_n}\mathcal{U}_\alpha\otimes\mathcal{S}_\alpha \tag{256}$$

$$= \dim(\mathbb{C}^d)^{\otimes n} \tag{257}$$

$$= d^n \tag{258}$$

holds, where we use Lem. 6 in Appendix A.

Therefore, (λ, W) given in Eqs. (215), (222) and (240) is a feasible solution of the dual SDP (214). As shown above, this gives a matching upper bound on the optimal fidelity of unitary inversion using general protocols, which completes the proof. $\square$

Proof of Lem. 19: We first consider the operator $\{E^\beta_{cd}\}$ for $\beta \in \mathbb{Y}^D_n$ and $c, d \in \{1, \ldots, m_\beta\}$ defined on $(\mathbb{C}^D)^{\otimes n+1}$ for $D \geq n+1$. For $\tau = (n, n+1) \in \mathfrak{S}_{n+1}$,

$$\operatorname{Tr}_{n+1}[V_\tau(E^\beta_{cd}\otimes\mathbb{1}_{\mathbb{C}^D})V_\tau^\dagger] = \operatorname{Tr}_n E^\beta_{cd}\otimes\mathbb{1}_{\mathbb{C}^D} \tag{259}$$

holds. The left-hand side is calculated as

$$\operatorname{Tr}_{n+1}[V_\tau(E^\beta_{cd}\otimes\mathbb{1}_{\mathbb{C}^D})V_\tau^\dagger]$$
$$= \sum_{\mu\in\beta+\square}\operatorname{Tr}_{n+1}[V_\tau(E^\mu_{c^\beta_\mu d^\beta_\mu})V_\tau^\dagger] \tag{260}$$

$$= \sum_{\mu\in\beta+\square}\sum_{i,j=1}^{m_\mu}[\tau_\mu]_{ic^\beta_\mu}[\tau^\dagger_\mu]_{d^\beta_\mu j}\operatorname{Tr}_{n+1}(E^\mu_{ij}) \tag{261}$$

$$= \sum_{\mu\in\beta+\square}\sum_{\alpha\in\mu-\square}\sum_{a,b=1}^{m_\alpha}[\tau_\mu]_{a^\alpha_\mu c^\beta_\mu}[\tau^\dagger_\mu]_{d^\beta_\mu b^\alpha_\mu}\frac{d_\mu}{d_\alpha}E^\alpha_{ab} \tag{262}$$

$$= \sum_{\alpha\in\mathbb{Y}^D_n}\sum_{\mu\in(\alpha+\square)\cap(\beta+\square)}\sum_{a,b=1}^{m_\alpha}[\tau_\mu]_{a^\alpha_\mu c^\beta_\mu}[\tau^\dagger_\mu]_{d^\beta_\mu b^\alpha_\mu}\frac{d_\mu}{d_\alpha}E^\alpha_{ab} \tag{263}$$

$$= \sum_{\alpha\in\mathbb{Y}^D_n}\sum_{\mu\in(\alpha+\square)\cap(\beta+\square)}\sum_{a,b=1}^{m_\alpha}[\tau_\mu]_{c^\beta_\mu a^\alpha_\mu}[\tau^\dagger_\mu]_{b^\alpha_\mu d^\beta_\mu}\frac{d_\mu}{d_\alpha}E^\alpha_{ab}. \tag{264}$$

Here, we use the relation $\tau_\mu^\mathsf{T} = (\tau_\mu^\dagger)^* = \tau_\mu^* = \tau_\mu$. The right-hand side is calculated as

$$\operatorname{Tr}_n E^\beta_{cd}\otimes\mathbb{1}_{\mathbb{C}^D}$$
$$= \sum_{\lambda\in\beta-\square}\sum_{p,q=1}^{m_\lambda}\frac{d_\beta}{d_\lambda}\delta_{c,p^\lambda_\beta}\delta_{d,q^\lambda_\beta}E^\lambda_{pq}\otimes\mathbb{1}_{\mathbb{C}^D} \tag{265}$$

$$= \sum_{\lambda\in\beta-\square}\sum_{p,q=1}^{m_\lambda}\sum_{\alpha\in\lambda+\square}\frac{d_\beta}{d_\lambda}\delta_{c,p^\lambda_\beta}\delta_{d,q^\lambda_\beta}E^\alpha_{p^\lambda_\alpha q^\lambda_\alpha} \tag{266}$$

$$= \sum_{\alpha \in \mathbb{Y}_n^D} \sum_{\lambda \in (\alpha - \square) \cap (\beta - \square)} \sum_{p,q=1}^{m_\lambda} \frac{d_\beta}{d_\lambda} \delta_{c, p_\beta^\lambda} \delta_{d, q_\beta^\lambda} E^\alpha_{p_\alpha^\lambda q_\alpha^\lambda}. \tag{267}$$

Therefore, we obtain

$$\sum_{\mu \in (\alpha + \square) \cap (\beta + \square)} \frac{d_\mu}{d_\alpha} [\tau_\mu]_{c_\mu^\beta a_\mu^\alpha} [\tau_\mu^\dagger]_{b_\mu^\alpha d_\mu^\beta}$$
$$= \sum_{\lambda \in (\alpha - \square) \cap (\beta - \square)} \frac{d_\beta}{d_\lambda} \delta_{a, p_\alpha^\lambda} \delta_{b, q_\lambda^\alpha} \delta_{c, p_\beta^\lambda} \delta_{d, q_\beta^\lambda}. \tag{268}$$

Due to the hook-content formula (43) shown in Appendix A for the dimensions of the irreducible representations of the unitary group and the symmetric group,

$$\lim_{D \to \infty} \frac{1}{D} \frac{d_\mu}{d_\alpha} = \lim_{D \to \infty} (n+1) \frac{D + i - j}{D} \frac{m_\mu}{m_\alpha} = (n+1) \frac{m_\mu}{m_\alpha}, \tag{269}$$
$$\lim_{D \to \infty} \frac{1}{D} \frac{d_\beta}{d_\lambda} = \lim_{D \to \infty} n \frac{D + k - l}{D} \frac{m_\beta}{m_\lambda} = n \frac{m_\beta}{m_\lambda} \tag{270}$$

hold, where $(i, j)((k, l))$ is the position of the box added to $\alpha(\beta)$ to obtain $\mu(\nu)$. Therefore, we obtain

$$A^{\alpha\beta}_{abcd} = \frac{1}{n+1} \sum_{\mu \in (\alpha + \square) \cap (\beta + \square)} \frac{m_\mu}{m_\alpha} [\tau_\mu]_{c_\mu^\beta a_\mu^\alpha} [\tau_\mu^\dagger]_{b_\mu^\alpha d_\mu^\beta} \tag{271}$$
$$= \frac{1}{n} \sum_{\lambda \in (\alpha - \square) \cap (\beta - \square)} \frac{m_\beta}{m_\lambda} \delta_{a, p_\alpha^\lambda} \delta_{b, q_\lambda^\alpha} \delta_{c, p_\beta^\lambda} \delta_{d, q_\beta^\lambda}. \tag{272}$$

□

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