Optimal Non-asymptotic Quantum Metrology with Hierarchical Strategies

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One of the main quests in quantum metrology is to attain the ultimate precision limit with given resources, where the resources are not only of the number of queries, but more importantly of the allowed strategies. With the same number of queries, the restrictions on the strategies constrain the achievable precision. In this work, we establish a systematic framework to identify the ultimate precision limit of different families of strategies, including the parallel, the sequential and the indefinite-causal-order strategies, and provide an efficient algorithm that determines an optimal strategy within the family of strategies under consideration. With our framework, we show there exists a strict hierarchy of the precision limits for different families of strategies.

Introduction.—Quantum metrology [1, 2] features a series of promising applications in the near future [3]. In the prototypical setting of quantum metrology, the goal is to estimate an unknown parameter carried by a quantum channel, given $N$ queries to it. A pivotal task is to design a strategy that utilizes these $N$ queries to generate a quantum state with as much information about the unknown parameter as possible. This often involves, for example, preparing a suitable input probe state [4–6] and applying intermediate quantum control [7–10] as well as quantum error correction [11–14].

In reality, the implementation of strategies is subject to physical restrictions. In particular, within the noisy and intermediate-scale quantum (NISQ) era [15], we have to adjust the strategy to accommodate the limitations on the system. For example, for systems with short coherence time it might be favorable to adopt the parallel strategy (Fig. 1(a)), where multiple queries of the unknown channel are applied simultaneously on a multipartite entangled state [4]. When the system has longer coherence time and can be better controlled, one could choose to query the channel sequentially (Fig. 1(b)), which may potentially enhance the precision. In addition to the parallel and sequential strategies, it was recently discovered that the quantum SWITCH [10], a primitive where the order of making queries to the unknown channel is in a quantum superposition (Fig. 1(c)), can be employed to generate new strategies of quantum metrology [17, 19] that may even break the Heisenberg limit [19].

Moreover, indefinite causal structures beyond the quantum SWITCH [10, 20, 21] (Fig. 1(d) and (e)) have recently been shown to further boost the performance of certain information processing tasks [22, 23]. The ultimate performance of these strategies in quantum metrology, however, remains unknown. This is mainly due to the lack of a systematic method that optimizes the probe state, the control and other degrees of freedom in a strategy in a unified fashion which leads to the ultimate precision limit.

Quantum Fisher information.—The uncertainty $\delta^2 \hat{\phi}$ of estimating an unknown parameter $\phi$ encoded in a quant-
tum state $\rho_\phi$, for any unbiased estimator $\hat{\phi}$, can be determined via the quantum Cramér-Rao bound (QCRB) as $\delta \hat{\phi} \geq 1/\sqrt{J_Q(\rho_\phi)}$ [23, 24], where $J_Q(\rho_\phi)$ is the quantum Fisher information (QFI) of the state $\rho_\phi$ and $\nu$ is the number of repeated measurements [27]. For single-parameter estimation, the QCRB is achievable, and the QFI thus quantifies the amount of information that can be extracted from the quantum state. One way to compute the QFI is [28, 29]:

$$J_Q(\rho_\phi) = 4 \min_{\text{Tr}_A(\hat{\psi} \rho_\phi \hat{\psi}) = \rho_\phi} \langle \hat{\psi} \rho_\phi \hat{\psi} \rangle,$$  

(1)

where $|\hat{\psi}_\phi\rangle$ is the purification of $\rho_\phi$ with an ancillary space $\mathcal{H}_A$. $\text{Tr}_A$ denotes the partial trace over $\mathcal{H}_A$, and $\hat{\psi} = \partial \hat{\psi}/\partial \phi$. When the parameter is carried by a quantum channel $\mathcal{E}_\phi$, i.e., a completely positive trace-preserving (CPTP) map, the channel QFI can be defined as the maximal QFI of output states using the optimal input assisted by arbitrary ancillae [25, 30–32]:

$$J_Q(\mathcal{E}_\phi) = \max_{\rho_\phi \in \mathcal{S}(\mathcal{H}_2 \otimes \mathcal{H}_A)} J_Q((\mathcal{E}_\phi \otimes \mathbb{I}_A)(\rho_\phi)),$$

where $\mathcal{S}(\mathcal{H})$ denotes the space of density operators on the Hilbert space $\mathcal{H}$, $\mathcal{H}_{S(A)}$ denotes the Hilbert space of the system/ancilla, and $\mathbb{I}_A$ is the identity on $\mathcal{H}_A$.

We denote by $\mathcal{L}(\mathcal{H})$ the set of linear operators on the finite-dimensional Hilbert space $\mathcal{H}$, and $\mathcal{L}(\mathcal{H}_{i1}, \mathcal{H}_{i2})$ denotes the set of linear maps from $\mathcal{L}(\mathcal{H}_i)$ to $\mathcal{L}(\mathcal{H}_i)$. By the Choi–Jamiołkowski (CJ) isomorphism, a parameterized quantum channel $\mathcal{E}_\phi \in \mathcal{L}(\mathcal{H}_{2i-1}, \mathcal{H}_{2i})$ for $1 \leq i \leq N$ can be represented by a positive semidefinite operator (called the CJ operator) $\mathcal{E}_\phi = \text{Choi}(\mathcal{E}_\phi) = \mathcal{E}_\phi \otimes \mathbb{I}(|I\rangle\langle I|)$, where $|I\rangle = \sum_i |i\rangle |i\rangle$. The CJ operator of $N$ identical quantum channels is $\mathcal{E}_\phi = E^\otimes N \in \mathcal{L}(\otimes_{i=1}^N \mathcal{H}_i)$.

**Strategy set in quantum metrology.**—A strategy is an arrangement of physical processes (the blue shaded area in Fig. 1) which, when concatenated with given queries to $\mathcal{E}_\phi$, generates an output quantum state carrying the information about $\phi$. A strategy can be described by a CJ operator on $\mathcal{L}(\mathcal{H}_{F} \otimes_{i=1}^N \mathcal{H}_i)$, where $\mathcal{H}_F$ denotes the output Hilbert space of the concatenation, referred to as the *global future* space. The concatenation of two processes is characterized by the link product [33, 34] of two corresponding CJ operators $A \in \mathcal{L}(\otimes_{i=1}^N \mathcal{H}_i)$ and $B \in \mathcal{L}(\otimes_{i=1}^N \mathcal{H}_i)$ as

$$A \ast B := \text{Tr}_{A \otimes B} \left((\mathbb{1}_{B} \otimes A^{\dagger} \otimes B)(B \otimes \mathbb{1}_{A \otimes B})\right).$$

(2)

where $T_i$ denotes the partial transpose on $\mathcal{H}_i$, and $\mathcal{H}_{A: B}$ denotes $\otimes_{i \neq A: B} \mathcal{H}_i$. The output state lies in the global future F, which should not affect any state in the past.

Following the above formalism, a sufficiently large ancillary Hilbert space, a strategy set determined by the relevant causal constraints is described by a subset $\mathcal{P}$ of

$$\text{Strat} := \{P \in \mathcal{L}(\mathcal{H}_F \otimes_{i=1}^N \mathcal{H}_i) | P \geq 0, \text{rank}(P) = 1\}.$$  

(3)

Here, without loss of generality [35], we have restricted $P$ to pure processes (rank-1 operators) due to the monotonicity of QFI [36]. Our goal is to identify the ultimate precision limit of parameter estimation characterized by the QFI within such constraints:

**Definition 1.** The QFI of $N$ quantum channels $\mathcal{E}_\phi$ given a strategy set $\mathcal{P}$ is

$$J_Q^{(P)}(\rho_\phi) := \max_{P \in \mathcal{P}} J_Q(P \ast \rho_\phi),$$

(4)

where $J_Q(\rho)$ is the QFI of the state $\rho$, and $\mathcal{P} \subseteq \mathcal{P}$ is the CJ operator of $N$ channels.

In general we can write the ensemble decomposition [28] of the CJ operator $\mathcal{N}_\phi$ as $\mathcal{N}_\phi = \sum_{i=1}^r |N_{\phi,i}\rangle \langle N_{\phi,i}| = \mathcal{N}_\phi \mathcal{N}_\phi^\dagger$, where $\mathcal{N}_\phi := (|N_{\phi,1}\rangle, \ldots, |N_{\phi,r}\rangle)$ and $r := \max_\phi \text{rank}(\mathcal{N}_\phi)$. We also define $\tilde{\mathcal{N}}_\phi := \mathcal{N}_\phi - i \mathcal{N}_\phi h$ for $h \in \mathbb{H}_r$, where $\mathbb{H}_r$ denotes the set of $r \times r$ Hermitian matrices, and the performance operator [35]

$$\Omega_\phi(h) := 4\left(\tilde{\mathcal{N}}_\phi \tilde{\mathcal{N}}_\phi^\dagger \right)^T.$$  

(5)

With these notations, we can show (see Appendix A which is analogous to the approach in [35]) that the QFI admits the form:

$$J_Q^{(P)}(\rho_\phi) = \min_{P \in \mathcal{P}} \text{Tr} \left[\hat{P} \Omega_\phi(h)\right];$$

(6)

with

$$\hat{P} := \left\{ \hat{P} = \text{Tr}_F P | P \in \mathcal{P} \right\}.$$  

(7)

To evaluate the QFI, we first exchange $\max_\phi$ and $\min_h$ without changing the optimal QFI, assured by the min-max theorem [39, 40] since the objective function is concave on $\hat{P}$ and convex on $h$ [41]. Hence, the problem is cast into

$$J_Q^{(P)}(\rho_\phi) = \min_{h} \max_{P \in \mathcal{P}} \text{Tr} \left[\hat{P} \Omega_\phi(h)\right].$$

(8)

Then we fix $h$ and formulate the dual problem of maximization over the set $\hat{P}$. Finally we further optimize the value of $h$. To simplify the calculation of QFI we require that

$$\hat{P} = \text{Conv} \left\{ \bigcup_{i=1}^K \left\{ S^i \geq 0 | S^i \in \mathbb{S}^i \right\} \right\},$$

(9)

where $\text{Conv}\{\cdot\}$ denotes the convex hull, and each $S^i$ for $i = 1, \ldots, K$ is an affine space of Hermitian operators. Adopting the above-mentioned method, we get:

**Theorem 1.** Given an arbitrary strategy set $\mathcal{P}$ such that $\hat{P}$ given by Eq. (7) satisfies the condition Eq. (9), the
QFI of $N$ quantum channels $\mathcal{E}_\phi$ can be expressed as the following optimization problem:

$$J^{(P)}(N_\phi) = \min_{\lambda, Q, h} \lambda,$$

$$\text{s.t. } \lambda Q^i \geq \Omega_\phi(h), \; Q^i \in \bar{S}^i, \; i = 1, \ldots, K,$$

where $\bar{S}^i := \{Q \text{ is Hermitian} | \text{Tr}(QS) = 1, S \in S^i \}$ is the dual affine space of $S^i$.

The proof can be found in Appendix IV. We remark that similar optimization ideas have been applied to other tasks, such as quantum Bayesian estimation [42], quantum network optimization [43], non-Markovian quantum metrology [38], and quantum channel discrimination [23]. The minimization problem in Theorem 1 can be further written in the form of SDP and solved efficiently, with detailed numerically solvable forms given in Appendix III where the constraints in Eq. 10 can be further simplified in some cases.

Optimal strategies.—By itself, the QFI does not reveal how to implement the optimal strategy achieving the highest precision. Here, in addition to Theorem 1, we design an algorithm that yields a strategy attaining the optimal QFI for any strategy set satisfying Eq. 9. The method, which generalizes the method of finding an optimal probe state for a single channel [44, 45], is summarized as Algorithm I (see Appendix C for its derivation).

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Algorithm 1. Find an optimal strategy in the set $P$.

- Given $N_\phi$ the CJ operator of $N$ channels, solve for an optimal value $h = h^{(\text{opt})}$ in Eq. 10 of Theorem 1 via SDP.
- Fixing $h = h^{(\text{opt})}$, solve for an optimal value $\hat{P}^{(\text{opt})}$ of $P \in P$ in Eq. 6 via SDP such that

$$\text{Re}\left\{\text{Tr}\left\{[\hat{P}^{(\text{opt})} - iN_\phi \mathcal{H} \left( N_\phi - iN_\phi h^{(\text{opt})} \right)]^T\right\}\right\} = 0 \quad \text{for all } \mathcal{H} \in \mathbb{H}_r,$$

where $N_\phi := \{|N_\phi, 1\}, \ldots, |N_\phi, N\rangle \rangle$. An optimal strategy $P^{(\text{opt})} \in P$ can be taken as a purification of $\hat{P}^{(\text{opt})}$.

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By Algorithm I we obtain the CJ operator of a strategy that attains the optimal QFI. For strategies following definite causal order, there exists an operational method of mapping the CJ operator of the strategy to a probe state and a sequence of in-between control operations with minimal memory space [46]. For causal order superposition strategies (see the strategy set $\text{Sup}$ later), we show that they can always be implemented by controlling the order of operations in a circuit with a quantum SWITCH (see Appendix E). In this way, we obtain a systematic method to identify optimal sequential and causal superposition strategies, one of the key problems in quantum metrology.

Strategy sets.—We consider the evaluation of QFI for five different families of strategies. In all the following definitions the subscript $i$ of an operator denotes the Hilbert space $\mathcal{H}_i$ it acts on.

The family of parallel strategies (see Fig. 4(a)) is the first and one of the most successful examples of quantum-enhanced metrology, featuring the usage of entanglement to achieve precision beyond the classical limit [17]. By making parallel use of $N$ quantum channels together with ancillae, we can regard these $N$ channels as one single channel from $\mathcal{L}(\mathcal{H}_{1}^N \otimes \mathcal{H}_{2k-1})$ to $\mathcal{L}(\mathcal{H}_{1}^N \otimes \mathcal{H}_{2k})$. A parallel strategy set $\text{Par}$ is defined as the collection of $P \in \text{Strat}$ such that [34]

$$\text{Tr}_F P = \mathbb{I}_{2, 4, \ldots, 2N} \otimes P^{(1)}, \; \text{Tr}_P P^{(1)} = 1.$$

Note that the optimal QFI of parallel strategies can also be evaluated using the method in [28, 30].

A more general protocol is to allow for sequential use of $N$ channels assisted by ancillae, where only the output of the former channel can affect the input of the latter channel, and any control gates can be inserted between channels (see Fig. 4(b)). A sequential strategy set $\text{Seq}$ is defined as the collection of $P \in \text{Strat}$ such that [34]

$$\text{Tr}_F P = \mathbb{I}_{2N} \otimes P^{(N)}, \; \text{Tr}_P P^{(1)} = 1,$$

$$\text{Tr}_{2k-1} P^{(k)} = \mathbb{I}_{2k-2} \otimes P^{(k-1)}, \; k = 2, \ldots, N.$$ (13)

Unlike the case of parallel strategies, there is no existing way of evaluating the exact QFI using sequential strategies.

We also consider families of strategies involving indefinite causal order. The first one, denoted by $\text{SWI}$, takes advantage of the (generalized) quantum SWITCH [15, 39], where the execution order of $N$ channels is entangled with the state of an $N$!-dimensional control system (see Fig. 4(c)). See Appendix E for the formal definition.

More generally, we consider the quantum superposition of multiple sequential orders, each with a unique order of querying the $N$ channels (see Fig. 4(d)). This can be implemented by entangling $N!$ definite causal orders with a quantum control system [50]. If $N = 2$ and the control system is traced out, this notion is equivalent to causal separability [20, 21]. A causal superposition strategy set $\text{Sup}$ is defined as the collection of $P \in \text{Strat}$ such that

$$\text{Tr}_F P = \sum_{\pi} q^{\pi} P^\pi, \; \sum_{\pi \in S_N} q^{\pi} = 1,$$

$$P^\pi \in \text{Seq}^\pi, \; q^{\pi} \geq 0, \; \pi \in S_N,$$ (14)

where each permutation $\pi$ is an element of the symmetric group $S_N$ of degree $N$, and each $\text{Seq}^\pi$ denotes a sequential strategy set whose execution order of $N$ channels is $\mathcal{E}_\phi^{(1)} \to \mathcal{E}_\phi^{(2)} \to \cdots \to \mathcal{E}_\phi^{(N)}$, having denoted by $\mathcal{E}_\phi^k$ the channel from $\mathcal{L}(\mathcal{H}_{2k-1})$ to $\mathcal{L}(\mathcal{H}_{2k})$. Note that $\text{SWI}$ is a
subset of $\text{Sup}$, where the intermediate control is trivial. There are other strategies, such as quantum circuits with quantum controlled causal order (QC-QCs) and probabilistic QC-QCs [50, 51], which we will not discuss here.

Finally we introduce the family of general indefinite-causal-order strategy (see Fig. 2(e)), which is the most general strategy set considered in this work. Here the only requirement is that the concatenation of the strategy $P$ with $N$ arbitrary channels results in a legitimate quantum state. The causal relations in this case [21] are a bit cumbersome, but for our purpose what matters is the dual affine space (see Theorem 1), which is simply the space of no-signalling channels [16, 43]. A general indefinite-causal-order strategy set ICO is defined as the collection of $P \in \text{Strat}$ such that

$$\rho_F = P \star (\otimes_{j=1}^N E^j)$$

for any $E^j$, $\rho_F \geq 0$, $\text{Tr} \rho_F = 1$, (15)

where $E^j \in \mathcal{L}(\mathcal{H}_{2j-1} \otimes \mathcal{H}_{2j} \otimes \mathcal{H}_{A_j})$ denotes the CJ operator of an arbitrary quantum channel with an arbitrary ancillary space $\mathcal{H}_{A_j}$.

We note that, unlike the previous strategies that can always be physically realized, the physical realization of the general ICO is untraceable [50, 51]. The optimal value obtained with general ICO nevertheless serves as a useful tool that can gauge the performances of different strategies. For example, as we will show, in some cases the optimal QFI $J^{(\text{Sup})}$ and $J^{(\text{ICO})}$ are equal or nearly equal. This then shows that the physically realizable strategy obtained from the set Sup is already optimal or nearly optimal among all possible strategies, which will not be able to tell without $J^{(\text{ICO})}$.

**Symmetry reduced programs for optimal metrology.—** The complexity of the original optimization problems in Theorem 1 and Algorithm 1 can be reduced by exploiting the permutation symmetry. In Appendix D, we prove that we can choose a permutation-invariant matrix $\pi$ for Theorem 1 and solve for a permutation-invariant optimal strategy [52] by Algorithm 1 based on this choice, if any permutation $\pi \in S_N$ bijectively maps each affine space $S^i$ (in Eq. (9)) to another affine space $S^j$. That is, for any $\pi \in S_N$ and any $i$, there exists a $j$ such that the mapping $S \mapsto G_{\pi} S G_{\pi}^\dagger$ on $S^j$ is a bijective function from $S^i$ to $S^j$, where $G_{\pi}$ is a unitary representation of $\pi$. Furthermore, if each space $S^i$ itself is permutation-invariant, we can restrict each $Q^i \in S^i$ to be permutation-invariant, further reducing the complexity of optimization. For both optimization problems we can apply the technique of group-invariant SDP to reduce the size as there exists an isomorphism which preserves positive semidefiniteness, from the permutation-invariant subspace to the space of block-diagonal matrices [53, Theorem 9.1]. Table 1 compares the number of variables involved in QFI evaluation with/without exploiting the symmetry (see Appendix E for its derivation as well as Appendix F for the complexity of Algorithm 1) where by group-invariant SDP we also numerically evaluate the growth of QFI $J^{(\text{ICO})}$ up to $N = 5$.

| SDP | Par | Seq | SWI | Sup | ICO |
|-----|-----|-----|-----|-----|-----|
| Ori. | $O(s^N)$ | $O(d^N)$ | $O(s^N)$ | $O(N!d^N)$ | $O(d^N)$ |
| Inv. | $O(N^{d-1})$ | $O(d^N)$ | $O(N^{d-1})$ | $O(d^N)$ | $O(N^{d-1})$ |

TABLE I. Complexity of QFI evaluation for each family of strategies (with respect to $N$). The asymptotic numbers of variables in optimization are compared between the original (Ori.) and group-invariant (Inv.) SDP. We denote $d := \text{dim}(\mathcal{H}_1)\text{dim}(\mathcal{H}_2)$ and $s := \max_{\phi} \text{rank}(E_\phi) \leq d$.

**Hierarchy of strategies.—** By substituting the definitions of different strategy sets into Theorem 1 we obtain the exact values of the optimal QFI. We find that a strict hierarchy of QFI exists quite prevalently. For demonstration purposes, here we show only the result for the amplitude damping channel for $N = 2$ and supplement our findings with bountiful numerical results in Appendix G. In this case, the process encoding $\phi$ is a $z$-rotation $U_z(\phi) = e^{-i\phi t|x|/2}$, where $t$ is the evolution time, followed by an amplitude damping channel described by two Kraus operators: $K_1^{(\text{AD})} = |0\rangle\langle 0| + \sqrt{1-p}|1\rangle\langle 1|$ and $K_2^{(\text{AD})} = \sqrt{p}|0\rangle\langle 1|$, with the decay parameter $p$.

![Fig. 2. Hierarchy of QFI using parallel, sequential and indefinite-causal-order strategies.](image) We take $N = 2$ and $\phi = 1.0$, fix $t = 1.0$ and vary the decay parameter $p$. The gaps can be seen more clearly by zooming in on the interval [0.35, 0.45] of the value of $p$. $J^{(\text{Sup})} = J^{(\text{ICO})}$ with an error tolerance of no more than $10^{-8}$ in this case, but the gap between $J^{(\text{Sup})}$ and $J^{(\text{ICO})}$ could exist for larger $N$ or for other types of noise, which can be observed by randomly sampling noise channels.

In Fig. 2 we plot the QFI versus $p$ for the amplitude damping noise with all 5 strategies for $N = 2$. A strict hierarchy of Par, Seq and ICO holds if $p$ is neither 1 nor 0, i.e., $J^{(\text{Par})} < J^{(\text{Seq})} < J^{(\text{ICO})}$. This is in contrast to the asymptotic regime of $N \rightarrow \infty$, where the relative difference between $J^{(\text{Seq})}$ and $J^{(\text{Par})}$ vanishes for this channel [15]. Besides, in this case general ICO cannot strictly
outperform $\text{Sup}$, implying that causally superposing two sequential strategies is sufficient to achieve the general optimality in this particular scenario. The gap between $J^{(\text{Sup})}$ and $J^{(\text{ICO})}$, however, could be observed for the same channel with larger $N$ or for other channels when $N = 2$ (see Appendix F). In fact, by randomly sampling noise channels from CPTP channel ensembles, we find that for 984 of 1000 random channels, a strict hierarchy $J^{(\text{Par})} < J^{(\text{Seq})} < J^{(\text{Sup})} < J^{(\text{ICO})}$ holds for $N = 2$, implying that there exist more powerful strategies than causal superposition strategies in these cases. We note that a strict hierarchy of strategies has been found for channel discrimination in [23], but much less is known in quantum metrology until our work.

Our method can also test the tightness of existing QFI bounds in the non-asymptotic regime, which has seldom been done till this work. Here we take the commonly used, asymptotically tight [4] upper bound for parallel strategies (see [28] Theorem 4 or [30] Eq. (16)). For $p = 0.5$, our result shows that the exact parallel QFI $J^{(\text{Par})} = 1.795$ is 32.7% lower than the asymptotically tight parallel upper bound 2.667, and even the exact sequential QFI $J^{(\text{Seq})} = 2.179$ is 18.3% lower than this parallel upper bound [54]. Similar phenomena are observed in other noise models and for different $N$ (see Appendix F).

With Algorithm 1 we can also construct strategies to achieve the optimal QFI. Remarkably, we find that a simple strategy of applying a quantum SWITCH using a control qubit $|\psi\rangle = (|0\rangle_C + |1\rangle_C)/\sqrt{2}$ (without any additional control operations on the probe) beats any sequential strategies (which can involve complex control) in certain cases (e.g. $p < 0.5$). To our best knowledge, this is the only instance of noisy quantum metrology so far, where the advantage of indefinite causal orders is established rigorously. In Appendix F we also present two explicit examples of implementing optimal sequential and causal superposition strategies, obtained by first applying Algorithm 1 and converting the CJ operators into quantum circuit consisting of single-qubit rotations and CNOT gates (as well as a quantum SWITCH for the case of $\text{Sup}$). For optimal causal superposition strategies, the permutation symmetry allows us to only control the execution order of channels while fixing state preparation and intermediate control ($\rho_1 = \rho_2$ and $U_1 = U_2$ in Fig. 11), which can be implemented by a $(2N - 1)$-quantum SWITCH of $N$ channels $E_\phi$ and $N - 1$ intermediate operations.

Our result serves as a versatile tool for the demonstration of optimal quantum metrology and the design of optimal quantum sensors, especially in the context of control optimization [55, 56] and indefinite causal orders [16, 23].

The code accompanying the paper is openly available [57].

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Appendix A: Proof of Eq. (6) of the main text

The formalism of this proof has been developed for strategies following a definite causal order in [38], and the generalization to indefinite-causal-order strategies considered here is straightforward.

In [28], the QFI of a quantum state is expressed as a minimization problem

\[ J_Q(\rho_\phi) = 4 \min_{\{\phi,i\}} \sum_{i=1}^N \text{Tr}(|\psi_{\phi,i}\rangle \langle \psi_{\phi,i}|), \]  

(A1)

for any integer \( q \geq \max_\phi \text{rank}(\rho_\phi) \), where \( \{ |\psi_{\phi,i}\rangle \} \) is a set of unnormalized vectors such that \( \rho_\phi = \sum_i |\psi_{\phi,i}\rangle \langle \psi_{\phi,i}| \)

In the main text, the QFI of \( N \) quantum channels \( E_\phi \) is defined as the QFI of the output state obtained from the concatenation of the CJ operator \( N_\phi \) of \( N \) quantum channels and an optimal strategy \( P \) in a given strategy set \( P \):

\[ J^{(P)}(N_\phi) := \max_{P \in P} J_Q(P \ast N_\phi). \]  

(A2)

Due to the monotonicity [36] of the QFI under CPTP maps (e.g., the partial trace operation over ancillary space in this case), by choosing a proper global future space \( \mathcal{H}_F \) an optimal \( P \) can be taken as a pure process (rank-1 operator) denoted by \( |P\rangle \langle P| \). For a fixed \( P = |P\rangle \langle P| \), minimization over decompositions of \( P \ast N_\phi \) is equivalent to minimization over decompositions of \( N_\phi \), as \( \text{rank}(P \ast N_\phi) \leq \text{rank}(N_\phi) \).

As a positive semidefinite operator, \( N_\phi \) has a decomposition as:

\[ N_\phi = \sum_{i=1}^r |N_{\phi,i}\rangle \langle N_{\phi,i}|, \]  

(A3)

where \( r := \max_\phi \text{rank}(N_\phi) \) \(^1\). Note that the decomposition is non-unique. Defining \( N_\phi := (|N_{\phi,1}\rangle, \ldots, |N_{\phi,r}\rangle) \), an arbitrary alternative decomposition \( \hat{N}_\phi := (|\hat{N}_{\phi,1}\rangle, \ldots, |\hat{N}_{\phi,r}\rangle) \) can be related to \( N_\phi \) by \( \hat{N}_\phi = N_\phi V_\phi \), where \( V_\phi \) is an \( r \times r \) unitary matrix. Then the QFI of \( N \) channels can be expressed as

\[ J^{(P)}(N_\phi) = \max_{P \in P} \min_{V_\phi} \text{Tr}[P (\mathbb{1}_F \otimes \Omega_\phi)], \]  

(A4)

\(^1\) We assume \( \{ |\psi_{\phi,i}\rangle \} \) is continuously differentiable with respect to \( \phi \).

\(^2\) We also assume \( \{ |N_{\phi,i}\rangle \} \) is continuously differentiable with respect to \( \phi \).
having defined the performance operator $\Omega_\phi := 4 \left( \hat{N}_\phi \hat{N}_\phi^\dagger \right)^T = 4 \sum_{i=1}^r \left( \left| \hat{N}_{\phi,i} \right| \right)^T$, where the superscript $T$ denotes the transpose. We can further define an $r \times r$ Hermitian matrix $h := i \hat{V}_\phi V_\phi^\dagger$ to take care of the freedom of choice for the decomposition $\hat{N}_\phi$, by noting that $\hat{N}_\phi \hat{N}_\phi^\dagger = \left( \hat{N}_\phi - iN_\phi \right) \left( \hat{N}_\phi - iN_\phi \right)^\dagger$. Now by redefining $\hat{N}_\phi := \left( \hat{N}_\phi - iN_\phi h \right)$, we rewrite $\Omega_\phi$ as $\Omega_\phi(h)$ to explicitly manifest its dependence on $h$. Hence, we finally arrive at Eq. (6) of the main text:

$$
J^{(p)}(N_\phi) = \max_{P \in \mathcal{P}} \min_{h \in \mathcal{H}_r} \text{Tr} \left( P \left[ \mathbb{1}_F \otimes \Omega_\phi(h) \right] \right)
$$

where $\mathcal{P} := \{ \hat{P} = \text{Tr}_F P | P \in \mathcal{P} \}$.

**Appendix B: Proof of Theorem 1**

Starting from Eq. (6) of the main text, we exchange the order of minimization and maximization thanks to Fan’s minimax theorem [39], since $\text{Tr} \left[ \hat{P} \Omega_\phi(h) \right]$ is concave on $\hat{P}$ and convex on $h$, and $\hat{P}$ is assumed to be a compact set. Then the problem of QFI evaluation can be rewritten as

$$
J^{(p)}(N_\phi) = \min_h \max_{\hat{P} \in \hat{P}} \text{Tr} \left[ \hat{P} \Omega_\phi(h) \right].
$$

Reformulating the condition of Theorem 1, we require that each operator $\hat{P} \in \hat{P}$ can be written as a convex combination of positive semidefinite operators $S^i$, $i = 1, \ldots, K$:

$$
\hat{P} = \sum_{i=1}^K q^i S^i, \quad \text{for} \quad \sum_{i=1}^K q^i = 1, \quad q^i \geq 0, \quad S^i \geq 0, \quad S^i \in \mathcal{S}^i, \quad i = 1, \ldots, K,
$$

where each $\mathcal{S}^i$ is an affine space of Hermitian operators. Thus Eq. (B1) can be reformulated as

$$
J^{(p)}(N_\phi) = \min_h \max_{\hat{P}} \text{Tr} \left[ \hat{P} \Omega_\phi(h) \right],
$$

s.t. \quad $\hat{P} = \sum_{i=1}^K q^i S^i$,

$$
\sum_{i=1}^K q^i = 1,
$$

$q^i \geq 0, \quad S^i \geq 0, \quad S^i \in \mathcal{S}^i, \quad i = 1, \ldots, K$.

For now we fix $h$ and consider the dual problem of maximization over $\hat{P}$. For each affine space $\mathcal{S}^i$ we have defined its dual affine space $\overline{\mathcal{S}}^i$, whose dual affine space in turn is exactly $\mathcal{S}^i$ [43]. Choose an affine basis $\{ Q^{i,j} \}$ for $\overline{\mathcal{S}}^i$ and the maximization problem is further expressed as

$$
\max_{\hat{P}} \text{Tr} \left[ \hat{P} \Omega_\phi(h) \right],
$$

s.t. \quad $\hat{P} = \sum_{i=1}^K q^i S^i$,

$$
\sum_{i=1}^K q^i = 1,
$$

$q^i \geq 0, \quad S^i \geq 0, \quad \text{Tr} \left( S^i Q^{i,j} \right) = 1, \quad i = 1, \ldots, K, \quad j = 1, \ldots, L_i.$
Defining \( P^i := q^i S^i \) to avoid the product of variables in optimization, we have

\[
\max \operatorname{Tr} \left[ \hat{P} \Omega_{\phi}(h) \right], \\
\text{s.t. } \hat{P} = \sum_{i=1}^{K} P^i, \\
\sum_{i=1}^{K} q^i = 1, \\
P^i \geq 0, \quad \operatorname{Tr} \left( P^i Q^{i,j} \right) = q^i, \quad i = 1, \ldots, K, \quad j = 1, \ldots, L_i,
\]

where the constraints \( q^i \geq 0 \) can be safely removed, since \( \operatorname{Tr} S^i = \prod_{j=1}^{N} d_{2j} \), implying that \( S^i \) includes a positive operator proportional to identity for any \( i = 1, \ldots, K \), having denoted \( d_j := \dim(\mathcal{H}_j) \) for simplicity. The Lagrangian of the problem is given by

\[
L = \sum_{i} \operatorname{Tr} \left[ P^i \Omega_{\phi}(h) \right] + \left( 1 - \sum_{i} q^i \right) \lambda + \sum_{i,j} \operatorname{Tr} \left( P^i \hat{Q}^{i,j} \right) + \sum_{i,j} q^i \left( \sum_{j} \lambda^{i,j} Q^{i,j} \right) - \lambda \sum_{i,j} \hat{Q}^{i,j} + \sum_{i,j} q^i \left( \sum_{j} \lambda^{i,j} Q^{i,j} \right),
\]

for \( \hat{Q}^{i,j} \geq 0 \). Hence, by removing \( \hat{Q}^{i,j} \) the dual problem is written as

\[
\min \lambda, \\
\text{s.t. } \sum_{j} \lambda^{i,j} Q^{i,j} \geq \Omega_{\phi}(h), \quad \lambda = \sum_{j} \lambda^{i,j}, \quad i = 1, \ldots, K, \quad j = 1, \ldots, L_i.
\]

We define \( Q^i := \sum_{j} \lambda^{i,j} Q^{i,j} / \lambda \) if \( \lambda \neq 0 \) (\( \lambda = 0 \) corresponds to a trivial case where the QFI is zero), and clearly \( Q^i \) is an arbitrary operator in the set \( \mathcal{S}^i \). Therefore, we cast the dual problem into

\[
\min \lambda, \\
\text{s.t. } \lambda Q^i \geq \Omega_{\phi}(h), \quad Q^i \in \mathcal{S}^i, \quad i = 1, \ldots, K.
\]

Slater’s theorem \cite{slater1974} implies that the strong duality holds, since the QFI is finite and the inequality constraints can be strictly satisfied for a positive semidefinite operator \( \Omega_{\phi}(h) \), by choosing \( \lambda Q^i = \mu \| \Omega_{\phi}(h) \| \mathbb{I}_{1,2,\ldots,2N} \) for \( \mu > 1 \) and any \( i = 1, \ldots, K \), having denoted the operator norm by \( \| \cdot \| \). Finally, by optimizing the choice of \( h \) we derive the result of Theorem \cite{main_text}.

**Appendix C: Proof of the validity of Algorithm** \cite{algorithm}

We first recall the minimax theorem:

\[
\min_{x} \max_{y} f(x, y) = \max_{y} \min_{x} f(x, y)
\]

for a function \( f(x, y) \) convex on \( x \) and concave on \( y \). Assume \((x_0, y_0)\) is a solution for the L.H.S. of Eq. \( \text{(C1)} \) and \((x_1, y_0)\) is a solution for the R.H.S. of Eq. \( \text{(C1)} \). It is easy to see that

\[
f(x_0, y_1) \geq f(x_0, y_0) \geq f(x_1, y_0). \tag{C2}
\]

In view of Eq. \( \text{(C1)} \) both equalities hold. Therefore, \((x_0, y_0)\) is a saddle point of \( f(x, y) \), i.e., \( x_0 = \arg\min_{x} f(x, y_0) \) and \( y_0 = \arg\max_{y} f(x_0, y) \). Since the objective function \( \operatorname{Tr} \left[ \hat{P} \Omega_{\phi}(h) \right] \) in the primal problem of estimating QFI is convex on \( h \) and concave on \( \hat{P} \), we can substitute \( x = h \) and \( y = \hat{P} \). Obviously, \( h^{(\text{opt})} \) is an optimal solution for \( \min_{h} \max_{P} \operatorname{Tr} \left[ \hat{P} \Omega_{\phi}(h) \right] \) and thus corresponds to a saddle point. Then \( x_0 = \arg\min_{x} f(x, y_0) \) can be satisfied by requiring \( \partial_{h} f \left( h, \hat{P}^{(\text{opt})} \right) \big|_{h=h^{(\text{opt})}} = 0 \), resulting in Eq. \( \text{(H1)} \) in the main text:

\[
\text{Re} \left\{ \operatorname{Tr} \left[ \hat{P}^{(\text{opt})} \left[ -i \mathcal{N}_{\phi} \left( \hat{N} - i \mathcal{N}_{\phi} h^{(\text{opt})} \right) \right]^T \right] \right\} = 0 \text{ for all } \mathcal{H} \in \mathbb{H}_{r}. \tag{C3}
\]
Meanwhile $y_0 = \arg\max_y f(x_0, y)$ corresponds to the optimal solution for $h = (h^{(\text{opt})})$. Therefore, $(h^{(\text{opt})}, \tilde{P}^{(\text{opt})})$ is a saddle point and an optimal solution for $\max_{\tilde{P}} \min_h \text{Tr} \left[ \tilde{P} \Omega_\phi(h) \right]$. By definition a purification of $\tilde{P}^{(\text{opt})}$ is an optimal physically implemented strategy, i.e., we can choose a strategy $\tilde{P}^{(\text{opt})}$ such that $\text{Tr}_F \tilde{P}^{(\text{opt})} = \tilde{P}^{(\text{opt})}$. \hfill \Box

We remark that Eq. (C.3) can be reformulated as a set of linear constraints by choosing a basis $\{\mathcal{H}^i\}_{i=1}^r$ for the space $\mathbb{H}_r$ of Hermitian matrices. For example, denoting by $E_{ij}$ the $r \times r$ matrix of which only the $(i,j)$-th element is 1 and all other elements are 0, we can choose $\mathcal{H} = E_{ij}$ for $j = 1, \ldots, r$, $\mathcal{H} = E_{jk} + E_{kj}$ and $\mathcal{H} = i(E_{jk} - E_{kj})$ for $k = 1, \ldots, r$ and $k \neq j$, and obtain a series of constraints, which are equivalent to Eq. (C.3).

### Appendix D: Symmetry reduced optimization

This section demonstrates how to reduce the size of the optimization problems concerned in Theorem 1 and Algorithm 1 by exploiting the permutation symmetry as applicable.

Let us begin with some notations. We consider the action of $S_N$, the symmetric group of degree $N$, on the finite-dimensional representation space $\otimes_{i=1}^N W_i$. $\mathcal{G}$ is a unitary (and orthogonal) operator on $\otimes_{i=1}^N W_i$ corresponding to the permutation $\pi \in S_N$: $\mathcal{G}_\pi = \sum_{i=\{i_1, \ldots, i_N\}} (\otimes_{j=1}^N |\pi(j)\rangle \langle \pi(j)|) \otimes_{k=1}^N |i_k\rangle$, where $|i_j\rangle$ denotes an orthonormal basis of $W_j$. Then an operator $X$ on $\otimes_{i=1}^N W_i$ is said to be permutation-invariant iff $\mathcal{G}_\pi X \mathcal{G}_\pi^\dagger = X$ for all $\pi \in S_N$. Analogously, a space $\mathcal{X}$ is permutation-invariant iff $\mathcal{G}_\pi X_{\mathcal{G}_\pi} \in \mathcal{X}$ for any $X \in \mathcal{X}$ and any $\pi \in S_N$.

We now explicitly express the components of the performance operator $\Omega_\phi(h)$. Given $N$ identical quantum channels $E_\phi(\rho) = \sum_i K_\phi^{i} \rho K_\phi^{i \dagger}$, we decompose the CJ operator $E_\phi = \sum_i |E_\phi,i\rangle \langle E_\phi,i|$ corresponding to each channel. Note that $|E_\phi,i\rangle$ is the vectorization of the Kraus operator $K_\phi$, i.e., $|E_\phi,i\rangle = \sum_{m,n} \langle m|K_\phi|n\rangle |m\rangle |n\rangle$. The CJ operator of $N$ identical quantum channels is $N_\phi = E_\phi \otimes^N = \sum_i |N_\phi,i\rangle \langle N_\phi,i|$, where we use the notation $|N_\phi,i\rangle = \bigotimes_{n=1}^N |E_\phi,i_n\rangle$. Taking the derivative results in (we omit the subscript $\phi$ in $|E_\phi,i\rangle$) $\dot{N}_\phi,i = \sum_{j=1}^N |E_{i,j}\rangle \langle E_{i,j}| E_{i,j+1} \langle E_{i,j+1}| E_{i,j+1} \langle E_{i,j+1}| \cdots |E_{i,N}\rangle$, from which we can obtain the performance operator $\Omega_\phi(h) = 4 \left( \dot{N}_\phi \dot{N}_\phi^\dagger \right)^T = 4 \sum_i \left( \dot{N}_\phi,i \dot{N}_\phi,i^\dagger \right)^T$, where $\dot{N}_\phi,i = \dot{N}_\phi - i \sum_k |N_\phi,k\rangle h_{kj}$.

1. **Symmetry reduced QFI evaluation**

With these notations, we first consider the optimization in QFI evaluation and have the following:

**Lemma 1.** In the optimization problem of Theorem 1, if, for any $\pi \in S_N$ and any $i$, there exists a $j$ such that the mapping $S \rightarrow G_{\pi} S G_{\pi}^\dagger$ on $S^i$ is a bijective function from $S^i$ to $S^j$, then there must exist a permutation-invariant $h$ as a feasible solution.

**Proof.** Without loss of generality we assume all $S^i$ are distinct spaces; otherwise, we just remove the duplicate ones. We first prove that, under any permutation operation $\mathcal{Q} \rightarrow G_{\pi} \mathcal{Q} G_{\pi}^\dagger$, for any $i \in \{1, \ldots, K\}$ there exists a unique $j \in \{1, \ldots, K\}$ such that the dual affine space $\overline{S^i}$ is isomorphically mapped to $\overline{S^j}$. The condition of the lemma implies that, for any $G_{\pi}$ and any $i$ we can find $j_i$ such that $G_{\pi} S_j G_{\pi}^\dagger \in \overline{S^j}$ for all $S^j \in S^i$. Due to the bijectivity, $S^i$ and the corresponding $\overline{S^j}$ are isomorphic, with different $j_i$ for different $i$. Apparently $\overline{S^i}$ and $\overline{S^j}$ are also isomorphic. If we choose any $Q^{j_i} \in \overline{S^j}$, i.e., $\text{Tr} \left( Q^{j_i} S^{j_i} \right) = 1$ for all $S^{j_i} \in S^{j_i}$, then we have $\text{Tr} \left( G_{\pi}^\dagger Q^{j_i} G_{\pi} S^{j_i} \right) = \text{Tr} \left( Q^{j_i} G_{\pi} S^{j_i} G_{\pi}^\dagger \right) = 1$ for all $S^{j_i} \in \overline{S^j}$. Therefore, $G_{\pi}^\dagger Q^{j_i} G_{\pi} \in \overline{S^j}$ for all $Q^{j_i} \in \overline{S^j}$. Furthermore, the permutation operation $\mathcal{Q} \rightarrow G_{\pi} \mathcal{Q} G_{\pi}$ from $\overline{S^j}$ to $\overline{S^i}$ is bijective as $\overline{S^j}$ and $\overline{S^i}$ are isomorphic. In particular, any set of $K$ operators $\{Q^i\}_{i=1}^K$ for $Q^i \in \overline{S^i}$ is mapped to a set $\{Q^i\}_{i=1}^K$ such that $Q^i \in \overline{S^j}$.

We then prove that there exists a permutation-invariant performance operator $\Omega_\phi(h)$ as a feasible solution. The group action is characterized by the permutation operator $G_{\pi}$ on the representation space $\otimes_i W_i = \otimes_i (\mathcal{H}_{2\lambda-1} \otimes \mathcal{H}_{2\lambda})$. Suppose $h^{(\text{opt})}$ is an optimal solution, i.e., for any $i \in \{1, \ldots, K\}$, there exist optimal values of $\lambda$ and $Q^j$ such that $\lambda Q^j \geq \Omega_\phi \left( h^{(\text{opt})} \right)$ for $Q^j \in \overline{S^j}$. Then for any permutation $\pi \in S_N$ we have

$$\lambda G_{\pi} Q^j G_{\pi}^\dagger \geq G_{\pi} \Omega_\phi \left( h^{(\text{opt})} \right) G_{\pi}^\dagger, \quad Q^j \in \overline{S^j}, \quad i = 1, \ldots, K.$$  

(D1)
Since $G_\pi$ maps $\{Q^i\}_i$ to a set $\{\tilde{Q}^i\}_i$ such that $\tilde{Q}^i \in \mathbb{S}^i$, the constraint Eq. (D1) becomes

$$\lambda \tilde{Q}^i \geq G_\pi \Omega_\phi \left(h^{(\text{opt})}\right) G_\pi^\dagger, \quad \tilde{Q}^i \in \mathbb{S}^i, \quad i = 1, \ldots, K,$$

(D2)

which implies that $G_\pi \Omega_\phi(h^{(\text{opt})}) G_\pi^\dagger$ is also a feasible solution for any $\pi$. Furthermore, the permutation-invariant solution of the performance operator $\frac{1}{N!} \sum_{\pi \in S_N} G_\pi \Omega_\phi(h^{(\text{opt})}) G_\pi^\dagger$ is feasible.

Next, we show that we can choose a permutation-invariant $h$ such that the performance operator $\Omega_\phi(h) = \frac{1}{N!} \sum_{\pi \in S_N} G_\pi \Omega_\phi \left(h^{(\text{opt})}\right) G_\pi^\dagger$ is an operator on $\otimes_{i=1}^N \mathbb{C}^s$, where $s := \max_\phi \text{rank}(E_\phi) \leq d$. For distinction we denote the group action on $h$ by $G_\pi^\dagger h G_\pi^\dagger$ and the group action on $\Omega_\phi(h)$ by $G_\pi \Omega_\phi(h) G_\pi^\dagger$. Writing $h$ in components, we have

$$\sum_{i,j} G_\pi^\dagger h_{ij} \mathbf{1}_j G_\pi = \sum_{i,j} h_{ij} |\pi(i)\rangle \langle \pi(j)| = \sum_{\pi^{-1}(i), \pi^{-1}(j)} h_{\pi^{-1}(i)\pi^{-1}(j)} |\pi(i)\rangle \langle \pi(j)| = \sum_{i,j} h_{\pi^{-1}(i)\pi^{-1}(j)} |\pi(i)\rangle \langle \pi(j)|,$$

(D3)

where $\pi(i) := (i_{\pi(1)}, \ldots, i_{\pi(N)})$. Note that $G_\pi |N_{\phi,i}\rangle = |N_{\phi,\pi(i)}\rangle$ and

$$G_\pi |\tilde{N}_{\phi,i}\rangle = \sum_{j=1}^N |E_{i_1}\rangle \cdots |E_{i_{j-1}}\rangle |\tilde{E}_{i_j}\rangle |E_{i_{j+1}}\rangle \cdots |E_{i_N}\rangle = \sum_{j=1}^N |E_{i_{\pi(1)}}\rangle \cdots |E_{i_{\pi^{-1}(j-1)}}\rangle |\tilde{E}_{i_j}\rangle |E_{i_{\pi^{-1}(j+1)}}\rangle \cdots |E_{i_{\pi(N)}}\rangle = \sum_{j=1}^N |E_{i_{\pi(1)}}\rangle \cdots |E_{i_{\pi(j-1)}}\rangle |\tilde{E}_{i_j}\rangle |E_{i_{\pi(j+1)}}\rangle \cdots |E_{i_{\pi(N)}}\rangle = |\tilde{N}_{\phi,\pi(i)}\rangle,$$

(D4)

which results in

$$G_\pi \Omega_\phi(h) G_\pi^\dagger = 4 \sum_j G_\pi \left(|\tilde{N}_{\phi,j}\rangle \langle \tilde{N}_{\phi,j}|\right) G_\pi^\dagger = 4 \sum_j G_\pi \left(|\tilde{N}_{\phi,j}\rangle \langle \tilde{N}_{\phi,j}|\right) G_\pi^\dagger = 4 \sum_j G_\pi \left(|\tilde{N}_{\phi,j}\rangle + i \sum_k |N_{\phi,k}\rangle h_{kj}^*\right) \left(|\tilde{N}_{\phi,j}\rangle - i \sum_l h_{lj} |N_{\phi,l}\rangle\right) G_\pi^\dagger = 4 \sum_j \left(|\tilde{N}_{\phi,\pi(j)}\rangle + i \sum_k |N_{\phi,\pi(k)}\rangle h_{kj}^*\right) \left(|\tilde{N}_{\phi,\pi(j)}\rangle - i \sum_l h_{lj} |N_{\phi,\pi(l)}\rangle\right) = 4 \sum_j \left(|\tilde{N}_{\phi,\pi(j)}\rangle + i \sum_k |N_{\phi,k}\rangle h_{\pi^{-1}(\pi(j))} \right) \left(|\tilde{N}_{\phi,\pi(j)}\rangle - i \sum_l h_{\pi^{-1}(\pi(j)) l} |N_{\phi,l}\rangle\right) = \Omega_\phi \left(G_\pi^\dagger h G_\pi^\dagger\right),$$

(D5)

where in the last equation we have used Eq. (D2). Therefore, by choosing the permutation-invariant solution $h = \frac{1}{N!} \sum_{\pi \in S_N} G_\pi \Omega_\phi \left(h^{(\text{opt})}\right) G_\pi^\dagger$ we obtain $\Omega_\phi(h) = \frac{1}{N!} \sum_{\pi \in S_N} G_\pi \Omega_\phi \left(h^{(\text{opt})}\right) G_\pi^\dagger$, and this permutation-invariant choice of $h$ is also a feasible solution.

If a stronger condition holds, then not only can we choose a permutation-invariant $h$, but we can also restrict $Q^i \in \mathbb{S}^i$ to be permutation-invariant. In this case all matrix variables concerned in the optimization are permutation-invariant.

**Lemma 2.** In the optimization problem of Theorem 1 if each affine space $S^i$ is permutation-invariant for any $i = 1, \ldots, K$, then there must exist a permutation-invariant $Q^i \in \mathbb{S}^i$ as a feasible solution for each $i$. 


Proof. By Lemma 1 we can restrict $h$ to be permutation-invariant in optimization, and therefore the performance operator $\Omega_\phi(h)$ is permutation-invariant. It is easy to see that each dual affine space $S^i$ is also permutation-invariant. Then for any $i = 1, \ldots, K$, for $Q^{i, (\text{opt})} \in S^i$ satisfying the constraint $\lambda Q^i \geq \Omega_\phi(h)$, we have the permutation-invariant solution $Q^i = \frac{1}{N} \sum_{\pi \in S_N} G^\dagger_\pi Q^{i, (\text{opt})} G^\dagger_\pi \in S^i$ which also satisfies the same constraint. Hence, this permutation-invariant choice of $Q^i$ is also a feasible solution.

Now since the optimization is restricted to the invariant subspace, we can reduce the matrix sizes by block diagonalization. Generally, for a group-invariant space of complex matrices $\mathbb{C}^{n \times n}_{\text{inv}}$, there exists an isomorphism preserving positive semidefiniteness between $\mathbb{C}^{n \times n}_{\text{inv}}$ and a direct sum of complex matrix spaces $\mathbb{C}^{n \times n}_{\text{inv}}$ [53 Theorem 9.1]:

$$\varphi : \mathbb{C}^{n \times n}_{\text{inv}} \rightarrow \bigoplus_{k=1}^{f} \mathbb{C}^{m_k \times m_k},$$

where $m_k$ is the multiplicity of the $k$-th inequivalent irreducible representation of the group, and $I$ is the number of inequivalent irreducible representations. To be more specific, for the symmetric group $S_N$, the representation space $W = (\mathbb{C}^{d^2})^N$ can be decomposed into $\bigoplus_{|\mu| = N} W^\mu$, where each partition $\mu := (\mu_1, \ldots, \mu_d)$ (with nonnegative integers $\mu_i \geq \mu_j$ for any $i < j$) corresponds to a Young diagram, and $|\mu| := \sum \mu_i$. Each isotypic component $W^\mu$ can be further decomposed into a direct sum of equivalent irreducible subspaces: $W^\mu = \bigoplus_{i=1}^{m_\mu} W^\mu_i$. We define the dimension of the irreducible representation $d_\mu := \dim(W^\mu_i)$. It is worth mentioning that the first decomposition into isotypic components is unique while the second decomposition into equivalent irreducible representations is not (see, e.g., [53]). In terms of the unitary group action $G_\pi$ on $W$, there exists a unitary transformation of basis $U$ such that for any $\pi$ we have

$$U^\dagger G_\pi U = \bigoplus_{|\mu| = N} G^\mu_\pi \otimes 1(m_\mu),$$

where $G^\mu_\pi$ is a unitary operator on the irreducible representation space associated with the Young diagram label $\mu$, $m_\mu$ is the corresponding multiplicity, and $1(m_\mu)$ is an $m_\mu \times m_\mu$ identity matrix acting on the multiplicity subspace. By Schur’s lemma, for any group-invariant operator $X$ on $W$, i.e., $X$ commuting with all $G_\pi$, we have

$$U^\dagger XU = \bigoplus_{|\mu| = N} 1(d_\mu) \otimes X^\mu,$$

for any $\pi$, where $X^\mu$ is an $m_\mu \times m_\mu$ matrix. With such block diagonalization of the permutation-invariant operator, we reduce the dimension from $d^2 N$ to [60 Eq. (57)]

$$\sum_{|\mu| = N} m_\mu^2 = \left( \frac{N + d^2 - 1}{d^2 - 1} \right) \leq (N + 1)^{d^2 - 1},$$

where the upper bound is obtained straightforwardly from the definition of the binomial coefficient. Specifically, if $X$ is further restricted to be a Hermitian matrix variable, then the number of real scalar variables contained in all elements of $X$ is reduced from $d^2 N$ to $\left( \frac{N + d^2 - 1}{d^2 - 1} \right)$.

Now let us turn to the optimization problem of QFI evaluation. If the Hermitian matrix $h$ is taken to be permutation-invariant by Lemma [1], the number of variables concerned in $h$ is reduced from $s^2 N$ to $\left( \frac{N + s^2 - 1}{s^2 - 1} \right)$. Similarly, if further by Lemma [2] each Hermitian matrix $Q^i$ is permutation-invariant, the number of variables in $Q^i$ is also reduced from $d^2 N$ to $\left( \frac{N + d^2 - 1}{d^2 - 1} \right)$, where we redefine $d := \dim(H_1)\dim(H_2)$. By this reduction the complexity gets polynomial rather than exponential, with respect to $N$.

We can then reformulate the optimization in Theorem 1 with the reduced form. We consider two cases relevant to the strategy sets mentioned in the main text. First, under certain circumstances we can reduce the number of constraints in optimization as follows:

**Theorem 2** (Symmetry reduced Theorem 1 first case). If, for any $\pi \in S_N$ and any $i$, there exists a $j$ such that the mapping $S \rightarrow G_\pi SG^j_\phi$ on $S^i$ is a bijective function from $S^i$ to $S^j$, and meanwhile for any $i, j$ there exists some permutation operation such that $S^i$ is bijectively mapped to $S^j$, then the QFI of $N$ quantum channels $E_\phi$ can be expressed as:

$$J^{(P)}(N_\phi) = \min_{\lambda, Q^{i, (\text{opt})}} \lambda,$$

s.t. $\lambda Q^i \geq \Omega_\phi(h)$, $Q^i \in S^i$, (D10)
where \( h = U^\dagger \left( \bigoplus_{|\mu|=N} \mathbb{1}(d_\mu) \otimes h^\mu \right) U \) with each \( h^\mu \) as an \( m_\mu' \times m_\mu' \) matrix variable and \( U^\dagger \) as a unitary transformation of basis.

Proof. We first prove that, for any \( i, j \) there exists some permutation operation \( Q \mapsto G_\pi Q G_\pi^\dagger \) such that \( \mathcal{S}^j \) is bijectively mapped to \( \mathcal{S}^j \). Given any \( i \) and \( j \), if we choose an arbitrary \( Q^j \in \mathcal{S}^j \), i.e., \( \text{Tr}(Q^j S^i) = 1 \) for all \( S^i \in \mathcal{S}^j \), then the condition of the theorem implies that there exists \( G_\pi \) such that \( G_\pi S^i G_\pi^\dagger \in \mathcal{S}^j \). As the map is bijective, in fact \( G_\pi S^i G_\pi^\dagger G_\pi \in \mathcal{S}^j \) for all \( S^i \in \mathcal{S}^j \). Therefore, following the same argument in the proof of Lemma 1 under \( Q \mapsto G_\pi Q G_\pi^\dagger \), \( \mathcal{S}^j \) is bijectively mapped to \( \mathcal{S}^j \).

By Lemma 1, we can take \( h \) to be permutation-invariant and apply the block diagonalization to \( h \) given by Eq. (D8). Then for any \( Q^j \in \mathcal{S}^j \) satisfying the constraint \( \lambda Q^j \geq \Omega_\phi(h) \), there exists \( G_\pi \) such that \( Q^j \in \mathcal{S}^j \) satisfying \( \lambda Q^j \geq \Omega_\phi(h) \) for any \( i = 2, \ldots, K \). Therefore, all the constraints except for \( \lambda Q^j \geq \Omega_\phi(h) \) are redundant and can be removed.

Now we consider the second case. If by Lemmas 1 and 2 \( h \) and each \( Q^j \) are permutation-invariant, we can then reformulate the constraints in optimization with reduced matrix dimensions. To relate the group representation on \( \bigoplus_1 (\mathcal{H}_{2i-1} \otimes \mathcal{H}_{2i}) \) to the representation on \( (C^*)^\otimes N \), we choose a unitary transformation of basis \( U^\dagger \) for \( h \), decompose \( h = U^\dagger \left[ \bigoplus_{|\mu|=N} \mathbb{1}(d_\mu) \otimes h^\mu \right] U \) with \( h^\mu \) as an \( m_\mu' \times m_\mu' \) matrix, and divide \( U^\dagger = \left( U^{\mu_1,1}, \ldots, U^{\mu_I,1} \right) \) into blocks, where \( \mu^i \) is the label of the \( i \)-th Young diagram, and \( U^{\mu_i} \) has \( d_\mu, m_\mu' \), columns. Thus by defining the matrix

\[
\tilde{\mathcal{N}}^\mu_\phi = \mathcal{N}_\phi U^{\mu} - i \mathcal{N}_\phi U^{\mu} \left[ \mathbb{1}(d_\mu) \otimes h^\mu \right],
\]

we have the permutation-invariant performance operator

\[
\Omega_\phi(h) = 4 \sum_{|\mu|=N} \left( \tilde{\mathcal{N}}^\mu_\phi \tilde{\mathcal{N}}^\mu_\phi^* \right)^T = 4 \sum_{|\mu|=N} \tilde{\mathcal{N}}^\mu_\phi \tilde{\mathcal{N}}^\mu_\phi^*. \tag{D12}
\]

Analogously, we apply the block diagonalization using a change of basis \( U \) to

\[
Q^j = U \left[ \bigoplus_{|\mu|=N} \mathbb{1}(d_\mu) \otimes Q^{i,\mu} \right] U^\dagger \in \mathcal{S}^j, \tag{D13}
\]

where \( Q^{i,\mu} \) is an \( m_\mu \times m_\mu \) matrix variable. The unitary transformation \( U = \left( U^{\mu_1,1}, \ldots, U^{\mu_I,1} \right) \) is first divided into blocks, and then each \( U^{\mu_i} = \left( U^{\mu_i,1}, \ldots, U^{\mu_i,d_\mu} \right) \) is divided into blocks for \( i = 1, \ldots, I \), where \( \mu^i \) is the label of the \( i \)-th Young diagram, and \( U^{\mu_i,j} \) has \( m_\mu \), columns for \( j = 1, \ldots, d_\mu \). Note that \( U \) also gives the block diagonalization of \( \Omega_\phi(h) \).

Before proceeding further we prove that the range of \( \tilde{\mathcal{N}}^\mu_\phi^* \) is exactly contained in the irreducible representation space corresponding to \( \mu \):

**Lemma 3.** If we decompose the representation space \( \mathcal{W} = \bigotimes_{i=1}^N (\mathcal{H}_{2i-1} \otimes \mathcal{H}_{2i}) \) by \( \bigoplus_{|\mu|=N} \mathcal{W}^\mu \), then \( \text{Range} \left( \tilde{\mathcal{N}}^\mu_\phi^* \right) \subseteq \mathcal{W}^\mu \) for any Young diagram label \( \mu \).

Proof. To characterize the representation space \( \mathcal{W}^\mu \) we introduce the key notion of Young symmetrizer as well as other related concepts very briefly (see, e.g., [59] for mathematical details). A Young tableau is a filling into the boxes of the Young diagram with positive integers weakly increasing along each row and strictly increasing along each column. For a standard Young tableau labeled by \( \nu \), i.e., a Young tableau filled with the entries \( 1, \ldots, N \), we define two permutation subgroups

\[
P_\nu := \{ \sigma \in S_N | \text{\sigma preserves each row} \} \tag{D14}
\]

and

\[
Q_\nu := \{ \sigma \in S_N | \text{\sigma preserves each column} \}. \tag{D15}
\]

In the group algebra \( \mathbb{C}S_N \) we define two elements \( a_\nu := \sum_{\sigma \in P_\nu} e_\sigma \) and \( b_\nu := \sum_{\sigma \in Q_\nu} \text{sgn}(\sigma) e_\sigma \), where \( e_\sigma \) is the unit vector corresponding to \( \sigma \) and \( \text{sgn}(\cdot) \) denotes the parity of the permutation. Then the Young symmetrizer is defined by

\[
c_\nu := a_\nu b_\nu = \sum_{\sigma \in P_\nu} \sum_{\pi \in Q_\nu} \text{sgn}(\pi) e_{\sigma \pi} \in \mathbb{C}S_N. \tag{D16}
\]
It is known that a Young diagram of $\mu$ corresponds to $d_{\mu}$ standard Young tableaux, with each Young tableau of $\nu$ characterizing an irreducible representation space, given by the image of $c_\nu$ on $\otimes_i \mathcal{W}_i$ under the natural group algebra representation $CS_N \to \text{End}(\otimes_i \mathcal{W}_i)$, where $\text{End}(V)$ denotes the set of endomorphisms on $V$.

With these notions we now have an explicit characterization of the representation space. Note that we can prove $\text{Range} \left( \hat{N}^\mu_\phi \right) \subseteq \mathcal{W}^\mu$ if $\text{Range} \left( \hat{N}^\mu_\phi U^{i,\mu^*} \right) \subseteq \mathcal{W}^\mu$ and $\text{Range} \left( \hat{N}^\mu_\phi U^{i,\mu^*} \right) \subseteq \mathcal{W}^\mu$. In the proof of Lemma 1 we have seen $G_{\pi} \left( \hat{N}_\phi i \right) = \left| \hat{N}_{\phi, \pi(i)} \right|$ and $G_{\pi} \left( \hat{N}_\phi d \right) = \left| N_{\phi, \pi(i)} \right|$, from which it follows that

$$G_{\pi} \hat{N}_\phi = \hat{N}_\phi G'_{\pi} \quad \text{(D17)}$$

and $G_{\pi} N_\phi = N_\phi G'_{\pi}$.

Now we prove that $\text{Range} \left( \hat{N}^\mu_\phi U^{i,\mu^*} \right) \subseteq \mathcal{W}^\mu$. From the discussions above we know that

$$\text{Range} \left( U^{i,\mu^*} \right) = \bigoplus_{\phi} c_\nu \left[ \otimes_i \mathbb{C}^n \right], \quad \text{(D18)}$$

for all Young tableau labels $\nu$ corresponding to the Young diagram of $\mu$. Explicitly, we have

$$c_\nu \left[ \otimes_i \mathbb{C}^n \right] = \text{Range} \left[ \sum_{\sigma \in \mathcal{P}_\nu} \sum_{\pi \in Q_\nu} \text{sgn}(\pi) G'_{\sigma \pi} \right]. \quad \text{(D19)}$$

Note that there always exists a unitary transformation of basis $V$ such that we can obtain a real matrix $U^{i,\mu}_{(\text{real})} = U^{i,\mu} V^d$, which leads to

$$\text{Range} \left( U^{i,\mu^*} \right) = \text{Range} \left( U^{i,\mu^*}_{(\text{real})} V^* \right) = \text{Range} \left( U^{i,\mu}_{(\text{real})} V^* \right) = \text{Range} \left( U^{i,\mu} \right). \quad \text{(D20)}$$

Thus $\text{Range} \left( \hat{N}^\mu_\phi U^{i,\mu^*} \right) = \text{Range} \left( \hat{N}^\mu_\phi U^{i,\mu} \right)$. Furthermore, from Eqs. (D18) and (D19) we have $\text{Range} \left( \hat{N}^\mu_\phi U^{i,\mu^*} \right) \subseteq \mathcal{W}^\mu$ if

$$\text{Range} \left[ \hat{N}^\mu_\phi \sum_{\sigma \in \mathcal{P}_\nu} \sum_{\pi \in Q_\nu} \text{sgn}(\pi) G'_{\sigma \pi} \right] \subseteq \mathcal{W}^\mu \quad \text{(D21)}$$

for all Young tableau labels $\nu$ corresponding to the Young diagram of $\mu$. To show Eq. (D21), note that by Eq. (D17) we have

$$\text{Range} \left[ \hat{N}^\mu_\phi \sum_{\sigma \in \mathcal{P}_\nu} \sum_{\pi \in Q_\nu} \text{sgn}(\pi) G'_{\sigma \pi} \right] = \text{Range} \left[ \sum_{\sigma \in \mathcal{P}_\nu} \sum_{\pi \in Q_\nu} \text{sgn}(\pi) G_{\sigma \pi} N^\mu_\phi \right]. \quad \text{(D22)}$$

Since the R.H.S. of Eq. (D22) is the image of the Young symmetrizer $c_\nu$ on $\text{Range} \left( \hat{N}^\mu_\phi \right)$, it is a subset of $\mathcal{W}^\mu$. Therefore, $\text{Range} \left( \hat{N}^\mu_\phi U^{i,\mu^*} \right) \subseteq \mathcal{W}^\mu$. In the same way we can also show that $\text{Range} \left( N^\mu_\phi U^{i,\mu^*} \right) \subseteq \mathcal{W}^\mu$ and thus complete the proof.

Therefore, $U^{i}\Omega_\phi(u^1)U$ is block diagonal with each block on the space $\text{Range} \left( \hat{N}^\mu_\phi \right)$. This results in:

**Theorem 3 (Symmetry reduced Theorem 1 second case).** If each affine space $S^i$ is permutation-invariant for any $i = 1, \ldots, K$, then the QFI of $N$ quantum channels $E_\phi$ can be expressed as:

$$J^{(P)}(N_\phi) = \min_{\lambda, Q^{i,\mu^*}, h^i} \lambda,$$

s.t. $\lambda Q^{i,\mu^*} \geq 4 U^{\mu_1} \left( \hat{N}^\mu_\phi \hat{N}^{\mu^*}_\phi \right)^T U^{\mu_1}, \quad i = 1, \ldots, K, \quad |\mu| = N,$

where $Q^{i,\mu^*}$ is given by Eq. (D13).

**Proof.** By Lemmas 1 and 2, $h^i$, $\Omega_\phi(h)$ and all $Q^i$ are taken to be permutation-invariant. The original constraint $\lambda Q^{i^*} \geq \Omega_\phi(h)$ on the permutation-invariant space is reformulated as

$$\lambda \bigoplus_{|\mu|=N} (d_\mu) \otimes Q^{i,\mu^*} \geq \bigoplus_{|\mu|=N} 4 U^{\mu_1} \sum_{|\mu|=N} \hat{N}^{\mu^*}_\phi \hat{N}^{\mu^*+}_\phi U^\mu. \quad \text{(D24)}$$
Since by Lemma 3 \( \text{Range} \left( \hat{N}^{\mu*}_{\phi} \right) \subseteq \mathcal{W}^{\mu} = \text{Range} \left( U^{\mu} \right) \) for any \( \mu \), we have \( U^{\mu}|_{\sum_{|\mu|=N} \hat{N}^{\mu*}_{\phi} \hat{N}^{\mu*}_{\phi}} U^{\mu} = U^{\mu}|_{\hat{N}^{\mu*}_{\phi} \hat{N}^{\mu*}_{\phi}} U^{\mu} \). Then Eq. (D24) can be reformulated as

\[
\lambda I (d_{\mu}) \otimes Q^{i,\mu} \geq 4U^{\mu}|_{\hat{N}^{\mu*}_{\phi} \hat{N}^{\mu*}_{\phi}} U^{\mu}, \quad |\mu| = N.
\]

(D25)

Furthermore, both sides of the inequality in Eq. (D25) are block diagonal with the same repeating blocks and we only need to compare one of the blocks. Without loss of generality, we choose the first block for comparison and obtain

\[
\lambda Q^{i,\mu} \geq 4U^{\mu}|_{\hat{N}^{\mu*}_{\phi} \hat{N}^{\mu*}_{\phi}} U^{\mu},
\]

(D26)

which holds for all \( i = 1, \ldots, K \) and \( |\mu| = N \). \( \square \)

We have not characterized each dual affine space \( \tilde{S}^i \) for \( i = 1, \ldots, K \) yet. If we choose an affine basis \( \{ S^{i,j} \}_{j=1}^{M_i} \) for each \( S^i \), then the constraint \( Q^i \in \tilde{S}^i \) can be reformulated as a set of linear constraints \( \text{Tr}(Q^i S^{i,j}) = 1 \) for all \( j = 1, \ldots, M_i \). If each affine space \( S^i \) is permutation-invariant, then by the proof of Lemma 3 we have, for a feasible solution of \( Q^i \in \tilde{S}^i \), \( G_{\pi} Q^i G_{\pi}^\dagger \) is also a feasible solution for any \( \pi \in S_N \). Then by defining

\[
\tilde{S}^{i,j} := \frac{1}{N!} \sum_{\pi \in S_N} G_{\pi} S^{i,j} G_{\pi}^\dagger,
\]

(D27)

each linear constraint \( \text{Tr}(Q^i S^{i,j}) = 1 \) can be replaced by \( \text{Tr}(Q^i \tilde{S}^{i,j}) = 1 \) without changing the problem. Since \( \tilde{S}^{i,j} \) is permutation-invariant, similar to Eq. (D13) it can be decomposed as

\[
\tilde{S}^{i,j} = U \left[ \bigoplus_{|\mu|=N} I (d_{\mu}) \otimes \tilde{S}^{i,j,\mu} \right] U^\dagger,
\]

(D28)

where \( \tilde{S}^{i,j,\mu} \) is an \( m_j \times m_j \) matrix. Combining Eqs. (D13) and (D28), we can reformulate the constraint \( Q^i \in \tilde{S}^i \) with reduced matrix sizes as

\[
\sum_{|\mu|=N} d_{\mu} \text{Tr}(Q^i,\mu \tilde{S}^{i,j,\mu}) = 1, \quad j = 1, \ldots, M_i.
\]

(D29)

Finally, it remains to be seen how to find the unitary transformation \( U \) and \( U' \) for block diagonalization. Known rigorous numerical algorithms for identifying the transformation are fairly expensive [61]. Fortunately, RepLAB [62], a numerical approach to decomposing representations based on randomized heuristics works very well in practice and is thus adopted here.

2. Symmetry reduced algorithm for optimal strategies

The idea is similar to the symmetry reduced evaluation of QFI. Since the first step of Algorithm 1 is simply solving the optimization problem in Theorem 1, now we only consider its second step, where we need to solve for the optimal value of \( \tilde{P} \) in

\[
\max_{\tilde{P} \in \mathcal{B}} \text{Tr} \left[ \tilde{P} \Pi_{\phi} \left( h^{(\text{opt})} \right) \right],
\]

(D30)

where \( \tilde{P} = \text{Conv} \left\{ \bigcup_{i=1}^K \{ S^i \geq 0 | S^i \in \tilde{S}^i \} \right\} \) and

\[
\text{Re} \left\{ \text{Tr} \left[ \tilde{P} \left[ -i \mathbf{N}_{\phi} \mathcal{H} \left( \hat{N}_{\phi} - i \mathbf{N}_{\phi} h^{(\text{opt})} \right) ^\dagger \right] ^T \right] \right\} = 0 \quad \text{for all } \mathcal{H} \in \mathbb{H}_r.
\]

(D31)

We have the following:

**Lemma 4.** If, for any \( \pi \in S_N \) and any \( i \), there exists a \( j \) such that the mapping \( S \mapsto G_{\pi} S G_{\pi}^\dagger \) on \( S^i \) is a bijective function from \( \tilde{S}^i \) to \( \tilde{S}^j \), then there must exist a permutation-invariant \( \tilde{P} \) as an optimal solution in Algorithm 1.
Proof. By definition \( \tilde{P} \) is permutation-invariant. By Lemma 1 we can choose a permutation-invariant \( h^{(\text{opt})} \) and thus \( \Omega_\phi (h^{(\text{opt})}) \) is also permutation-invariant. If \( \tilde{P}^{(\text{opt})} \) is an optimal solution of \( \tilde{P} \), then \( G_\pi \tilde{P}^{(\text{opt})} G_\pi^\dagger \) for any \( \pi \in S_N \) is also an optimal solution, since

\[
\text{Tr} \left[ G_\pi \tilde{P}^{(\text{opt})} G_\pi^\dagger \Omega_\phi \left( h^{(\text{opt})} \right) \right] = \text{Tr} \left[ \tilde{P}^{(\text{opt})} G_\pi^\dagger \Omega_\phi \left( h^{(\text{opt})} \right) G_\pi \right] = \text{Tr} \left[ \tilde{P}^{(\text{opt})} \Omega_\phi \left( h^{(\text{opt})} \right) \right]
\]

and for all \( \mathcal{H} \in \mathbb{H}_r \)

\[
\text{Re} \left\{ \text{Tr} \left[ G_\pi \tilde{P}^{(\text{opt})} G_\pi^\dagger \left[ -iN_\phi G_\pi^\dagger \mathcal{H} G_\pi \left( N_\phi - iN_\phi h^{(\text{opt})} \right)^\dagger \right]^T \right] \right\} = \text{Re} \left\{ \text{Tr} \left[ \tilde{P}^{(\text{opt})} G_\pi^\dagger \left[ -iN_\phi \mathcal{H} \left( N_\phi - iN_\phi h^{(\text{opt})} \right)^\dagger \right]^T \right] \right\} = 0,
\]

having used \( G_\pi^\dagger N_\phi = N_\phi G_\pi^\dagger \) and \( G_\pi^\dagger N_\phi = N_\phi G_\pi^\dagger \) for any \( \pi \in S_N \) in the second equality of Eq. (D33). Therefore, there exists a permutation-invariant solution \( \tilde{P} = \frac{1}{N^2} \sum_{\pi \in S_N} G_\pi \tilde{P}^{(\text{opt})} G_\pi^\dagger \).

Now by following the same line of arguments as used from Eqs. (D27) to (D29), we define

\[
O := \frac{1}{N^2} \sum_{\pi \in S_N} G_\pi \left[ -iN_\phi \mathcal{H} \left( N_\phi - iN_\phi h^{(\text{opt})} \right)^\dagger \right] G_\pi^\dagger = \left[ -iN_\phi \mathcal{H} \left( N_\phi - iN_\phi h^{(\text{opt})} \right)^\dagger \right] G_\pi^\dagger
\]

having defined the permutation-invariant \( \tilde{\mathcal{H}} := \frac{1}{N^2} \sum_{\pi \in S_N} G_\pi^\dagger \mathcal{H} G_\pi \). Similar to the arguments in Appendix C, by choosing a basis \( \{ \tilde{\mathcal{H}}^i \}_{i=1}^J \) for the permutation-invariant subspace of \( \mathbb{H}_{r \times r} \), where \( J = \binom{N}{2} \), Eq. (C3) can be reformulated as a set of \( J \) linear constraints. We further define

\[
O^i := \left[ -iN_\phi \tilde{\mathcal{H}}^i \left( N_\phi - iN_\phi h^{(\text{opt})} \right)^\dagger \right]^T
\]

for \( i = 1, \ldots, J \). Now we can decompose \( O^i = U \left[ \bigoplus_{|\mu| = N} 1 \left( d_\mu \right) \otimes \tilde{O}^{i,\mu} \right] U^\dagger, \tilde{P} = U \left[ \bigoplus_{|\mu| = N} 1 \left( d_\mu \right) \otimes \tilde{\mu} \right] U^\dagger, \Omega_\phi \left( h^{(\text{opt})} \right) = U \left[ \bigoplus_{|\mu| = N} 1 \left( d_\mu \right) \otimes \Omega_\phi \left( h^{(\text{opt})} \right) \right] U^\dagger \), and then reformulate the optimization problem as the following reduced form:

\[
\max_{\tilde{P}^{\mu}} \sum_{|\mu| = N} d_\mu \text{Tr} \left[ \tilde{P}^{\mu} \Omega_\phi \left( h^{(\text{opt})} \right) \right], \quad \text{s.t.} \quad \sum_{|\mu| = N} d_\mu \text{Re} \left[ \text{Tr} \left( \tilde{P}^{\mu} O^i \right) \right] = 0 \text{ for all } i = 1, \ldots, J.
\]

Recall that \( \tilde{P} = \sum_{i=1}^K q^i S^i \) for \( S^i \in S^i \). By choosing an affine basis \( \{ Q^{i,j} \}_{j=1}^{L_i} \) for \( S^i \) we can also characterize \( S^i \in S^i \) by a set of linear constraints \( \text{Tr} \left( S^i Q^{i,j} \right) = 1 \) for \( i = 1, \ldots, K \) and \( j = 1, \ldots, L_i \), and follow the same routine to tackle the constraints on the permutation-invariant subspace. Thus both the number of variables and the number of constraints are polynomial with respect to \( N \).

**Appendix E: Evaluation of QFI using different strategies**

In this section we provide explicit formulas of the QFI for all strategy sets considered in the main text, in the forms which can be numerically solved by SDP. Without the positivity constraints, parallel, sequential and general indefinite-causal-order strategy sets are affine spaces themselves, while quantum SWITCH and causal superposition strategy sets are convex hulls of affine spaces. In some cases the result of Theorem 1 can be simplified a bit, as it is possible to trace over certain subspace while formulating the primal problem at the beginning.
1. Parallel strategies

When definite causal order is obeyed, a strategy can be described by a quantum comb \[33, 34, 63\]. The dual affine space is the set of dual combs without the positivity constraint [33]. For parallel strategies the primal problem can be written as

\[
J^{(\text{pr})}(N_\phi) = \min_{h \in \mathbb{H}_r} \max_P \text{Tr} \left[ \hat{P} \Omega_\phi(h) \right],
\]

s.t. \( \hat{P} \geq 0, \)
\[
\hat{P} = \mathbb{1}_{2,4,\ldots,2N} \otimes \hat{P}^{(1)},
\]
\[
\text{Tr} \hat{P}^{(1)} = 1.
\]

(E1)

Equivalently, the problem can be formulated as

\[
\min_{h \in \mathbb{H}_r} \max_P \text{Tr} \left[ P \text{Tr}_{2,4,\ldots,2N} \Omega_\phi(h) \right],
\]

s.t. \( P \geq 0, \)
\[
\text{Tr} P = 1.
\]

(E2)

The dual problem is given by

\[
\min_{\lambda, h} \lambda, \]

s.t. \( \lambda \mathbb{1}_{1,3,\ldots,2N-1} \geq \text{Tr}_{2,4,\ldots,2N} \Omega_\phi(h), \)

(E3)

which simplifies the result directly obtained from Theorem 1 a bit. To solve the problem via SDP, we define a block matrix

\[
A := \begin{pmatrix}
\frac{\lambda}{2} \mathbb{1} & \left( r \prod_{i=1}^N d_{2i} \right) \\
\left( n_{1,1} \right) & \vdots \\
\left( n_{r, \prod_{i=1}^N d_{2i}} \right) & \mathbb{1}_{1,3,\ldots,2N-1}
\end{pmatrix},
\]

(E4)

wherein \( \mathbb{1}(d) \) denotes a \( d \)-dimensional identity matrix, and

\[
|n_{i,j} \rangle := \left( \hat{J} \hat{N}_{\phi,j}^{\ast} \right),
\]

(E5)

where \( \hat{N}_{\phi,j} = [\hat{N}_{\phi,j} - i \sum_k |N_{\phi,k} \rangle \langle h_k |] \) and \( \{|j\rangle, j = 1, \ldots, \prod_{i=1}^N d_{2k} \} \) forms an orthonormal basis of \( \otimes_{k=1}^N \mathcal{H}_{2k} \), having assumed that the identity map trivially acts on the subspace where the dual vector \( \langle j \rangle \) does not affect. Note that

\[
\sum_{i,j} |n_{i,j} \rangle \langle n_{i,j} | = \frac{1}{4} \text{Tr}_{2,4,\ldots,2N} \Omega_\phi(h).
\]

(E6)

By Schur complement lemma [64, Theorem 1.12], the constraint in Eq. (E3) is equivalent to the requirement that \( A \geq 0 \). Hence, the QFI for parallel strategies is solved by

\[
\min_{\lambda, h} \lambda,
\]

s.t. \( A \geq 0, \)
\[
h \in \mathbb{H}_r.
\]

(E7)

The problem can be solved by SDP since \( h \) is incorporated linearly in the blocks of \( A \).

**Symmetry reduction.**—We can reduce the problem using permutation symmetry. For Par, the set \( \hat{P} \) is given by \( \hat{P} = \{ S \geq 0 | S \in \mathbb{S} \} \), and the affine space \( \mathbb{S} \) is permutation-invariant. As explained in Appendix D, we can decompose the permutation-invariant \( h = U^\dagger \left[ \otimes_{\mu=1}^m \mathbb{1}_{(d_\mu) \otimes h^\mu} \right] U^\mu \) with \( h^\mu \) as an \( m_\mu \times m_\mu \) matrix. \( Q \in \mathbb{S} \) is characterized by the
constraint $\text{Tr}_{2,4,\ldots,2N} Q = 1_{1,3,\ldots,2N-1}$, and we can decompose $Q = U \left[ \bigoplus_{|\mu| = N} \mathbf{1} (d_{\mu}) \otimes Q^\mu \right] U^\dagger$ with $Q^\mu$ as an $m_{\mu} \times m_{\mu}$ matrix. If we define

$$A^\mu := \begin{pmatrix} \frac{1}{4} \mathbf{1} (d_{\mu} m_{\mu}^\prime) & \left( U_{\mu,1}^\dagger \hat{N}_{\phi,\mu}^* \right)^\dagger \\ U_{\mu,1}^\dagger \hat{N}_{\phi,\mu}^\dagger & Q^\mu \end{pmatrix},$$

(E8)

where $\hat{N}_{\phi,\mu}^\dagger$ is given by Eq. (D11), then by Theorem 3 we can reformulate the optimization problem as

$$\min_{\lambda, Q^\mu, h} \lambda,$n
s.t. $A^\mu \succeq 0$, $h^\mu \in \mathbb{H}_{m_{\mu}^\prime}$, $|\mu| = N,$
$$\text{Tr}_{2,4,\ldots,2N} Q = 1_{1,3,\ldots,2N-1}.$$ (E9)

The constraint $\text{Tr}_{2,4,\ldots,2N} Q = 1_{1,3,\ldots,2N-1}$ only requires to be explicitly characterized on the permutation-invariant subspace, since $\text{Tr}_{2,4,\ldots,2N} Q$ is permutation-invariant. Therefore, not only the number of scalar variables but also the number of constraints in terms of scalar variables are polynomial with respect to $N$.

2. Sequential strategies

For sequential strategies the problem can be written as (having traced over $\mathcal{H}_{2N}$)

$$J^{(\text{Seq})}(N_{\phi}) = \min_{h \in \mathcal{H}_r} \max_{P^{(k)}} \text{Tr} \left[ P^{(N)} \text{Tr}_{2N} \Omega_{\phi} (h) \right],$$

s.t. $P^{(N)} \succeq 0$,
$$\text{Tr}_{2k-1} P^{(k)} = 1_{2k-2} \otimes P^{(k-1)}$, $k = 2, \ldots, N,$
$$\text{Tr} P^{(1)} = 1,$$

(E10)

from which it follows that the dual problem is

$$\min_{\lambda, Q^{(k),h}} \lambda,$n
s.t. $\lambda 1_{2N-1} \otimes Q^{(N-1)} \succeq \text{Tr}_{2N} \Omega_{\phi} (h),$n
$$\text{Tr}_{2k} Q^{(k)} = 1_{2k-1} \otimes Q^{(k-1)},$ $k = 2, \ldots, N - 1,$
$$\text{Tr}_2 Q^{(1)} = 1,$$

(E11)

where $Q^{(N-1)}$ is Hermitian.

Similarly, in order to solve the problem via SDP we rewrite it as

$$\min_{\lambda, Q^{(k),h}} \lambda,$n
s.t. $A \succeq 0$,
$$\text{Tr}_{2k} Q^{(k)} = 1_{2k-1} \otimes Q^{(k-1)},$ $k = 2, \ldots, N - 1,$
$$\text{Tr}_2 Q^{(1)} = 1,$n
$$h \in \mathbb{H}_r,$$

(E12)

for

$$A := \begin{pmatrix} \frac{1}{4} \mathbf{1} (rd_{2N}) & \langle n_{1,1} \rangle \\ \vdots & \vdots \\ \langle n_{r,d_{2N}} \rangle & \mathbf{1}_{2N-1} \otimes Q^{(N-1)} \end{pmatrix},$$

(E13)

having defined

$$|n_{i,j} \rangle := \langle j | \hat{N}_{\phi,i}^* \rangle,$$

(E14)

where $\hat{N}_{\phi,j} = |N_{\phi,j} \rangle - i \sum_{k} |N_{\phi,k} \rangle h_{kj}$ and $\{ |j \rangle, j = 1, \ldots, d_{2N} \}$ forms an orthonormal basis of $\mathcal{H}_{2N}$. 
3. Quantum SWITCH strategies

We first formally define a quantum SWITCH strategy set $\mathcal{SW}$ as the collection of $P \in \text{Strat}$ such that

$$P = (\rho_{T,A,C}) \star |P^{(\text{SW})}| P^{(\text{SW})}|, \quad \rho_{T,A,C} \geq 0, \quad \text{Tr} \rho_{T,A,C} = 1,$$

(E15)

where $|P^{(\text{SW})}| := |\pi\rangle_{A,F,N} \sum_{\pi \in S_N} \{\pi\}_C |\pi\rangle_{T,2\pi-1}(\mathbf{\Phi}_{i=1}^{N-1} |\pi\rangle_{2\pi(i),2\pi(i+1)-1} |\pi\rangle_{2\pi(N),F_T} |\pi\rangle_{F_C})$ corresponds to a (generalized) quantum SWITCH for $N$ operations, each permutation $\pi$ is an element of the symmetric group $S_N$ whose order is $N!$, and $\{\pi\}_C$ forms an orthonormal basis. We suppose each $\mathcal{H}_i$ for $i = 1, \ldots, 2N$ has the same dimension $d_1$, and $\mathcal{H}_T \cong \mathcal{H}_A$ denotes the input space of the target system, $\mathcal{H}_A$ the ancillary space, and $\mathcal{H}_C$ the space of the control system. Correspondingly, $\mathcal{H}_{F_T}, \mathcal{H}_{F_A}$ and $\mathcal{H}_{F_C}$ denote the future output spaces of each part. The global future space $\mathcal{H}_F = \mathcal{H}_{F_T} \otimes \mathcal{H}_{F_A} \otimes \mathcal{H}_{F_C}$.

Using the quantum SWITCH strategy set, after tracing over the global future space $\mathcal{H}_F$, the QFI evaluation problem is written as

$$J^{(\text{SW})}(N_\phi) = \min_{h \in \mathcal{H}_I} \max_{\rho \in \rho_2(1)} \sum_{\pi \in S_N} \text{Tr} \left[ q^{\pi} \rho^{\pi}_{2\pi(1)-1} \left( \mathbf{\Phi}_{i=1}^{N-1} |\pi\rangle_{2\pi(i),2\pi(i+1)-1} \langle \pi|_{2\pi(N),2\pi(N-1)-1} \right) \otimes 1_{2\pi(N)} \right],$$

(E16)

s.t. $\sum_{\pi \in S_N} q^{\pi} = 1,$

$$\rho^{\pi}_{2\pi(1)-1} \geq 0, \quad \text{Tr} \rho^{\pi}_{2\pi(1)-1} = 1, \quad q^{\pi} \geq 0, \quad \pi \in S_N,$$

where the superscript $\pi$ of an operator denotes a permutation label, and the subscript denotes the subspace it lies in. Note that the primal set of $P$ is a convex hull of affine spaces. Equivalently the problem can be rewritten as

$$\min_{h \in \mathcal{H}_I} \max_{\rho \in \rho_2(1)} \sum_{\pi \in S_N} \text{Tr} \left[ q^{\pi} \rho^{\pi}_{2\pi(1)-1} \left( \mathbf{\Phi}_{i=1}^{N-1} |\pi\rangle_{2\pi(i),2\pi(i+1)-1} \langle \pi|_{2\pi(N),2\pi(N-1)-1} \right) \otimes 1_{2\pi(N)} \right],$$

(E17)

s.t. $\sum_{\pi \in S_N} q^{\pi} = 1,$

$$\rho^{\pi}_{2\pi(1)-1} \geq 0, \quad \text{Tr} \rho^{\pi}_{2\pi(1)-1} = 1, \quad q^{\pi} \geq 0, \quad \pi \in S_N.$$

Following the method in the proof of Theorem 1, the dual problem is given by

$$\min_{\lambda, \rho} \lambda \mathbb{1}_{2\pi(1)-1} \geq \Omega^{\pi}_{\phi}(h), \quad \Omega^{\pi}_{\phi}(h) := \left( \mathbf{\Phi}_{i=1}^{N-1} |\pi\rangle_{2\pi(i),2\pi(i+1)-1} \langle \pi|_{2\pi(N),2\pi(N-1)-1} \right) \text{Tr} \rho^{\pi}_{2\pi(N)} \langle \pi|_{2\pi(N),2\pi(N-1)-1} \right), \quad \pi \in S_N.$$

(E18)

Equivalently in an SDP form the problem is written as

$$\min_{\lambda, \rho} \lambda h, \quad \text{s.t.} \quad A^{\pi} \geq 0, \quad \pi \in S_N, \quad h \in \mathcal{H}_I,$$

(E19)

having defined

$$A^{\pi} := \begin{pmatrix} \frac{1}{4} \mathbb{1}_{(rd_1)} & \langle \pi |_{1} \rangle & \cdots & \langle \pi |_{r,d_1} \rangle \\ \langle \pi |_{1} \rangle & \cdots & \langle \pi |_{r,d_1} \rangle & \mathbb{1}_{2\pi(1)-1} \end{pmatrix},$$

(E20)

for

$$|n^{\pi}_{r,j} \rangle := \langle j^{\pi}| \left( \mathbf{\Phi}_{k=1}^{N-1} |\pi\rangle_{2\pi(k),2\pi(k+1)-1} \langle \pi|_{2\pi(N),2\pi(N-1)-1} \right) \hat{N}^{\pi}_{\phi,i},$$

(E21)

where $\hat{N}^{\pi}_{\phi,j} = |\hat{N}_{\phi,j} \rangle - i \sum_k |N_{\phi,k} \rangle h_{kj}$ and $\{\langle j^{\pi}\rangle\}$ forms an orthonormal basis of $\mathcal{H}_{2\pi(N)}$. 
**Symmetry reduction.**—For SWI, by Theorem 2, \( h \) can be taken to be permutation-invariant and the constraint corresponding to one permutation \( \pi \) (e.g., the identity element of \( S_N \)) is sufficient. As explained in Appendix D, we can decompose the permutation-invariant \( h = U[\otimes_{|\phi|=N} 1 (d_\mu) \otimes h^\mu] U^\dagger \) with \( h^\mu \) as an \( m'_\mu \times m'_\mu \) matrix. We define

\[
n_{j2N}^\mu := \langle j_{2N}^\mu | \bigotimes_{i=1}^{N-1} \langle I_{2i,2i+1} \rangle \hat{N}_{\phi}^\dagger, \quad (E22)
\]

where \( \{\langle j_{2N}^\mu \rangle\} \) forms an orthonormal basis of \( H_{2N} \) and \( \hat{N}_{\phi}^\dagger \) is given by Eq. [D11]. If we define

\[
A^{(\text{inv})} := \begin{pmatrix}
n_1^\mu \otimes 1 & \mathbb{I} (rd_{1}) & \cdots & \mathbb{I} (rd_{\mu}) \\
n_2^\mu \otimes 1 & \vdots & \ddots & \vdots \\
\vdots & \vdots & \ddots & \vdots \\
\vdots & \vdots & \vdots & \vdots \\
n_{d_\mu}^\mu \otimes 1 & \mathbb{I} (rd_{d_\mu}) & \cdots & \mathbb{I} (rd_{d_\mu}) \\
\end{pmatrix}, \quad (E23)
\]

then by Theorem 2 we can reformulate the optimization problem as

\[
\begin{align*}
\min_{\lambda, h^\mu} & \lambda, \\
\text{s.t.} & A^{(\text{inv})} \geq 0, \\
& h^\mu \in \mathbb{H}_{m'_\mu}, \ |\mu| = N. \quad (E24)
\end{align*}
\]

4. **Causal superposition strategies**

Following a similar route for the causal superposition strategy set the problem can be written as

\[
J^{(\text{Sup})}(N_\phi) = \min_{h \in \mathbb{H}_r} \max_{P^{\pi,(N)}, \mu} \sum_{\pi \in S_N} \text{Tr} (q^\pi P^{\pi,(N)} \text{Tr}_{2\pi(N)} \Omega_\phi(h)), \\
\text{s.t.} \sum_{\pi \in S_N} q^\pi = 1, \quad q^\pi \geq 0, \quad P^{\pi,(N)} \geq 0, \quad \text{Tr} P^{\pi,(1)} = 1, \quad \text{Tr}_{2k-1} P^{\pi,(k)} = 1_{2k-2} \otimes P^{\pi,(k-1)} \quad \text{for} \ k = 2, \ldots, N, \ \pi \in S_N. \quad (E25)
\]

For each causal order in the superposition the dual affine space is the set of dual combs without the positivity constraint. Thus the dual problem is given by

\[
\begin{align*}
\min_{\lambda, h} & \lambda, \\
\text{s.t.} & \lambda 1_{2\pi(N)-1} \otimes Q^{\pi,(N-1)} \geq \text{Tr}_{2\pi(N)} \Omega_\phi(h), \quad \text{Tr}_{2\pi(1)} Q^{\pi,(1)} = 1_{2\pi(1)-1}, \ \pi \in S_N, \\
& \quad \text{Tr}_{2\pi(k)} Q^{\pi,(k)} = 1_{2\pi(k)-1} \otimes Q^{\pi,(k-1)} \quad \text{for} \ k = 2, \ldots, N-1, \ \pi \in S_N, \quad (E26)
\end{align*}
\]

where the constraints hold for any \( \pi \in S_N \). To solve the problem via SDP we can formulate it as

\[
\begin{align*}
\min_{\lambda, h} & \lambda, \\
\text{s.t.} & A^\pi \geq 0, \ \text{Tr}_{2\pi(1)} Q^{\pi,(1)} = 1_{2\pi(1)-1}, \ \text{Tr}_{2\pi(k)} Q^{\pi,(k)} = 1_{2\pi(k)-1} \otimes Q^{\pi,(k-1)} \quad \text{for} \ k = 2, \ldots, N-1, \ \pi \in S_N, \quad (E27)
\end{align*}
\]

having defined

\[
A^\pi := \begin{pmatrix}
\frac{1}{4} \mathbb{I} (rd_{2\pi(N)}) & \langle n_{1,1}^\pi \rangle \\
\vdots & \vdots \\
n_{1,1}^\pi & \mathbb{I} (rd_{2\pi(N)}) \\
\vdots & \vdots \\
n_{2,1}^\pi & \mathbb{I} (rd_{2\pi(N)}) \\
\end{pmatrix}, \quad (E28)
\]

for

\[
|n_{i,j}^\pi \rangle := \langle j^\pi | \hat{N}_{\phi,i}^\dagger, \quad (E29)
\]
where \( |\hat{N}_{\phi,j}\rangle = |\hat{N}_{\phi,j}\rangle - i \sum_k |N_{\phi,k}\rangle h_{kj} \) and \( \{j^2\} \) forms an orthonormal basis of \( \mathcal{H}_{2N(N)} \).

**Symmetry reduction.**—Similar to SWI, by Theorem 2 for Sup we take a permutation-invariant \( h \) and only need the constraint corresponding to the identity element of \( S_N \). As explained in Appendix D we can decompose the permutation-invariant \( h = U' \left( \bigoplus_{|\mu|=N} 1 \ (d_\mu) \otimes h^\mu \right) U'' \) with \( h^\mu \) as an \( m_\mu' \times m_\mu' \) matrix. We define

\[
\mathbf{n}_{j2N}^\mu := \langle j_{2N}| \hat{N}_{\phi}^{\mu*},
\]

where \( \{j_{2N}\} \) forms an orthonormal basis of \( \mathcal{H}_{2N} \) and \( \hat{N}_{\phi}^\mu \) is given by Eq. [D11]. If we define

\[
A^{(inv)} := \begin{pmatrix}
\frac{\lambda}{4} \mathbb{1} (rd_{2N}) & \mathbf{n}_{1\dagger}^\mu

\vdots

\mathbf{n}_{d_1\dagger}^\mu

\mathbf{n}_{d_1}^{\mu*} & \mathbf{n}_{d_1}^{\mu*}

\end{pmatrix},
\]

then by Theorem 2 we can reformulate the optimization problem as

\[
\min_{\lambda, Q^{(\phi)}, h} \lambda,
\]

s.t. \( A^{(inv)} \geq 0 \),

\[
\begin{align*}
\Tr Q^{(k)} &= \mathbb{1}_{2k-1} \otimes Q^{(k-1)}, \ k = 2, \ldots, N - 1, \\
\Tr Q^{(1)} &= \mathbb{1}_1, \\
\forall k & \in \mathbb{H}_{m_\mu'}, |\mu| = N.
\end{align*}
\]

5. General indefinite-causal-order strategies

In this case the explicit linear constraints on strategies have been derived in [21], and the dual affine space turns out to be the set of CJ operators of \( N \)-partite no-signalling quantum channels without the positivity constraint [16] [43], mathematically defined by

\[
\begin{align*}
\Tr Q &= \prod_{i=1}^{N} d_{2i-1}, \\
\forall k & \in \mathbb{H}_r, \\
\end{align*}
\]

The intuitive interpretation for no-signaling channels is that locally the input of each channel only affects the output of this single channel, but cannot transmit any information to \( N - 1 \) other channels. To solve the QFI evaluation problem via SDP we can write it in the form

\[
\min_{\lambda, Q, h} \lambda,
\]

s.t. \( A \geq 0 \),

\[
\begin{align*}
\Tr Q &= \prod_{i=1}^{N} d_{2i-1}, \\
\forall k & \in \mathbb{H}_r,
\end{align*}
\]

having defined

\[
A = \begin{pmatrix}
\frac{\lambda}{4} \mathbb{1} (r) & \langle \hat{N}_{\phi,1}^{*} \rangle \\
\vdots & \vdots \\
\langle \hat{N}_{\phi,r}^{*} \rangle & \langle \hat{N}_{\phi,r}^{*} \rangle

\end{pmatrix}.
\]

(E35)
Symmetry reduction. For ICO, by Lemmas 1 and 2, both $h$ and $Q$ can be taken to be permutation-invariant. As explained in Appendix C, we can decompose the permutation-invariant $h = U^\dagger \left( \bigoplus_{|\mu|=N} 1 \left( d_\mu \right) \otimes h^\mu \right) U$ with $h^\mu$ as an $m'_\mu \times m'_\mu$ matrix, and decompose the permutation-invariant $Q = U \left[ \bigoplus_{|\mu|=N} 1 \left( d_\mu \right) \otimes Q^\mu \right] U^\dagger$ with $Q^\mu$ as an $m_\mu \times m_\mu$ matrix. If we define

$$A^\mu := \left( \frac{1}{\bar{\mu}} \left( \sum_{i} \frac{1}{\mu_i} m'_i \right) \left( U_{\mu,11} \hat{\mathcal{N}}_{\phi}^{\mu} \right)^{\frac{1}{2}} \right),$$

where $\hat{\mathcal{N}}_\phi^{\mu}$ is given by Eq. (D11), then by Theorem 3 we can reformulate the optimization problem as

$$\begin{aligned}
\min_{\lambda, Q^\mu, h} \frac{\lambda}{Q^\mu}, \\
\text{s.t. } A^\mu \geq 0, & \quad h^\mu \in \mathbb{H}_{m'_\mu}, \quad |\mu| = N, \\
\text{Tr}_{2N} Q = & \frac{1_{_{2N-1}}}{d_{2N-1}} \otimes \text{Tr}_{2N-1,2N} Q, \\
\sum_{|\mu|=N} d_\mu \text{Tr} Q^\mu = & \prod_{i=1}^{N} d_{2i-1},
\end{aligned}$$

having removed the redundant constraints on $Q$ by permutation symmetry. Similar to the case of Par, we only need to consider the constraint on $Q$ on the permutation-invariant subspace, since both $Q$ and $\text{Tr}_{2N-1,2N} Q$ are permutation-invariant. Therefore, both the number of scalar variables and the number of constraints in terms of scalar variables are polynomial with respect to $N$.

Appendix F: Complexity analysis

Here we refer to the number of real scalar variables concerned in optimization as the complexity. In Appendix E we have presented both the original and the symmetry reduced QFI evaluation for all families of strategies considered in this work as applicable, from which we can obtain Table II in the main text.

Now we consider the algorithm for identifying an optimal strategy. Since the algorithm is based on Theorem 1, its complexity is no less than that of the QFI evaluation. For the second step of the algorithm, by Lemma 3 there exists a permutation-invariant optimal strategy for all families of strategies except for the sequential one, and thus we can apply the group-invariant SDP to achieve the permutation-invariant solution. Recall that $\hat{P} = \sum_{i=1}^{K} q_i S^i$ for $S^i \in \mathcal{S}^1$. In fact, for SWI and Sup, we only need to characterize $S^1 \in \mathcal{S}^1$ and obtain $\bar{P} = \sum_{i=1}^{K} \frac{1}{2} S^1$ due to the permutation invariance. In summary, taking both steps of the algorithm into account, we obtain Table III.

| SDP    | Par       | Seq       | SWI       | Sup       | ICO       |
|--------|-----------|-----------|-----------|-----------|-----------|
| Ori.   | $O \left( \max(s, d_1)^N \right)$ | $O \left( d^{N} \right)$ | $O \left( N! \right)$ | $O \left( N! d^{N} \right)$ | $O \left( d^{N} \right)$ |
| Inv.   | $O \left( N^{d_1^2-1} \right)$ | $O \left( d^{N} \right)$ | $O \left( N^{d_1^2-1} \right)$ | $O \left( d^{N} \right)$ | $O \left( N^{d_1^2-1} \right)$ |

TABLE II. Complexity of Algorithm I for each family of strategies (with respect to $N$). The asymptotic numbers of variables in optimization are compared between the original (Ori.) and group-invariant (Inv.) SDP. We denote $d := d_1 d_2$ for $d_i := \dim(H_i)$ and $s := \max_{\phi} \text{rank}(E_{\phi}) \leq d$.

As a concrete example, we apply the group-invariant SDP to the evaluation of the QFI $J^{(ICO)}$ for the general indefinite-causal-order strategies up to $N = 5$. We consider the amplitude damping noise and take $\phi = 1.0$, $t = 1.0$ and $p = 0.5$. As illustrated in Fig. 3 the growth of $J^{(ICO)}$ is faster than linear growth but slower than quadratic growth. Table III compares the complexity between the original and the group-invariant SDP and indicates that the symmetry reduced approach can save the computational resources dramatically.
FIG. 3. **Growth of QFI** $J^{(ICO)}$ **as** $N$ **increases.** For the amplitude damping noise, we take $\phi = 1.0$, $t = 1.0$ and $p = 0.5$. The dashed and dotted lines illustrate the linear and quadratic growth with respect to $N$ respectively, while matching the QFI at $N = 1$.

| $N$ | 1   | 2   | 3   | 4     | 5     |
|-----|-----|-----|-----|-------|-------|
| No. of variables in the original SDP | 21 | 273 | 4161| 65793 | 1049601 |
| No. of variables in the group-invariant SDP | 21 | 147 | 837 | 3912 | 15561 |

**TABLE III. Number of real scalar variables concerned in the evaluation of** $J^{(ICO)}$. For the original SDP the total number of real scalar variables for $Q$, $h$ and $\lambda$ is $16N + 4^N + 1$, while for the group-invariant SDP the total number of real scalar variables for $Q^\mu$, $h^\mu$ and $\lambda$ for all Young diagram labels $|\mu| = N$ is $\binom{N+15}{15} + \binom{N+3}{3} + 1$.

**Appendix G: Supplementary numerical results**

1. **Hierarchy for the $N = 3$ case**

Numerical results in this work are obtained by implementing SDP using the open source Python package CVXPY [65, 66] with the solver MOSEK [67]. We plot the QFI for $N = 3$, amplitude damping noise in Fig. 4 and observe a similar hierarchy of the estimation performance using parallel, sequential and indefinite-causal-order strategies. Different from the $N = 2$ case presented in the main text, general indefinite-causal-order strategies indeed provide a small advantage over causal superposition strategies, which is presented in Table. IV.

On the other hand, analogous to the $N = 2$ case, simple quantum SWITCH strategies without any additional intermediate control operations could have advantage over any definite-causal-order strategies when the decay parameter $p$ is small, but this advantage becomes more insignificant. This should not be surprising since the control can make a bigger difference as $N$ grows.
FIG. 4. Hierarchy of QFI using parallel, sequential and indefinite-causal-order strategies for $N = 3$, the amplitude damping noise. We take $\phi = 1.0$, fix the evolution time $t = 1.0$ and vary the decay parameter $p$. To see the gaps between different strategies more clearly we insert an inset plot where the decay parameter $p$ ranges from 0.1 to 0.2.

| $p$ | $J^{(\text{Sup})}(N_\phi)$ | $J^{(\text{ICO})}(N_\phi)$ |
|-----|-----------------|-----------------|
| 0.1 | 8.185           | 8.200           |
| 0.2 | 7.364           | 7.375           |
| 0.3 | 6.523           | 6.524           |
| 0.4 | 5.642           | 5.647           |
| 0.5 | 4.725           | 4.743           |
| 0.6 | 3.786           | 3.815           |
| 0.7 | 2.832           | 2.870           |
| 0.8 | 1.871           | 1.909           |
| 0.9 | 0.918           | 0.930           |

TABLE IV. Hierarchy of QFI using ICO and Sup.

2. Estimation of randomly sampled channels

To demonstrate the universality of the hierarchy of different families of strategies considered in the main text, we randomly sample noise channels drawn from an ensemble of CPTP maps defined by Bruzda et al. in [68]. In this work we only sample rank-2 qubit channels for $N = 2$, which is enough to show the hierarchy. The sampling process is implemented via an open source Python package QuTiP [69, 70]. We set an error tolerance of $10^{-8}$, i.e., we claim $J_1 > J_2$ only if the gap is no smaller than $10^{-8}$. We find that for 984 of 1000 random channels, a strict hierarchy $J^{(\text{Par})} < J^{(\text{Seq})} < J^{(\text{Sup})} < J^{(\text{ICO})}$ holds, implying that general indefinite-causal-order strategies can provide advantage
over causal superposition strategies. In addition, we find that of the same 1000 channels \( J^{(\text{Par})} < J^{(\text{SW})} \) for 34 channels and \( J^{(\text{Seq})} < J^{(\text{SW})} \) only for 1 channel, so with a high probability quantum SWITCH strategies cannot outperform strategies following definite causal order for a random noise channel, which highlights the estimation enhancement from intermediate control in the general case.

Appendix II: Comparison with asymptotic results

In this section we focus on strategies following definite causal order, i.e., parallel and sequential ones, and compare our results and those of the extensively studied asymptotic theory.

1. Preliminaries

We first introduce some basic notions. If we write the operation-sum representation of the channel \( \mathcal{E}_\phi(\rho) = \sum_{i=1}^r K_{\phi,i}^\dagger \rho K_{\phi,i} \), where \( \{K_{\phi,i}\} \) are a set of Kraus operators and \( r \) is the rank of the channel, the channel QFI can be evaluated by optimization:

\[
J_Q^{(\text{chan})}(\mathcal{E}_\phi) = 4 \min_{h \in \mathbb{H}_r} |\alpha|,
\]

where \( |\cdot| \) denotes the operator norm and \( \alpha = \sum_i \hat{K}_{\phi,i}^\dagger \hat{K}_{\phi,i} \). Here \( \hat{K}_{\phi,i} = \hat{K}_{\phi,i} - i \sum_{j=1}^r h_{ij} K_{\phi,j} \) is nothing but the derivative of an equivalent Kraus representation, given an \( r \times r \) Hermitian matrix \( h \).

The asymptotically tight upper bounds on QFI of \( N \) quantum channels have been derived for both sequential and parallel strategies. For parallel strategies an asymptotically tight upper bound is \( \{28, 30\} \):

\[
J^{(\text{Par})}(N_\phi) \leq 4 \min_{h \in \mathbb{H}_r} [N|\alpha| + N(N-1)|\beta|^2],
\]

where \( \beta = \sum_i K_{\phi,i}^\dagger \hat{K}_{\phi,i} \). An asymptotically tight upper bound was also derived for sequential strategies \( \{27, 35\} \):

\[
J^{(\text{Seq})}(N_\phi) \leq 4 \min_{h \in \mathbb{H}_r} [N|\alpha| + N(N-1)|\beta|(|\beta| + 2\sqrt{|\alpha|})].
\]

It has been shown that the QFI follows the standard quantum limit if and only if there exists an \( h \) such that \( \beta = 0 \) \( \{43\} \). In this case sequential strategies provide no advantage asymptotically, and we have

\[
\lim_{N \to \infty} \frac{1}{N} J^{(\text{Par})}(N_\phi) = \lim_{N \to \infty} \frac{1}{N} J^{(\text{Seq})}(N_\phi) = 4 \min_{h \in \mathbb{H}_r, \beta=0} |\alpha|.
\]

We remark that the minimization in Eq. \( (H2) \) can be efficiently evaluated via SDP \( \{30\} \).

2. Tightness of QFI bounds in non-asymptotic channel estimation

We compare our non-asymptotic results and existing asymptotically tight bounds for two types of quantum channels. Apart from the amplitude damping noise described by \( K_{1}^{(\text{AD})} = |0\rangle\langle 0| + \sqrt{1-p} |1\rangle\langle 1| \) and \( K_{2}^{(\text{AD})} = \sqrt{p} |0\rangle \langle 1| \) considered in the main text, here we also present a second example, where the noise is described by a SWAP-type interaction \( V_{\text{int}} = e^{-ig\tau} H_{\text{SWAP}} \) between a qubit system \( S \) and a qubit environment \( E \), where \( g \) is the interaction strength, \( \tau \) is the interaction time and the Hamiltonian is given by \( H_{\text{SWAP}}(|i\rangle_{S} |j\rangle_{E}) = |j\rangle_{S} |i\rangle_{E} \). The initial environment state is \( |0\rangle \), and the Kraus operators can be written as \( K_{1}^{(\text{SWAP})} = |0\rangle_{E} V_{\text{int}} |0\rangle_{E} = e^{-ig\tau} |0\rangle_{0} + \cos(g\tau) |1\rangle_{1} \), and \( K_{2}^{(\text{SWAP})} = |1\rangle_{E} V_{\text{int}} |0\rangle_{E} = -i \sin(g\tau) |0\rangle_{1} \).

We plot the QFI for the two examples in Fig. 5. Both of them show the advantage of sequential strategies over parallel ones, and the gaps between exact results of QFI for sequential strategies and the parallel upper bounds given by Eq. \( (H2) \).
Thus there exists the asymptotically tight bound on the maximal QFI of parallel strategies. We plot the QFI versus the evolution time in FIG. 5. Comparison of our results with the existing asymptotically tight QFI bound.

3. Elusive advantage of sequential strategies in the asymptotic limit

We observe a gap between parallel and sequential strategies for amplitude damping channels and SWAP-type interactions for $N = 2$ and 3. Now we show that for both examples there is no advantage of sequential strategies asymptotically since there exists an $h$ such that $\beta = 0$.

For the amplitude damping channel, $K_{\phi,i}^{(AD)} = K_i^{(AD)}U_z(\phi)$, $i = 1, 2$. Direct calculation leads to

$$\beta^{(AD)} = \left(\frac{t}{2} + h_{11}^{(AD)}\right)|0\rangle\langle 0| + \left[h_{11}^{(AD)} - \frac{t}{2} + \left(h_{22}^{(AD)} - h_{11}^{(AD)}\right)p\right]|1\rangle\langle 1|.$$ (H5)

To obtain $\beta^{(AD)} = 0$ we just need to take $h_{11}^{(AD)} = -t/2$ and $h_{22}^{(AD)} = (2 - p)t/2p$.

Similarly, for the SWAP-type interaction we have

$$\beta^{(SWAP)} = \left(\frac{t}{2} + h_{11}^{(SWAP)}\right)|0\rangle\langle 0| + \left[h_{11}^{(SWAP)} - \frac{t}{2} + \left(h_{22}^{(SWAP)} - h_{11}^{(SWAP)}\right)\sin^2(g\tau)\right]|1\rangle\langle 1|.$$ (H6)

Thus there exists $h_{11}^{(SWAP)} = -t/2$ and $h_{22}^{(SWAP)} = \left[2 - \sin^2(g\tau)\right]t/2\sin^2(g\tau)$ such that $\beta^{(SWAP)} = 0$.

Appendix I: Implementation of optimal strategies with universal quantum gates

In this section we apply Algorithm 1 in the main text to numerically solve for an optimal strategy in the set of sequential and causal superposition ones respectively. The CJ operator of an optimal sequential strategy corresponds to a sequence of isometries with a minimal ancilla-space implementation provided by [46], and can then be decomposed into single-qubit gates and CNOT gates [71]. By taking advantage of the freedom of choosing a parameter-independent
unitary on the final output state, we can adjust the strategy to reduce the CNOT count without affecting the QFI. In terms of an optimal causal superposition strategy we follow the same routine for each sequential strategy branch respectively in the superposition.

1. Optimal sequential strategy

Let \( \mathcal{H}_0 = \mathbb{C} \) and \( \mathcal{H}_{2N+1} = \mathcal{H}_F \), and we have the CJ operator of a sequential strategy \( P \in \mathcal{L} \left( \mathcal{H}_F \otimes \mathcal{H}_{i=0}^{2N} \mathcal{H}_i \right) \) (an \((N+1)\)-step quantum comb), as illustrated in Fig. 6. In this way of relabeling Hilbert spaces we have

\[
P = P^{(N+1)} \geq 0, \quad \text{Tr} P_{2k-1}^{(k)} = \mathbb{I}_{2k-2} \otimes P^{(k-1)} \quad \text{for} \ k = 2, \ldots, N + 1, \quad \text{Tr} P^{(1)} = 1.
\]  

\[
P_{2k-1}^{(k)} = \mathbb{I}_{2k-2} \otimes P^{(k)}
\]

FIG. 6. Concatenation of a sequential strategy and \( N \) quantum channels. \( P \) is the CJ operator of a sequential strategy and \( E_\phi \) is the CJ operator of a parameterized quantum channel. \( H_0 = \mathbb{C} \) is a trivial one-dimensional Hilbert space, and therefore the first step of the strategy is the process of state preparation.

According to Theorems 1 and 2 in [46], \( P \) corresponds to a sequence of isometries \( \{ V^{(k)} \} \) for \( k = 1, \ldots, N + 1 \) by Stinespring dilation:

\[
\mathcal{P}(\rho) = \text{Tr}_{A_{N+1}} \left[ \left( V^{(N+1)} \otimes \mathbb{I}_{1,3,\ldots,2N-1} \right) \cdots \left( V^{(1)} \otimes \mathbb{I}_{2,4,\ldots,2N} \right) \rho \left( V^{(1)} \otimes \mathbb{I}_{2,4,\ldots,2N} \right)^\dagger \cdots \left( V^{(N+1)} \otimes \mathbb{I}_{1,3,\ldots,2N-1} \right)^\dagger \right]
\]  

\[
\mathcal{P}(\rho) = \text{Tr}_{A_{N+1}} \left[ \left( V^{(N+1)} \otimes \mathbb{I}_{1,3,\ldots,2N-1} \right) \cdots \left( V^{(1)} \otimes \mathbb{I}_{2,4,\ldots,2N} \right) \rho \left( V^{(1)} \otimes \mathbb{I}_{2,4,\ldots,2N} \right)^\dagger \cdots \left( V^{(N+1)} \otimes \mathbb{I}_{1,3,\ldots,2N-1} \right)^\dagger \right]
\]  

\[
\mathcal{P}(\rho) = \text{Tr}_{A_{N+1}} \left[ \left( V^{(N+1)} \otimes \mathbb{I}_{1,3,\ldots,2N-1} \right) \cdots \left( V^{(1)} \otimes \mathbb{I}_{2,4,\ldots,2N} \right) \rho \left( V^{(1)} \otimes \mathbb{I}_{2,4,\ldots,2N} \right)^\dagger \cdots \left( V^{(N+1)} \otimes \mathbb{I}_{1,3,\ldots,2N-1} \right)^\dagger \right]
\]  

for any input state \( \rho \in \mathcal{L} \left( \otimes_{i=0}^{N} \mathcal{H}_{2i} \right) \), where the whole process corresponding to \( P \) is described by an isometry \( \mathcal{P} \in \mathcal{L} \left( \otimes_{i=0}^{N} \mathcal{H}_{2i} \right) \), and in each step a choice of isometry \( V^{(k)} \in \mathcal{L} \left( \mathcal{H}_{2k-2} \otimes \mathcal{H}_{A_{k-1}} \right) \) with minimal ancilla space is given by

\[
V^{(k)} = \mathbb{I}_{2k-1} \otimes (P^{(k)})^\star \frac{1}{2} \left[ (I_{2k-1,(2k-2)'} \mathbb{I}_{2k-2-(2k-2)'} \otimes (P^{(k-1)}\ast)^{\frac{1}{2}} \right],
\]

\[
V^{(k)} = \mathbb{I}_{2k-1} \otimes (P^{(k)})^\star \frac{1}{2} \left[ (I_{2k-1,(2k-2)'} \mathbb{I}_{2k-2-(2k-2)'} \otimes (P^{(k-1)}\ast)^{\frac{1}{2}} \right],
\]

\[
V^{(k)} = \mathbb{I}_{2k-1} \otimes (P^{(k)})^\star \frac{1}{2} \left[ (I_{2k-1,(2k-2)'} \mathbb{I}_{2k-2-(2k-2)'} \otimes (P^{(k-1)}\ast)^{\frac{1}{2}} \right],
\]

\[
V^{(k)} = \mathbb{I}_{2k-1} \otimes (P^{(k)})^\star \frac{1}{2} \left[ (I_{2k-1,(2k-2)'} \mathbb{I}_{2k-2-(2k-2)'} \otimes (P^{(k-1)}\ast)^{\frac{1}{2}} \right],
\]

where \( \mathcal{H}_{A_k} = \text{Supp}(P^{(k)}\ast) \) is an ancillary space given by the support of \( P^{(k)} \) with \( \mathcal{H}_{A_0} = \mathbb{C} \), \( \mathcal{H}_{i} \) is a copy of the Hilbert space \( \mathcal{H}_{i} \), \( \mathbb{I}_{2k-2-(2k-2)} := \sum_{i} |i\rangle_{(2k-2)'} \langle i|_{2k-2} \) is an identity map from \( \mathcal{H}_{2k-2} \) to \( \mathcal{H}_{(2k-2)'} \), and \((P^{(k-1)}\ast)^{\frac{1}{2}}\) denotes the Moore–Penrose pseudoinverse of \( (P^{(k-1)}\ast)^{\frac{1}{2}} \) with its support on \( \mathcal{H}_{A_{k-1}} \).

As the last isometry \( V^{(N+1)} \) preserves the QFI, it is therefore only necessary to consider the implementation of \( P^{(N)} \) instead of the full strategy \( P^{(N+1)} \). From this explicit construction it follows that the minimal dimension of the ancilla space for implementing the sequential strategy \( P \) is \( \text{dim}(\mathcal{H}_{A_1}) = \text{rank}(P^{(N)}) \). In the case of \( N = 2 \) for the amplitude damping noise considered in the main text, it is easy to see that \( \text{dim}(\mathcal{H}_{A_1}) \leq 2 \) and \( \text{dim}(\mathcal{H}_{A_2}) \leq 8 \), so \( V^{(1)} \) is an isometry from 0 to (at most) 2 qubits and \( V^{(2)} \) is an isometry from 2 to (at most) 4 qubits, as illustrated in Fig. 7.

\[
|0\rangle \quad V^{(1)} \quad \mathcal{E}_\phi \quad V^{(2)} \quad |0\rangle
\]

\[
|0\rangle \quad V^{(1)} \quad \mathcal{E}_\phi \quad V^{(2)} \quad |0\rangle
\]

FIG. 7. A sequence of isometries corresponding to a sequential strategy for \( N = 2 \). The first qubit is the system qubit going through the channel \( \mathcal{E}_\phi \) twice, while the three other qubits are ancillary.

Next, we apply a circuit decomposition of each isometry into single-qubit gates and CNOT gates. In practice it is often desirable to achieve a CNOT count as low as possible. Note that \( V^{(1)} \) actually corresponds to the preparation of
a 2-qubit state, which in general requires only one CNOT gate. In terms of $V^{(2)}$, an isometry from 2 to 4 qubits, the state-of-the-art decomposition scheme is the column-by-column approach which requires at most 54 CNOT gates. However, as an arbitrary parameter-independent unitary on 3 ancillae can always be deferred and regrouped into $V^{(3)}$ and therefore does not affect the QFI, in fact we can choose a proper $V^{(2)}$ to further reduce the worst CNOT count to 47 without changing the QFI. To see this we need to briefly introduce the main ideas behind the column-by-column decomposition scheme.

An isometry $V$ from $m$ to $n$ qubits ($m \leq n$) can be represented in the matrix form by $V = U^\dagger (2^m \times 2^n)$, where $U^\dagger$ is a $2^n \times 2^n$ unitary matrix and $1 (2^n \times 2^n)$ is the first $2^m$ columns of the $2^n \times 2^n$ identity matrix. If we obtain a decomposition of $U^\dagger$, then we can simply initialize the state of the first $n - m$ qubits to $|0\rangle$ to implement $V$. Equivalently we can find a decomposition of $U$ such that $UV = 1 (2^n \times 2^n)$ and then inverse the circuit representing $U$. The idea is to find a sequence of unitary operations such that $U = U_{2m-1} \cdots U_0$ transforms $V$ into $1 (2^n \times 2^n)$ column by column. More specifically, we first choose a proper $U_0$ to map the first column of $V$ to the first column of $1 (2^n \times 2^n)$, i.e., $U_0 V |0\rangle_m = |0\rangle_n$, then choose $U_1$ satisfying $U_1 U_0 V |1\rangle_m = |1\rangle_n$ as well as $U_1 U_0 V |0\rangle_m = |0\rangle_n \ldots$ until we determine $U_{2m-1}$.

Here we only focus on $U_0$, the inverse of which can be seen as a process preparing a state $V |0\rangle_m$ from $|0\rangle_n$. In terms of decomposing $V^{(2)}$ from $m = 2$ to $n = 4$ qubits, preparing a 4-qubit state in general requires 8 CNOT gates. Fortunately, without changing the QFI, we have the freedom to choose a unitary $U_{\text{anc}}$ on the ancillae after applying $V^{(2)}$ such that the state $V^{(2)} |0\rangle_2 = U_{\text{anc}} V^{(2)} |0\rangle_2$ can be prepared using only one CNOT gate. This can be seen by dividing the 4 qubits into two parties, including the single system qubit (in the space $H_S$) and the three ancillary qubits (in the space $H_A$), and taking the Schmid decomposition of the 4-qubit state $V^{(2)} |0\rangle_2$

$$|\psi\rangle_{SA} := V^{(2)} |0\rangle_2 = \sum_{i=0}^1 \lambda_i |e_i\rangle_S |f_i\rangle_A,$$

where $\{e_i/f_i\}_{S/A}$ forms an orthonormal basis of $H_{S/A}$, and $\lambda_i$ is a set of non-negative real numbers satisfying $\sum_i \lambda_i^2 = 1$. Therefore, to prepare $V^{(2)} |0\rangle_2$, we only need a local unitary on $H_S$ to generate $\sum_{i=0}^1 \lambda_i |i\rangle_S \langle i|_A$, then apply one CNOT gate taking the system qubit as the control to obtain $\sum_{i=0}^1 \lambda_i |i\rangle_S \langle i|_A$, and finally apply local unitary operations $U_S = \sum_i |e_i\rangle_S \langle i|_S$ on the system and $U_A = \sum_i |f_i\rangle_A \langle i|_A$ on the ancillae respectively. If we take $U_{\text{anc}} = U_A^\dagger$, then it is easy to see that $V^{(2)} |0\rangle_2 = U_{\text{anc}} V^{(2)} |0\rangle_2 = \sum_{i=0}^1 \lambda_i |e_i\rangle_S \langle i|_A$ can thus be prepared using one CNOT gate. This choice of $V^{(2)}$ saves 7 CNOT gates compared to the general state preparation scheme, and leads to a worst CNOT count of 47 in total.

Now we present numerical results of the circuit implementation of an optimal sequential strategy. The decomposition of isometries is implemented using the Mathematica package UniversalQCompiler [44] based on the method described above. As in the main text, we consider the amplitude damping noise and take $N = 2$, $\phi = 1.0$, $p = 0.5$ and $t = 1.0$. The circuits implementing $V^{(1)}$ and $V^{(2)}$ are illustrated in Fig. 8. The state preparation $V^{(1)}$ requires 1 CNOT gate and the intermediate control operation $V^{(2)}$ requires 33 CNOT gates.

(a) Decomposition of $V^{(1)}$. For simplicity the angles of single-qubit rotation gates are not depicted.

(b) Decomposition of $V^{(2)} = U_{\text{anc}} V^{(2)}$. For simplicity single-qubit gates, which might be required in addition to CNOT gates, are not depicted.

FIG. 8. Decomposition of isometries corresponding to an optimal sequential strategy for $N = 2$. We apply $V^{(2)}$ instead of $V^{(2)}$ to achieve the maximal QFI with fewer CNOT gates.
2. Optimal causal superposition strategy

A causal superposition strategy for estimating \( N \) channels can be implemented by an \( N! \)-dim quantum control system entangled with \( N! \) sequential strategies of applying the channels:

\[
P = |P\rangle\langle P| \quad \text{for} \quad |P\rangle = \sum_{\pi \in S_N} |P^\pi\rangle |\pi\rangle_C,
\]

where \( |\pi\rangle_C \) forms an orthonormal basis of the Hilbert space \( \mathcal{H}_C \) of the control system, and each \( P^\pi = |P^\pi\rangle\langle P^\pi| \) is a sequential strategy. Once we obtain an optimal causal superposition strategy by applying Algorithm I (we can apply the circuit decomposition for each sequential strategy in the superposition, following the method described in Appendix I). Taking account of the permutation symmetry, we can choose an optimal causal superposition strategy such that apart from the execution order of two channels, sequential strategies in the decomposition of the strategy are the same, containing the same state preparation and intermediate control.

As a concrete example, we again take \( N = 2 \), \( \phi = 1.0 \), \( p = 0.5 \) and \( t = 1.0 \) for the amplitude damping noise and present numerical results of the circuit implementation of an optimal causal superposition strategy. As illustrated in Fig. 9 we use the qubit \( |\psi\rangle_C \) to coherently control which sequential order is executed. Due to the permutation invariance of the optimal strategy, we can simply control the query order of the identical channels while fixing \( V^{(1)} \) and \( V^{(2)} \) for all sequential orders. In view of this, generally we can use a \((2N - 1)\)-quantum SWITCH to control the order of \( N \) channels \( \mathcal{E}_\phi \) and \( N - 1 \) intermediate control operations \( V^{(i)} \).

![FIG. 9. Sequences of isometries corresponding to each sequential order in the causal superposition for \( N = 2 \). The first qubit of the circuit is the system qubit, and the query order of two identical channels \( \mathcal{E}^{(1)}_\phi \) and \( \mathcal{E}^{(2)}_\phi \) is entangled with the state of the control qubit \( |\psi\rangle_C \). When \( |\psi\rangle_C \) is a superposition of the two states shown in the figure, the causal order is also in a superposition given by Eq. (15).](image)

Further decomposition shows that each sequential branch requires one CNOT gate for state preparation \( V^{(1)} \) and 36 CNOT gates for intermediate control \( V^{(2)} \), as illustrated in Fig. 10.

![FIG. 10. Decomposition of isometries corresponding to one causal order in the decomposition of an optimal causal superposition strategy for \( N = 2 \). We have already taken advantage of the freedom to choose a \( V^{(2)} \) implemented by fewer CNOT gates, as explained in Appendix I.](image)