Amount of quantum coherence needed for measurement incompatibility

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A pair of quantum observables diagonal in the same "incoherent" basis can be measured jointly, so *some* coherence is obviously required for measurement incompatibility. Here we first observe that coherence in a single observable is linked to the diagonal elements of any observable jointly measurable with it, leading to a general criterion for the coherence needed for incompatibility. Specializing to the case where the second observable is incoherent (diagonal), we develop a concrete method for solving incompatibility problems, tractable even in large systems by analytical bounds, without resorting to numerical optimization. We verify the consistency of our method by a quick proof of the known noise bound for mutually unbiased bases, and apply it to study emergent classicality in the spin-boson model of an N-qubit open quantum system. Finally, we formulate our theory in an operational resource-theoretic setting involving "genuinely incoherent operations" used previously in the literature, and show that if the coherence is insufficient to sustain incompatibility, the associated joint measurements have sequential implementations via incoherent instruments.

I. INTRODUCTION

Coherence typically refers to nonzero off-diagonal elements in a quantum state, and is an essential resource for quantum information tasks [1–5]. Coherence in *measurements* (observables) [6,7] is equally fundamental, with an obvious relation to the noncommutativity of projective measurements, which has recently been refined [8–10]. It is therefore natural to ask how coherence is related to incompatibility of general observables—positive operator valued measures (POVMs). Incompatibility is a resource as well [5,11], specifically for steering [12–17] and state discrimination [18–20], and clearly requires noncommutativity, hence coherence.

As usual [2], we define coherence relative to a fixed "incoherent" basis (there is also a basis-independent approach [21]). Our key observation is the following: while incompatibility of POVMs is not linked to the overall coherence in their matrices, there is an asymmetric entrywise relation: coherences in *one* POVM are linked to the corresponding diagonal probabilities of any POVM jointly measurable with it. Heuristically, an observable that sharply distinguishes a pair of basis elements is incompatible with observables detecting coherence between that pair. An extreme case is any basis observable mutually unbiased [22] to the incoherent basis—it is both complementary and maximally coherent.

We warm up in Sec. II by formalizing the above observation into a simple but completely general inequality, the violation of which witnesses incompatibility. Combined with a sufficient condition for incompatibility, this leads to an analytical method for tackling the incompatibility problem, generalizing the usual robustness idea [23,24], and easily reproducing the known noise bound for incompatible mutually unbiased bases (MUBs) [19,25–28]. In Sec. III we special-

ize to the physically motivated setting where measurement coherence is given by a fixed "pattern matrix" describing decoherence [29–31], and subsequently use it to study emergent classicality in the spin-boson model [31–33], including the role of decoherence-free subspaces [33–36]. Unlike existing results on incompatibility in open systems [37], our method works for arbitrary system size. Finally, in Sec. IV, we formulate the idea in general operational terms motivated by resource theory, including genuinely incoherent operations [4,38,39] and introducing incoherent instruments, which turn out to provide sequential implementations for any joint measurement in an instance of channel-observable compatibility [40–42].

II. GENERAL FORMULATION

Let $\mathcal{H}$ be a Hilbert space of dim $\mathcal{H} = d < \infty$, and $\{|n\rangle\}_{n=1}^d$ its incoherent basis [2]. An observable (POVM) M with a finite outcome set Ω consists of positive semidefinite (PSD) matrices $\mathsf{M}(i) \geqslant 0$, for which $\sum_{i\in\Omega} \mathsf{M}(i) = \mathbb{1}$ (the identity matrix). For any POVM M we define the entrywise coherence

$$\mathrm{coh}_{nm}(\mathsf{M}) := \sum_{i\in\Omega} |\langle n|\mathsf{M}(i)|m\rangle|, \text{ for each } n, m.$$

We note that $0 \leqslant \mathrm{coh}_{nm}(\mathsf{M}) \leqslant 1$, and call M maximally coherent if $\mathrm{coh}_{nm}(\mathsf{M}) = 1$ for all $n \neq m$. We now observe (Appendix A) that any maximally coherent M with d outcomes is mutually unbiased to the incoherent basis $\{|n\rangle\}$, i.e., $\mathsf{M}(i) = |\psi_i\rangle\langle\psi_i|$ with $|\langle\psi_i|n\rangle|^2 = d^{-1}$ for all n, i. This reflects the importance of MUBs in the context of measurement coherence.

For any M we let $p_n^{\mathsf{M}}(j) := \langle n|\mathsf{M}(j)|n\rangle$ be the outcome distribution in state $|n\rangle$. The ability of M to distinguish $|n\rangle$

from $|m\rangle$ can be quantified by f divergences [43] between p_n^M and p_m^M; we use the Hellinger distances [44]

$$d_{nm}^2(\mathsf{M}) := 1 - \sum_j \sqrt{p_n^M(j)p_m^M(j)}.$$

Finally, an observable M is jointly measurable with an observable F if there is a joint observable $\mathsf{G} = (\mathsf{G}(i,j))_{(i,j)}$ with $\sum_j \mathsf{G}(i,j) = \mathsf{M}(i)$ for all i, and $\sum_i \mathsf{G}(i,j) = \mathsf{F}(j)$ for all j; otherwise M and F are incompatible [45].

A. Joint measurability criteria

The following observation provides a simple tradeoff between distinguishability and coherence, under the assumption of joint measurability:

Proposition 1. If M and F are jointly measurable, then

$$\mathrm{coh}_{nm}(\mathsf{M}) + d_{nm}^2(\mathsf{F}) \leqslant 1 \text{ for all } n, m. \qquad (1)$$

Proof. We have $\mathrm{coh}_{nm}(\mathsf{M}) \leqslant \sum_{i,j} |\langle n|\mathsf{G}(i,j)|m\rangle|$ for any joint POVM G of M and F. But $\mathsf{G}(i,j)$ is PSD, and hence $|\langle n|\mathsf{G}(i,j)|m\rangle| \leqslant \sqrt{p_n^G(i,j)p_m^G(i,j)}$ so $\sum_i |\langle n|\mathsf{G}(i,j)|m\rangle| \leqslant \sqrt{\sum_i p_n^G(i,j)\sum_i p_m^G(i,j)} = \sqrt{p_n^F(j)p_m^F(j)}$ by the Schwarz inequality. $\blacksquare$

Hence, M and F are incompatible if (1) is violated for at least one pair n, m; the result is an *upper* bound for the coherence needed for incompatibility. The interpretation is that coherence between $|n\rangle$ and $|m\rangle$ cannot be precisely detected by a measurement capable of distinguishing these states. In particular, if $\mathrm{coh}_{nm}(\mathsf{M}) = 1$ then M is incompatible with any F having $p_n^F \neq p_m^F$.

Necessary conditions for incompatibility require finding joint observables, equivalent to hidden variable models for quantum steering [12–17]. This is hard to tackle analytically, and often restricted to single qubits or highly symmetric cases. Surprisingly, we now obtain a very general result using the Schur product theorem [46], which states that the entrywise (Hadamard or Schur) product $A * B$ of PSD matrices A and B is also PSD. We call an observable P incoherent if $\mathsf{P}(i) = \sum_{n=1}^d p_n^P(i)|n\rangle\langle n|$ for all $i \in \Omega_\mathsf{P}$, and define a matrix $\mathfrak{S}(\mathsf{P})$ by $\mathfrak{S}_{nm}(\mathsf{P}) = (1 - d_{nm}^2(\mathsf{P}))^{-1}$ if $d_{nm}^2(\mathsf{P}) < 1$ for all n, m.

Proposition 2. If P is incoherent and $\mathfrak{S}(\mathsf{P}) * \mathsf{M}(i) \geqslant 0$ for all $i \in \Omega_\mathsf{M}$, then M and P are jointly measurable.

Proof. Define $C^P(j) \geqslant 0$ by $c_{nm}^P(j) = \sqrt{p_n^P(j)p_m^P(j)}$. Then $\mathsf{G}(i,j) := \mathfrak{S}(\mathsf{P}) * \mathsf{M}(i) * C^P(j) \geqslant 0$ by the assumption and the Schur product theorem. But $\sum_j \mathsf{G}(i,j) = \mathsf{M}(i)$, and $\sum_i \mathsf{G}(i,j) = \mathfrak{S}(\mathsf{P}) * \mathbb{1} * C^P(j) = \mathsf{P}(j)$ as P is incoherent. Hence G is a joint observable for M and P. $\blacksquare$

To appreciate how this result describes the coherence needed for incompatibility, note that the diagonal elements of P enter into the matrix $\mathfrak{S}(\mathsf{P})$, while the positivity condition describes the (lack of) coherence in M. More specifically, when the coherences $\mathrm{coh}_{nm}(\mathsf{M})$ are small enough relative to $1 - d_{nm}^2(\mathsf{P})$, then the off-diagonal elements $\langle n|\mathsf{M}(i)|m\rangle(1 - d_{nm}^2(\mathsf{P}))^{-1}$ of the matrix $\mathfrak{S}(\mathsf{P}) * \mathsf{M}(i)$ are small relative to the unit diagonal, and hence (e.g., by the Sylvester determinant criterion) the positivity condition $\mathfrak{S}(\mathsf{P}) * \mathsf{M}(i)$ of Proposition 2 will hold. This ensures the existence of a joint observable, showing that the (collective) coherence in M is *not* enough for incompatibility. In examples with suitable parametriza-

tion, this then translates into a lower bound for the coherence needed for incompatibility.

B. Basic examples

We now link the above results to the noise bounds for incompatibility [5,23–25]: consider

$$\mathsf{P}_\alpha(j) = \alpha|j\rangle\langle j| + (1-\alpha)d^{-1}\mathbb{1}, \quad 0 \leqslant \alpha \leqslant 1. \quad (2)$$

Let α_M be the minimal α for which a given observable M is incompatible with P_α; this is a way of quantifying incompatibility robustness of P_1 relative to M [23]. Now P_α has only one Hellinger distance; $d_{nm}^2(\mathsf{P}_\alpha) = 1 - g_d(\alpha)$ and $\mathfrak{S}_{nm}(\mathsf{P}_\alpha) = 1/g_d(\alpha)$ for $n \neq m$, with

$$g_d(\alpha) = \frac{1}{d}((d-2)(1-\alpha) + 2\sqrt{1-\alpha}\sqrt{1+(d-1)\alpha}).$$

Here $\alpha \mapsto d_{nm}^2(\mathsf{P}_\alpha)$ is monotone increasing, setting up a correspondence between α_M and the Hellinger distance, the latter providing a link to coherence via Propositions 1 and 2:

$$\max_{n, m \neq n} \mathrm{coh}_{nm}(\mathsf{M}) \leqslant g_d(\alpha_\mathsf{M}) \leqslant \max_{n,i} \sum_{m \neq n} \frac{|\langle n|\mathsf{M}(i)|m\rangle|}{p_n^M(i)}.$$

The upper bound follows from Proposition 2, as $\mathfrak{S}(\mathsf{P}_\alpha) * \mathsf{M}(i)$ is diagonally dominant [47], hence PSD, if $g_d(\alpha)$ exceeds this bound. As a simple example take a qubit with σ_z basis as the incoherent basis. Then $\mathsf{P}_\alpha(0) = \frac{1}{2}(\mathbb{1} + \alpha\sigma_z)$, so *any* observable M with $\mathrm{coh}_{01}(\mathsf{M}) > g_2(\alpha) = \sqrt{1-\alpha^2}$ is incompatible with P_α. If M is binary with $\mathsf{M}(0) = \frac{1}{2}(\mathbb{1} + \mathbf{m} \cdot \sigma)$, we have

$$1 \leqslant \frac{g_2(\alpha_\mathsf{M})^2}{m_1^2 + m_2^2} \leqslant \max\left\{\frac{1}{1+m_3}, \frac{1}{1-m_3}\right\}.$$

We can check this using the standard qubit criterion [48], according to which $g_2(\alpha_\mathsf{M})^2 = (m_1^2 + m_2^2)/(1 - m_3^2)$; hence our bounds are exact if and only if (iff) $m_3 = 0$.

Next we obtain a quick proof for the known noise bound for the incompatibility of MUBs [19,25–28].

Proposition 3. Let $\mathsf{M}(i) = \lambda\mathsf{Q}_0(i) + (1-\lambda)d^{-1}\mathbb{1}$ where Q_0 is mutually unbiased to the incoherent basis. Then $\alpha_\mathsf{M} = g_d(\lambda)$ for any $\lambda \in [0, 1]$.

Proof. The crucial observation is that $\mathsf{M} = C * \mathsf{Q}_0$, where C has unit diagonal and $c_{nm} = \lambda$ for $n \neq m$. Hence $\mathrm{coh}_{nm}(\mathsf{M}) = \lambda$, so $\lambda \leqslant g_d(\alpha)$ by Proposition 1 if M and P_α are jointly measurable. Conversely, if $\lambda \leqslant g_d(\alpha)$ then $\mathfrak{S}(\mathsf{P}_\alpha) * C \geqslant 0$, so $\mathfrak{S}(\mathsf{P}_\alpha) * \mathsf{M}(i) = \mathfrak{S}(\mathsf{P}_\alpha) * C * \mathsf{Q}_0(i) \geqslant 0$, so P_α and M are jointly measurable by Proposition 2. Therefore $\alpha_\mathsf{M} = g_d(\lambda)$ as $g_d^{-1} = g_d$ on [0,1]. $\blacksquare$

We note that $g_d(\lambda)$ is precisely the bound obtained in the cited literature by other methods. We will return to this example later.

III. INCOMPATIBILITY DUE TO A COHERENCE PATTERN

Here we specialize to the physically relevant class of observables, introducing first their general structure, and then focusing on the spin-boson model.

A. General consideration of coherence matrices

Starting with a brief motivation, we consider again the above qubit example: when $m_3 = 0$, we have $\mathsf{M} = C * \mathsf{Q}_0$ where C is a PSD matrix with $c_{00} = c_{11} = 1$, $c_{01} = m_1 - im_2$, and $\mathsf{Q}_0(0) = \frac{1}{2}(\mathbb{1} + \sigma_x)$. Note that $\mathrm{coh}_{01}(\mathsf{Q}_0) = 1$ (maximal coherence), and M is a "noisy" version of Q_0 obtained via *pure decoherence* [29,31,39]. The same structure appears in the case of MUBs (proof of Proposition 3), in any dimension. Accordingly, we call any PSD matrix C with unit diagonal a coherence (pattern) matrix, and consider noisy observables $\mathsf{M}(i) = C * \mathsf{Q}(i)$. In the special case where Q_0 is maximally coherent, we have $\mathrm{coh}_{nm}(\mathsf{M}) = |c_{nm}|$ so the coherence in M is "imprinted" by C. This setting captures a remarkable interplay of maximal incompatibility and coherence. Indeed, in Appendix C we use dilation theory to prove the following result:

Theorem 1. Let C be a coherence matrix and Q_0 a maximally coherent observable. If an incoherent observable P is jointly measurable with $C * \mathsf{Q}_0$, it is jointly measurable with $C * \mathsf{Q}$ for *every* observable Q.

Hence, any maximally coherent observable (such as one mutually unbiased to the incoherent basis) is also maximally incompatible in this setting (which is not true in general [25]). Incompatibility arising from coherence is now described as follows:

Definition 1. For a coherence matrix C, we denote by $\mathcal{C}_C$ the set of incoherent observables P jointly measurable with $C * \mathsf{Q}$ for every observable Q. If $\mathsf{P} \notin \mathcal{C}_C$ we say that P has incompatibility due to the coherence (pattern) C.

Note that to find out whether a given P lies in $\mathcal{C}_C$, it suffices (by Theorem 1) to check whether P is jointly measurable with $C * \mathsf{Q}_0$ for some *fixed* maximally coherent observable Q_0. The general results of the preceding section have the following useful corollaries:

Corollary 1. Let C be a coherence matrix. Any $\mathsf{P} \in \mathcal{C}_C$ has $d_{nm}^2(\mathsf{P}) \leqslant 1 - |c_{nm}|$ for all n, m.

Proof. Follows by Proposition 1, as $\mathrm{coh}_{nm}(C * \mathsf{Q}_0) = |c_{nm}|$. ∎

Corollary 2. Let C be a coherence matrix and P an incoherent observable. If $C * \mathfrak{S}(\mathsf{P}) \geqslant 0$ then $\mathsf{P} \in \mathcal{C}_C$.

Proof. Let Q be an arbitrary observable, and $\mathsf{M} = C * \mathsf{Q}$. Then $\mathfrak{S}(\mathsf{P}) * \mathsf{M}(i) = (C * \mathfrak{S}(\mathsf{P})) * \mathsf{Q}(i) \geqslant 0$ by the Schur product theorem, so P is jointly measurable with M by Proposition 2, hence $\mathsf{P} \in \mathcal{C}_C$. ∎

The coherence matrix model is strongly motivated by open quantum systems. In fact, quantum coherence is notoriously fragile against noise, and one of the basic mechanisms by which it decays is *pure decoherence* (i.e., no dissipation), typically arising as subsystem dynamics from a unitary evolution on a larger system which leaves the incoherent basis unchanged (see Chap. 4 of [31]). While incompatibility seems rarely tractable under general dynamics (see [37] for a qubit case), our theory applies neatly to this type of dynamics. Each incoherent observable represents a conserved quantity, whose incompatibility with all other system observables is lost when the decaying coherence fails to sustain it; this characterizes the emergent classicality of the open system in a more operational way than the decoherence itself.

More formally, suppose we have a family of coherence matrices $C[\lambda]$ depending on a parameter $\lambda \in [0, 1]$. If $\lambda = \lambda(t)$ depends on a time parameter $0 \leqslant t < \infty$, the map $\Lambda_t(\rho) := C[\lambda(t)] * \rho$ defines a quantum dynamical map, i.e., a family of completely positive trace-preserving maps on the set of density matrices. A natural "Markovianity" property in this setting is

$$C[\lambda\lambda'] = C[\lambda] * C[\lambda'], \quad \lambda, \lambda' \in [0, 1], \tag{3}$$

which leads to the CP-divisibility of the dynamical map if the function $\lambda(t)$ is monotone decreasing. Then the loss of incompatibility is irreversible, and (as the Heisenberg picture evolution has the same form) the above corollaries can be used to bound the critical time at which a given incoherent observable loses its incompatibility by entering the set $\mathcal{C}_{\lambda(t)}$. Next we show, by considering a specific model, that this approach is amenable to analytical results even in large systems.

B. Spin-boson model

We consider the spin-boson model with collective interaction [31–33]: N qubits coupled to bosonic modes b_k via the total spin $S_z = \frac{1}{2} \sum_{l=1}^{N} \sigma_z^{(l)}$. The total Hamiltonian is

$$H = H_S + \sum_k \omega_k b_k^\dagger b_k + \sum_k S_z(g_k b_k^\dagger + \bar{g}_k b_k),$$

where $H_S = \omega_0 S_z$ is the system Hamiltonian. The incoherent basis is the σ_z basis $\{|\mathbf{m}\rangle\}$, where $\mathbf{m} = (m_1, \ldots, m_N)$, and we let $|\mathbf{m}| = \sum_l m_l$. With the bath initially in a thermal state, the system state at time t is $\rho(t) = C[\lambda(t)] * \rho_0$, where $C[\lambda]$ is the coherence matrix $c_{\mathbf{n},\mathbf{m}}[\lambda] = \lambda^{(|\mathbf{n}|-|\mathbf{m}|)^2}$, and $\lambda(t) \in [0, 1]$ is given by the bath temperature and spectral density (see Sec. 4.2 of [31]). In the Heisenberg picture, the dynamics transform the system observables Q into $C[\lambda(t)] * \mathsf{Q}$, which is precisely of the form considered above, and has the divisibility property (3). The task is to characterize the set $\mathcal{C}_{C[\lambda]}$ for $\lambda \in [0, 1]$.

If $t \mapsto \lambda(t)$ is monotone decreasing (as in p. 230 of [31]), the loss of incompatibility is irreversible due to (3). However, the model also has decoherence-free subspaces (DFSs) $\mathcal{D}_j = \mathrm{span}\{|\mathbf{n}\rangle \mid |\mathbf{n}| = j\}$ [33–36]; basis elements in the same DFS have $c_{\mathbf{n},\mathbf{m}}[\lambda] = 1$ for all λ. By Corollary 1, each DFS "protects" the incompatibility of any P not proportional to $\mathbb{1}$ inside it. Observables P exhibiting a transition to classicality therefore have $p_{\mathbf{n}}^\mathsf{P} = p_{\mathbf{m}}^\mathsf{P}$ when $|\mathbf{n}\rangle, |\mathbf{m}\rangle$ lie in the same DFS. In Appendix D we show that for these P the problem reduces to an $(N + 1)$-dimensional space with incoherent basis $\{|k\rangle\}$ indexed by the DFS labels $k = 0, \ldots, N$: we have $\mathsf{P} \in \mathcal{C}_{C[\lambda]}$ iff $\tilde{\mathsf{P}} \in \mathcal{C}_{\tilde{C}[\lambda]}$ where $p_k^{\tilde{\mathsf{P}}} = p_{\mathbf{n}}^\mathsf{P}$ for $|\mathbf{n}\rangle \in \mathcal{D}_k$, and the coherence matrix is

$$\tilde{C}[\lambda] = \begin{pmatrix} 1 & \lambda & \lambda^4 & \cdots & \cdots & \lambda^{N^2} \\ \lambda & 1 & \lambda & \ddots & & \vdots \\ \lambda^4 & \lambda & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \lambda & \lambda^4 \\ \vdots & & \ddots & \lambda & 1 & \lambda \\ \lambda^{N^2} & \cdots & \cdots & \lambda^4 & \lambda & 1 \end{pmatrix}. \tag{4}$$
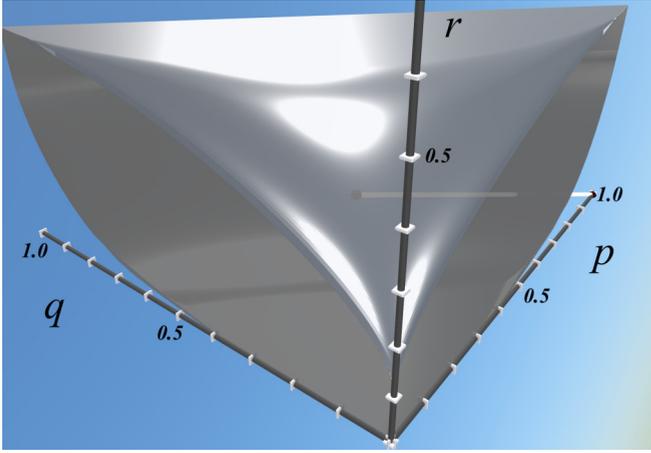
FIG. 1. The convex set $\mathcal{C}^{\text{sym}}_{C[\lambda]}$ for $N = 2$, $\lambda = 0.7$, parametrized by (p, q, r) where $p = p^{\mathsf{P}}_1(0)$, $q = p^{\mathsf{P}}_4(0)$, $r = p^{\mathsf{P}}_2(0) = p^{\mathsf{P}}_3(0)$. The line $\{\mathsf{P}^C_\alpha \mid \alpha \in [0, 1]\}$ is shown connecting $(\frac{1}{4}, \frac{1}{4}, \frac{1}{4})$ to $(1, 0, 0)$; it enters the set at $\alpha = \alpha_2(0.7) \approx 0.58$.

We further focus on the measurements of the DFS label $j = 0, \ldots, N$ which are *covariant* for the permutation $j \mapsto N - j$ leaving $C[\lambda]$ invariant, i.e., $p^{\mathsf{P}}_{\mathbf{n}}(j) = p^{\mathsf{P}}_{\mathbf{m}}(N - j)$ when $|\mathbf{n}| = N - |\mathbf{m}|$. We denote by $\mathcal{C}^{\text{sym}}_{C[\lambda]}$ the set of covariant $\mathsf{P} \in \mathcal{C}_{C[\lambda]}$. This set has affine dimension $\frac{1}{2}N(N + 1)$, and we find it analytically for $N = 2$ in Appendix G (see Fig. 1). In Sec. IV C and Appendix D we develop a general theory of covariance systems for coherence matrices.

For larger N we focus on covariant observables $\mathsf{P}^C_\alpha := \alpha \mathsf{P}^C + (1 - \alpha)\mathsf{P}^C_{\text{dep}}$, $\alpha \in [0, 1]$, where P^C is the spectral resolution of H_S [so $\mathsf{P}^C(j)$ is the projector onto the DFS $\mathcal{D}_j$], and $\mathsf{P}^C_{\text{dep}}$ its depolarization $\mathsf{P}^C_{\text{dep}}(j) := \frac{1}{2^N}\text{tr}[\mathsf{P}^C(j)]\mathbb{1} = c_N(j)\mathbb{1}$ into the "coin toss" distribution $c_N(j) = \binom{N}{j}\frac{1}{2^N}$. The proportion of $\{\mathsf{P}^C_\alpha \mid \alpha \in [0, 1]\}$ having lost incompatibility at time t is $\alpha_N(\lambda(t))$ where

$$\alpha_N(\lambda) := \max\{\alpha > 0 \mid \mathsf{P}^C_\alpha \in \mathcal{C}_{C[\lambda]}\}.$$

With reduction (4) we find $\alpha_N(\lambda) = \max\{\alpha > 0 \mid \tilde{\mathsf{P}}^C_\alpha \in \mathcal{C}_{\tilde{C}[\lambda]}\}$, where $\tilde{\mathsf{P}}^C_\alpha(j) = \alpha|j\rangle\langle j| + (1 - \alpha)c_N(j)\mathbb{1}$. The task is to find analytical bounds for $\alpha_N(\lambda)$. For $N = 2$ we can explicitly solve (Appendix G) $\alpha_2(\lambda) = 1 - \frac{4\lambda^2}{3 + \lambda^4 + 2\sqrt{2}(1 - \lambda^2)}$. Crucially, the Hellinger distances are tractable for *any* N: $d_{kk'}(\tilde{\mathsf{P}}^C_\alpha) = 1 - \beta_{kk'}(\alpha)$ when $k \neq k'$, with $\beta_{kk'}(\alpha) = 1 - \alpha + u_k + u_{k'}$, $u_k = \sqrt{c_N(k)(1 - \alpha)(\alpha + c_N(k)(1 - \alpha))} - c_N(k)(1 - \alpha)$. Each $\alpha \mapsto \beta_{kk'}(\alpha)$ is decreasing in α; using the inverse functions $[\beta_{01}]^{-1}$, $[\beta_{00}]^{-1}$ we set $U_N(\lambda) = [\beta_{01}]^{-1}(\lambda)$ and $L_N(\lambda) = [\beta_{00}]^{-1}(1 - \vartheta_3(\frac{\pi}{2}, \lambda))$, where $\vartheta_3(x, \lambda) = 1 + 2\sum_{k=1}^\infty \lambda^{k^2}\cos(2kx)$ is the Jacobi theta function [49]. The following result holds:

Proposition 4. $\vartheta_3(\frac{\pi}{2}, \lambda) \leqslant L_N(\lambda) \leqslant \alpha_N(\lambda) \leqslant U_N(\lambda)$ for all $N = 1, 2, \ldots$, and $\lambda \in [0, 1]$.

Proof. We fix $\lambda \in [0, 1]$ (and hence also $\tilde{C}[\lambda]$, $U_N = U_N(\lambda)$, $L_N = L_N(\lambda)$, $\alpha_N = \alpha_N(\lambda)$). Now if α is such that $\tilde{\mathsf{P}}^C_\alpha \in \mathcal{C}_{\tilde{C}}$, then $\lambda \leqslant \beta_{01}(\alpha)$ by Corollary 1, i.e., $U_N \geqslant \alpha$, so $U_N \geqslant \alpha_N$; this establishes the upper bound. For the lower bounds, define $B = (b_{nm})$ by $b_{nm} = 1/\beta_{nm}$ for each n, m.

(Notice that $\beta_{nn} \neq 1$, as $1 - \beta_{nm}$ only coincides with the corresponding Hellinger distance on the off-diagonal elements.) Now $B \geqslant 0$, as $b_{nm} = \int_0^1 x^{\beta_{nm}-1}dx = \int_0^1 x^{-\alpha}x^{u_n}x^{u_m}dx$. Now $b_{nm} = (1 - d^2_{nm}(\tilde{\mathsf{P}}^C_\alpha))^{-1}$ when $n \neq m$, but $b_{nn} = 1/\beta_{nn} \geqslant 1$, so $\tilde{C} * \mathfrak{S}(\tilde{\mathsf{P}}^C_\alpha) = \tilde{C} * B + D$ with D diagonal, $d_{nn} = 1 - b_{nn}$. Since $B \geqslant 0$, we get $(\tilde{C} - r\mathbb{1}) * B \geqslant 0$, where r is the bottom eigenvalue of $\tilde{C}$. By the theory of Toeplitz matrices (pp. 194 and 211 of [50], and Lemma 1 of [49]),

$$r \geqslant \min_{x \in [0, 2\pi]}\sum_{k=-\infty}^\infty \tilde{c}_{k0}\, e^{ikx} = \min_{x \in [0, 2\pi]}\vartheta_3\left(\frac{x}{2}, \lambda\right) = \vartheta_3\left(\frac{\pi}{2}, \lambda\right).$$

Hence, if $\vartheta_3(\frac{\pi}{2}, \lambda) \geqslant 1 - \beta_{00}(\alpha)$ then $\tilde{C} * \mathfrak{S}(\tilde{\mathsf{P}}^C_\alpha) \geqslant r(\mathbb{1} - D) + D \geqslant (1 - \beta_{00})(\mathbb{1} - D) + D \geqslant 0$ as $1 - \beta_{00} = \max_n(1 - \beta_{nn})$, and so $\tilde{\mathsf{P}}^C_\alpha \in \mathcal{C}_{\tilde{C}}$ by Corollary 2. Hence $\tilde{\mathsf{P}}^C_\alpha \in \mathcal{C}_{\tilde{C}}$ for all $\alpha \leqslant L_N$, so $\alpha_N \geqslant L_N$. Finally, $\vartheta_3(\frac{\pi}{2}, \lambda) \leqslant L_N$ since $\alpha \geqslant 1 - \beta_{00}(\alpha)$ for all α. This completes the proof. ∎

Figure 2 shows the bounds for $N = 2, 10$, and the analytical curve $\alpha_2(\lambda)$ with a numerical consistency check (blue dots) computed with a generic joint measurability SDP available in [51] applied to $(\tilde{C}[\lambda] * \mathsf{Q}_0, \tilde{\mathsf{P}}^C_\alpha)$ (see Theorem 1). This SDP is not practical for large N; to compute $\alpha_{10}(\lambda)$ we used the efficient SDP (5) adapted to our setting as described in the next section (implemented in PYTHON [52]). Proposition 4 says that at any time t, at least the proportion $1 - U_N(\lambda(t))$ of the line $\{\mathsf{P}^C_\alpha \mid \alpha \in [0, 1]\}$ has incompatibility due to coherence, while at least the proportion $L_N(\lambda(t)) \geqslant \vartheta_3(\frac{\pi}{2}, \lambda(t))$ has lost it. Remarkably, the last bound is independent of N; i.e., it holds for any system size. Finally, the bound U_N is tight near the classical limit (small λ):

Proposition 5. For each fixed N, the curves $\alpha = \alpha_N(\lambda)$ and $\alpha = U_N(\lambda)$ have the same asymptotic form: $\lambda = \frac{1 + \sqrt{N}}{2^{N/2}}\sqrt{1 - \alpha} + O(1 - \alpha)$ as $\alpha \to 1$ ($\lambda \to 0$).

We prove this (Appendix H) by explicitly constructing relevant joint observables in the operational framework of the next section. Note that the square-root behavior near the classical limit is distinct from the "middle" regime for λ,
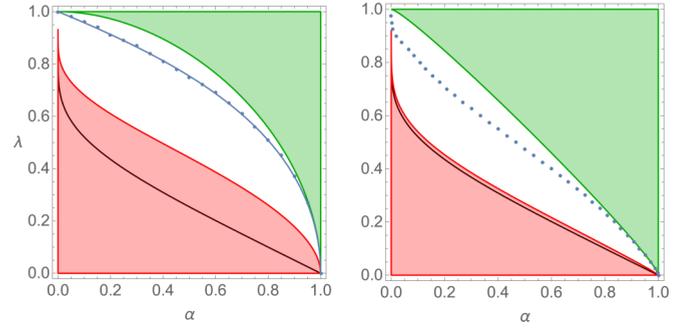

FIG. 2. Incompatibility of the incoherent observables arising as α-weighted averages of the system Hamiltonian and its depolarization, in the spin-boson model with coherence parameter λ, for $N = 2$ (left) and $N = 10$ (right). The green (red) region has incompatibility (loss thereof) "certified" by the *analytical* bound U_N (L_N) of Proposition 4. Below the $\vartheta_3(\frac{\pi}{2}, \lambda)$ bound (black line), incompatibility is lost for *all* N. The true boundary α_N is given for comparison, by a semidefinite program (SDP) (blue dots), and analytically for $N = 2$ (solid blue line).

where $U_N(\lambda)$ decreases towards $1 - \lambda$ as N increases. Clearly, incompatibility is much more intricate than the coherence which sustains it in this model.

IV. OPERATIONAL FRAMEWORK FOR COHERENCE AND INCOMPATIBILITY

Having demonstrated our theory in applications, we now gain further insight by reformulating it in resource-theoretic terms, in the context of quantum measurement theory.

A. Resource-theoretic aspects

Here we describe how our theory formally integrates into the resource theory of quantum coherence, and especially measurement coherence. We stress that our aim is *not* to develop a comprehensive joint resource theory for coherence and incompatibility, but rather to focus on the most relevant aspects.

The "free resources" are the incoherent observables $P(i) = \sum_n p_n^P(i)|n\rangle\langle n|$ [6,7] already used above; they are jointly measurable with each other. Their nonclassicality is quantified by the Hellinger distances: $d_{nm}^2(P_1) = 1$ for all $n \neq m$, while $d_{nm}(P) = 0$ for all n, m iff each $P(j)$ is a multiple of the identity, i.e., P is jointly measurable with *every* observable. An observable P is incoherent iff $\mathrm{coh}_{nm}(P) = 0$ for all $n \neq m$.

Any quantum channel, a completely positive (CP) trace-preserving map Λ, is a "free operation" for incompatibility [5,11,13], acting on observables via preprocessing $\Lambda^*(M)(i) = \Lambda^*(M(i))$, where Λ^* is defined by $\mathrm{tr}[\Lambda^*(X)\rho] = \mathrm{tr}[X\Lambda(\rho)]$ for all matrices X, ρ. If $\Lambda(|n\rangle\langle n|) = |n\rangle\langle n|$ for all n, i.e., Λ leaves each incoherent observable unchanged, then Λ is also "free" for coherence, called a genuinely incoherent operation (GIO) [4,38]. These have already appeared in our setting: each GIO has the form $\Lambda_C^*(M)(i) = C * M(i)$ for some coherence matrix C [4,29]. The entrywise coherence is monotonic in GIOs, as $\mathrm{coh}_{nm}(\Lambda_C^*(M)) = |c_{nm}|\mathrm{coh}_{nm}(M) \leqslant \mathrm{coh}_{nm}(M)$.

Observables are measured by instruments $I = (I_i)_{i\in\Omega}$, where each I_i is a CP map such that $\sum_i I_i$ is a channel [45]. The observable measured by I is $M(i) = I_i^*(\mathbb{1})$. For a state (density matrix) ρ the postmeasurement state given outcome i is $I_i(\rho)$. Instruments are needed for sequential implementation of joint measurements: measuring first M with I, and then an observable F, we get a joint POVM $G(i, j) = I_i^*(F(j))$ for M and $\Lambda^*(F)$. Joint measurements usually do not have sequential implementations (unless one "cheats" by allowing a larger output space; see Proposition 2 of [53]). We define a genuinely incoherent instrument (GII) as one whose channel $\sum_i I_i$ is a GIO. It follows (Appendix B) that any GII with channel Λ_C has the form $I_i^*(X) = C(i) * X$ for some PSD matrices $C(i)$ with $\sum_i C(i) = C$; we call C the coherence matrix of I. GIIs are free operations also for coherence: they cannot create coherent observables from incoherent ones by sequential combination. The observable measured by a GII is incoherent, namely, $P(i) := I_i^*(\mathbb{1}) = \sum_n c_{nn}(i)|n\rangle\langle n|$.

B. Sequential measurement setting

Given the above concepts, the operational scheme in Fig. 3 naturally emerges; in this setting, coherence needed for incompatibility can now be characterized as follows:
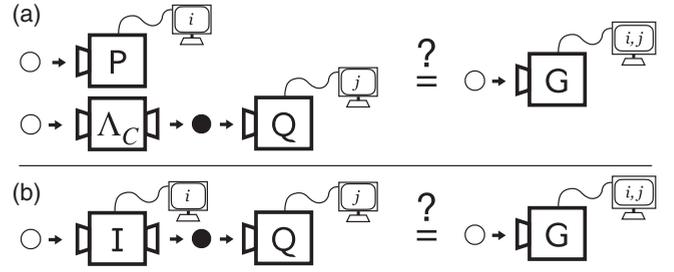

FIG. 3. (a) Operational setting for linking incompatibility and coherence. Here P is an incoherent observable and Λ_C a channel which imprints a coherence pattern $C = (c_{nm})$ into a coherent observable Q by Hadamard multiplication. If $C * Q$ is jointly measurable with P (via a joint POVM G) for *every* Q, the coherence C cannot sustain any (pairwise) incompatibility involving P, and we write $P \in \mathcal{C}_C$. (b) Sequential implementation of the joint POVM G in (a), given a GII I with observable P and channel Λ_C. By Theorems 1 and 2, the existence of I is equivalent to joint measurability in (a) when Q is a maximally coherent.

Theorem 2. Let C be a coherence matrix and P an incoherent observable. The following are equivalent:

(i) $P \in \mathcal{C}_C$.

(ii) There exists a GII with coherence matrix C and observable P, that is, matrices $C(j)$ satisfying

$$C(j) \geqslant 0, \qquad \sum_j C(j) = C, \qquad c_{nn}(j) = p_n^P(j). \qquad (5)$$

In that case a joint measurement of P and $C * Q$, for any observable Q, can be implemented sequentially by first measuring P using the GII in (ii), and subsequently Q.

The crucial part of the proof of this result is the construction of the special joint observable given in the proof of Theorem 1 (see Appendix C). The result is surprising, as joint observables with a GII implementation are quite special, requiring channel-observable compatibility [40–42]. We note that (5), as a SDP [54], is more efficient than a generic joint measurability SDP due to lower dimensionality, but still not analytically solvable except in simple cases (see Appendix F for a $d = 3$ example). However, there is a useful class of GIIs: for each incoherent observable P define $C^P(j)$ as in the proof of Proposition 2; this is a GII with coherence matrix C^P given by the Hellinger distances, $c_{nm}^P = \sum_j c_{nm}^P(j) = 1 - d_{nm}^2(P)$. Following the proof of Proposition 2 we obtain a GII for the setting in Corollary 2:

Proposition 6. If $C * \mathfrak{S}(P) \geqslant 0$ then $C(j) = C * \mathfrak{S}(P) * C^P(j)$ defines a GII with coherence matrix C and observable P.

Proof. Now $\sum_j C(j) = C * \mathfrak{S}(P) * \sum_j C^P(j) = C$, and $c_{nn}(j) = c_{nn}^P(j) = p_n^P(j)$. If $C * \mathfrak{S}(P) \geqslant 0$ then $C(j) \geqslant 0$ by the Schur product theorem, so (5) holds for $C(j)$. ∎

As an example of a GII we consider the qubit case:

$$C = \begin{pmatrix} 1 & c \\ \bar{c} & 1 \end{pmatrix}, \quad P(j) = \begin{pmatrix} p_j & 0 \\ 0 & q_j \end{pmatrix}, \quad j \in \mathbb{N},$$

with $c \in \mathbb{C}$, $|c| \leqslant 1$, and (q_j), (p_j) being probability distributions. The Hellinger distance is $d_{01}^2(P) = 1 - \gamma$ with $\gamma = \sum_j \sqrt{p_j q_j}$, and we obtain $P \in \mathcal{C}_C$ iff $|c| \leqslant \gamma$. Indeed, $P \in \mathcal{C}_C$ implies $|c| \leqslant \gamma$ by Corollary 1, while $|c| \leqslant \gamma$ implies $P \in \mathcal{C}_C$

by Corollary 2, with the GII

$$C(j) = \begin{pmatrix} p_j & c\gamma^{-1}\sqrt{q_j p_j} \\ \overline{c}\gamma^{-1}\sqrt{q_j p_j} & q_j \end{pmatrix}.$$

Revisiting the noisy MUB example (see Proposition 3), we note that any $-(d-1)^{-1} \leqslant \lambda \leqslant 1$ defines a valid coherence matrix C, and P_α is an incoherent observable for the same range of α. When $\lambda < 0$ the bounds of Corollaries 1 and 2 do not coincide, but our general method applies (Appendix E), reproducing the result in [28], and (additionally) yielding a sequential GII implementation for all jointly measurable cases, including the "corner" $\lambda = \alpha = -(d-1)^{-1}$ where the Lüders instrument fails. We consider this interesting exceptional case here, and postpone the rest of the proof to the Appendix. We have $\mathsf{P}_\alpha(j) = (d-1)^{-1}(\mathbb{1} - |j\rangle\langle j|)$, and

$$C = d(d-1)^{-1}(\mathbb{1} - |\phi_d\rangle\langle\phi_d|),$$

where $\phi_d = d^{-\frac{1}{2}}\sum_k |k\rangle$. In this case the two corollaries do not tell us anything: the tradeoff in Corollary 1 is not violated, and the matrix in Corollary 2 is not positive semidefinite. However, now $\mathsf{P}_\alpha \in \mathcal{C}_C$ directly by Theorem 2, as we can construct a GII $C(j)$ satisfying (5):

$$C(j) := (d-2)^{-1}(\mathbb{1} - |\phi_d\rangle\langle\phi_d| - |\varphi_d^j\rangle\langle\varphi_d^j|),$$

where $\varphi_d^j := \sqrt{d(d-1)^{-1}}(|j\rangle - d^{-\frac{1}{2}}\phi_d)$. Indeed, positivity follows from the fact that φ_d^j is orthogonal to ϕ_d for each j [so each $C(j)$ is a multiple of a projection], and it is easy to check that $\sum_j C(j) = C$ and $c_{nn}(j) = (d-1)^{-1}(1 - \delta_{jn}) = p_n^{\mathsf{P}_\alpha}(j)$.

In addition to these examples, in Appendix H we explicitly construct a GII for the spin-boson model: it establishes the tight bound for the coherence needed for incompatibility near the classical limit, and proves Proposition 5.

C. Reduction by symmetry

One of the main obstacles in our joint measurability problem is the difficulty of finding the form of a suitable GII. Symmetries in the coherence pattern C can be used to simplify the search, and also single out relevant incoherent observables. We outline this reduction here; detailed derivations are given in Appendix D.

First note that the matrix D of a unitary GIO $\Lambda_D(\rho) = U^\dagger\rho U$ has $d_{nm} = u_n\overline{u_m}$ with $|u_n| = 1$ for all n; then Λ_D changes neither incompatibility nor coherence. For coherence matrices C, C', we write $C \simeq C'$ if $C = D * C'$ for a unitary GIO Λ_D. Clearly, $\mathcal{C}_C = \mathcal{C}_{C'}$.

Second, we call an incoherent P *adapted to* C if $p_n^{\mathsf{P}} = p_m^{\mathsf{P}}$ (P does not distinguish n from m) whenever (n, m) has maximal coherence $|c_{nm}| = 1$. Crucially, each $\mathsf{P} \in \mathcal{C}_C$ is adapted to C, as $|c_{nm}| = 1$ implies $d_{nm}^2(\mathsf{P}) = 0$ by Corollary 1. So every P *not* adapted to C has incompatibility due to coherence. Now $\{1, \ldots, d\}$ splits into $n_C \leqslant d$ disjoint equivalence classes $I_k^C, k \in \Omega_C := \{1, \ldots, n_C\}$, such that $I_k^C = \{m \mid |c_{nm}| = 1\}$ for any $n \in I_k^C$. Let $\tilde{\mathcal{H}}$ be the Hilbert space with incoherent basis $\{|k\rangle\}_{k \in \Omega_C}$ and define $L : \tilde{\mathcal{H}} \to \mathcal{H}$ by $L|k\rangle = \sum_{n \in I_k^C} |n\rangle$. Then $C \simeq L\tilde{C}L^\dagger$ for a "reduced" coherence matrix $\tilde{C}$ acting on $\tilde{\mathcal{H}}$.

As an example, consider the spin-boson model: we have the coherence matrix $C = C[\lambda]$ with $n_C = N + 1$ equivalence

classes $I_k^C = \{\mathbf{n} \mid \sum_l n_l = k\}, k \in \Omega_C = \{0, 1, \ldots, N\}$ of size $|I_k^C| = \binom{N}{k}$, corresponding to the decoherence-free subspaces span$\{|\mathbf{n}\rangle \mid \mathbf{n} \in I_k^C\}$. The resulting reduced coherence matrix $\tilde{C}$ is easily seen to be the one given by (4).

Next, let S_d, the group of permutations of $\{1, \ldots, d\}$, act on $\mathcal{H}$ via $U_\pi|n\rangle = |\pi(n)\rangle$. We define

$$G_C := \{\pi \in S_d \mid U_\pi^\dagger C U_\pi \simeq C\}.$$

In Appendix D we show that G_C is a permutation group, i.e., a subgroup of S_d, and we call it the symmetry group of C. It moves each class I_k^C as a whole, and hence gives rise to a map $\phi : G_C \to G_{\tilde{C}}$ through $\pi(I_k^C) = I_{\phi(\pi)(k)}^C$. Now let G be any subgroup of G_C. We then say that an incoherent observable P is G covariant if it has outcome set Ω_C, and $p_{\pi^{-1}(n)}^{\mathsf{P}}(j) = p_n^{\mathsf{P}}(\phi(\pi)(j))$ for $\pi \in G$, $j \in \Omega_C$. These observables have their outcomes directly linked to the equivalence classes of the basis labels. The joint measurability problem reduces considerably when restricted to them; we set

$$\mathcal{C}_C[G] := \{\mathsf{P} \in \mathcal{C}_C \mid \mathsf{P} \text{ is } G \text{ covariant}\}.$$

The case of the full symmetry group is denoted by $\mathcal{C}_C^{\text{sym}} := \mathcal{C}_C[G_C]$. In Appendix D we show that for $\mathsf{P} \in \mathcal{C}_C^{\text{sym}}$, the SDP (5) can be constrained by a corresponding covariance condition at the GII level without any loss. Furthermore, we also link the incoherent observables on $\tilde{\mathcal{H}}$ and $\mathcal{H}$ as $\mathcal{L}(|k\rangle\langle k|) = \sum_{n \in I_k^C} |n\rangle\langle n|$; the reduction by symmetry is then given by

$$\mathcal{C}_C^{\text{sym}} = \{\mathcal{L}(\mathsf{P}(\cdot)) \mid \mathsf{P} \in \mathcal{C}_{\tilde{C}}[\phi(G_C)]\}. \tag{6}$$

We note that $\phi(G_C)$ may be different from $G_{\tilde{C}}$. However, they coincide when $|I_k^C| = |I_{\pi(k)}^C|$ for each $\pi \in G_{\tilde{C}}$ and $k \in \Omega_C$; i.e., the equivalence classes linked by permutations in the reduced symmetry group have equal size. In that case we have the straightforward reduction $\mathcal{C}_C^{\text{sym}} = \{\mathcal{L}(\mathsf{P}(\cdot)) \mid \mathsf{P} \in \mathcal{C}_{\tilde{C}}^{\text{sym}}\}$. An example is provided by the spin-boson model, where the reduced coherence matrix $\tilde{C} = \tilde{C}[\lambda]$ is invariant under the exchange permutation π_0 defined by $\pi_0(k) = N - k$ for $k \in \Omega_C$. In fact, $G_{\tilde{C}} = \{e, \pi_0\}$ for all λ, and $|I_k^C| = |I_{\pi_0(k)}^C|$ for each k, so $\phi(G_C) = \{e, \pi_0\}$. Hence, by (6), the set $\mathcal{C}_C^{\text{sym}}$ is isomorphic to $\mathcal{C}_{\tilde{C}}^{\text{sym}}$, as stated in Sec. III B.

Finally, we give a simple example involving also complex phase factors, and demonstrating the case $\phi(G_C) \neq G_{\tilde{C}}$. Let $\lambda \in [0, 1)$, and consider the following:

$$C := \begin{pmatrix} 1 & i & \lambda i \\ -i & 1 & \lambda \\ -\lambda i & \lambda & 1 \end{pmatrix} \simeq \begin{pmatrix} 1 & 1 & \lambda \\ 1 & 1 & \lambda \\ \lambda & \lambda & 1 \end{pmatrix} \longrightarrow \tilde{C} = \begin{pmatrix} 1 & \lambda \\ \lambda & 1 \end{pmatrix}.$$

Here $d = 3$, $n_C = 2$, $\Omega_C = \{1, 2\}$, $I_1^C = \{1, 2\}$, $I_2^C = \{3\}$, $G_C = \{e, (12)\}$, $G_{\tilde{C}} = S_2$, and $\phi(G_C) = \{e\}$. Note that the symmetry of C is "revealed" after factoring out a unitary GIO in the first step. As a further subtlety, the exchange symmetry of $\tilde{C}$ is excluded as $|I_1^C| \neq |I_2^C|$. The point of the reduction is that we can use the simpler two-dimensional case to solve the original three-dimensional joint measurability problem. Indeed, we first characterize $\mathcal{C}_{\tilde{C}}[\{e\}]$ as described in the qubit case after Proposition 6 above, and then use (6): $\mathcal{C}_C^{\text{sym}}$ consists

of the binary observables P of the form

$$\mathsf{P}(1) = \begin{pmatrix} p & 0 & 0 \\ 0 & p & 0 \\ 0 & 0 & q \end{pmatrix}, \quad \mathsf{P}(2) = \mathbb{1} - \mathsf{P}(1),$$

where $p, q \in [0, 1]$ and $\sqrt{pq} + \sqrt{(1-p)(1-q)} \geqslant \lambda$.

V. CONCLUSION

We considered a general operational setting where quantum coherence is tightly linked to measurement incompatibility. We derived two explicit conditions for the coherence needed for incompatibility, and demonstrated that these are amenable to analytical calculations even in large open quantum systems. Topics of further study include the infinite-dimensional case and adaptation to quantum steering.

ACKNOWLEDGMENTS

APPENDIX A: PROPERTIES OF THE ENTRYWISE COHERENCE

Recall that an observable is a POVM M on a Hilbert space $\mathcal{H} = \mathbb{C}^d$ with (finite) outcome set Ω_M, i.e., $\mathsf{M}(i) \geqslant 0$ for each $i \in \Omega_\mathsf{M}$, and $\sum_{i \in \Omega_\mathsf{M}} \mathsf{M}(i) = \mathbb{1}$. We assume that the outcome set is taken minimal, i.e., $\mathsf{M}(i) \neq 0$ for each $i \in \Omega_\mathsf{M}$. We fix a basis $\{|n\rangle \mid n = 1, \dots, d\}$ and call it the incoherent basis. For any observable we denote $p_n^\mathsf{M}(i) := \langle n|\mathsf{M}(i)|n\rangle$ for all $n \in \{1, \dots, d\}, i \in \Omega_\mathsf{M}$.

An observable M is incoherent if each POVM element $\mathsf{M}(i)$ is diagonal, i.e., $\mathsf{M}(i) = \sum_{n=1}^d p^\mathsf{M}(i)|n\rangle\langle n|$ for all $i \in \Omega_\mathsf{M}$. It is mutually unbiased to the incoherent basis if $\mathsf{M}(i) = |\psi_i\rangle\langle\psi_i|$ where $\{\psi_i \mid i \in \Omega_\mathsf{M}\}$ is a basis of $\mathcal{H}$ such that $|\langle n|\psi_i\rangle|^2 = d^{-1}$ for each $n \in \{1, \dots, d\}$ and $i \in \Omega_\mathsf{M}$. Note that incoherent observables can have arbitrary outcome set Ω_M, while $|\Omega_\mathsf{M}| = d$ for any if M is mutually unbiased to the incoherent basis.

In the main text we introduced the entrywise coherence and Hellinger distances for each $n, m \in \{1, \dots, n\}$:

$$\text{coh}_{nm}(\mathsf{M}) = \sum_{i \in \Omega_\mathsf{M}} |\langle n|\mathsf{M}(i)|m\rangle|,$$

$$d_{nm}^2(\mathsf{M}) = 1 - \sum_{i \in \Omega_\mathsf{M}} \sqrt{p_n^\mathsf{M}(i) p_m^\mathsf{M}(i)}.$$

We are not aware of the entrywise coherence having appeared in the literature as such, but it has been used recently in the construction of overall l_p-type measures [7]. Hellinger distance is a known f divergence [44], but (as far as we know) has not been used in the present context before. It is an actual metric in the space of probability distributions; in particular, if $d_{nm}^2(\mathsf{M}) = 0$ for some n, m, then $p_n^\mathsf{M}(i) = p_m^\mathsf{M}(i)$ for all $i \in \Omega_\mathsf{M}$. Furthermore, $0 \leqslant d_{nm}^2(\mathsf{M}) \leqslant 1$ by a simple application of the classical Schwarz inequality.

We say that M is maximally coherent if $\text{coh}_{nm}(\mathsf{M}) = 1$ for all $n, m = 1, \dots, d$. The following proposition summarizes the basic properties of the entrywise coherence:

Proposition 7. Let M be an observable.

(a) Bounds: $0 \leqslant \text{coh}_{nm}(\mathsf{M}) \leqslant 1 - d_{nm}^2(\mathsf{M}) \leqslant 1$ for all n, m.

(b) Zero coherence: $\text{coh}_{nm}(\mathsf{M}) = 0$ for all $n \neq m$, if and only if M is incoherent.

(c) Maximal coherence: The following are equivalent:

(i) M is maximally coherent.

(ii) M has has rank one, and p_n^M is the same probability distribution for each $n = 1, \dots, d$.

(iii) There is a probability distribution $i \mapsto p(i)$ on Ω_M, and a sequence of unit vectors $\psi_i \in \mathcal{H}$ with $|\langle n|\psi_i\rangle|^2 = d^{-1}$ for each $n = 1, \dots, d$, $i \in \Omega_\mathsf{M}$, such that $\mathsf{M}(i) = p(i)d|\psi_i\rangle\langle\psi_i|$ for each $i \in \Omega_\mathsf{M}$.

If M has exactly d outcomes, then M is maximally coherent if and only if M is a MUB to the incoherent basis.

Proof. Denote $\psi_i^n = \sqrt{\mathsf{M}(i)}|n\rangle$, for each $n = 1, \dots, d$, $i \in \Omega_\mathsf{M}$. Then $\|\psi_i^n\|^2 = p_n^\mathsf{M}(i)$, and hence $\sum_{i \in \Omega_\mathsf{M}} \|\psi_i^n\|^2 = \sum_i p_n^\mathsf{M}(i) = 1$ for each n by the normalization of the observable M. To prove (a) we use Cauchy-Schwarz inequality:

$$\text{coh}_{nm}(\mathsf{M}) = \sum_i |\langle n|\mathsf{M}(i)|m\rangle| = \sum_i |\langle\psi_i^n|\psi_i^m\rangle|$$

$$\leqslant \sum_i \|\psi_i^n\|\|\psi_i^m\| = 1 - d_{nm}^2(\mathsf{M}) \leqslant 1.$$

If $\text{coh}_{nm}(\mathsf{M}) = 0$ for all $n \neq m$ we have $\langle n|\mathsf{M}(i)|m\rangle = 0$ for all $n \neq m$, and hence M is incoherent; this proves (b).

To prove (c), assume (i), so that $\text{coh}_{nm}(\mathsf{M}) = 1$ for each pair (n, m). Then the second inequality in the above calculation is saturated, so $d_{nm}^2(\mathsf{M}) = 0$ for all $n \neq m$, which implies $p(i) := p_n^\mathsf{M}(i) = p_m^\mathsf{M}(i)$ for each pair $n, m = 1, \dots, d$, and all $i \in \Omega_\mathsf{M}$, so $\|\psi_i^n\|^2 = p(i)$ for each n, i (i.e., the norm only depends on i). Note that $p(i) > 0$ for each i (since otherwise $\mathsf{M}(i) = 0$). Also the first inequality is saturated, that is, $\sum_i (\|\psi_i^n\|\|\psi_i^m\| - |\langle\psi_i^n|\psi_i^m\rangle|) = 0$, so $|\langle\psi_i^n|\psi_i^m\rangle| = \|\psi_i^n\|\|\psi_i^m\|$ for all n, m, i, as each term in the sum is nonnegative. Hence the Cauchy-Schwarz inequality is saturated for each pair ψ_i^n, ψ_i^m, so $\psi_i^n = c_i^{nm}\psi_i^m$ for some constants $c_i^{nm} \in \mathbb{C}$ which must have modulus one as $\|\psi_i^n\|^2 = \|\psi_i^m\|^2 = p(i)$. Define $\psi_i := p(i)^{-\frac{1}{2}}\psi_i^1$ for each $i \in \Omega_\mathsf{M}$. Then $\|\psi_i\| = 1$, and $\sqrt{\mathsf{M}(i)}|n\rangle = \psi_i^n = c_i^{n1}\psi_i^1 = c_i^{n1}\sqrt{p(i)}\psi_i$ for all n, i, showing that $\sqrt{\mathsf{M}(i)}$ [and hence also $\mathsf{M}(i)$] has rank one with range spanned by ψ_i. Hence (ii) holds. Assume now (ii). Since M has rank one we can write $\mathsf{M}(i) = p(i)d|\psi_i\rangle\langle\psi_i|$ where $p(i) := \text{tr}[\mathsf{M}(i)]/d$ is a probability distribution and ψ_i is a unit vector for each $i \in \Omega_\mathsf{M}$. Since $p_n^\mathsf{M} = p_m^\mathsf{M}$ for all n, m, we must have $p(i) = \frac{1}{d}\sum_m p_m^\mathsf{M}(i) = p_n^\mathsf{M}(i) = \langle n|\mathsf{M}(i)|n\rangle = p(i)d|\langle\psi_i|n\rangle|^2$ for all n, i, which shows that $|\langle\psi_i|n\rangle|^2 = d^{-1}$ for all n, i. Hence (iii) holds. Finally, assuming (iii) we easily check that M has maximal coherence, i.e., (i) holds, and we have established the equivalences in (c). The last claim follows immediately from (iii) and the well-known fact (which is easy to prove) that any rank one observable in dimension d with d outcomes is necessarily a basis observable. $\blacksquare$

As noted above, any observable mutually unbiased to the incoherent basis is incoherent. Moreover, any refinement of

a such an observable is maximally coherent: if $q_k(i)_{i \in \Omega_k}$ defines a probability distribution for each $k = 1, \ldots, d$ (where Ω_k are distinct sets), and $\{\psi_k \mid k = 1, \ldots, d\}$ is mutually unbiased to the incoherent basis, let $\Omega = \cup_k \Omega_k$, and $\mathsf{M}(i) := q_k(i)|\psi_k\rangle\langle\psi_k|$ whenever $i \in \Omega_k$. Another class of maximally coherent observables is given as follows: take any pair of MUBs $\{\phi_k \mid k = 1, \ldots N\}$ and $\{\xi_k \mid k = 1, \ldots, N\}$ in a larger Hilbert space $\mathcal{M} = \mathbb{C}^N$, and define an isometry $V : \mathcal{H} \to \mathcal{M}$ by $V|n\rangle = \xi_n$ for $n = 1, \ldots, d$. Then $\mathsf{M}(i) := |V^*\phi_i\rangle\langle V^*\phi_i|$, $i \in \Omega_\mathsf{M} := \{1, \ldots, N\}$ is a maximally coherent observable with the distribution $p(i) = 1/N$ in the above proposition. An explicit example of this type is obtained by taking $\Omega_\mathsf{M} = \{0, \ldots, N\}$, $p(i) = 1/N$ and $|\psi_i\rangle = \frac{1}{\sqrt{d}} \sum_{j=0}^{d-1} \omega_N^{ji}|j\rangle$ for $i = 0, \ldots, N - 1$, where $\omega_N = e^{2\pi i/N}$.

APPENDIX B: DILATION THEORY

We review here briefly some well-known aspects of dilation theory of quantum channels and observables (see, e.g., [45]), applied to our framework introduced in the main text.

First recall that the Naimark dilation of an observable $\mathsf{M} = (\mathsf{M}(i))_{i \in \Omega_\mathsf{M}}$ on a Hilbert space $\mathcal{H}$ is a projection valued observable A on a larger Hilbert space $\mathcal{H}_\oplus$ such that $\mathsf{M}(i) = J^\dagger \mathsf{A}(i)J$ for all i, where $J : \mathcal{H} \to \mathcal{H}_\oplus$ is an isometry, i.e., $J^\dagger J = \mathbb{1}$. The dilation is minimal if $\mathcal{H}_\oplus = \mathrm{span}\{\mathsf{A}(i)J\varphi \mid \varphi \in \mathcal{H}, i \in \Omega_\mathsf{M}\}$. The following is a basic joint measurability result:

Theorem 3 ([53]). Let $\mathsf{F} = (\mathsf{F}(j))_{j \in \Omega_\mathsf{F}}$ be any observable jointly measurable with M and $(\mathcal{H}_\oplus, \mathsf{A}, J)$ a minimal Naimark dilation of M. Then each joint observable G of M and F is of the form $\mathsf{G}(i, j) = J^\dagger \mathsf{A}(i)\mathsf{B}(j)J$ where B is a unique POVM of $\mathcal{H}_\oplus$ such that $[\mathsf{A}(i), \mathsf{B}(j)] = 0$ for all $i \in \Omega_\mathsf{M}$, $j \in \Omega_\mathsf{F}$.

Any quantum channel Λ of $\mathcal{H} \simeq \mathbb{C}^d$ has a minimal Stinespring dilation, i.e., its Heisenberg picture [a completely positive unital map on the matrix algebra $M_d(\mathbb{C})$] can be written in the form $\Lambda^*(X) = J^\dagger(X \otimes \mathbb{1})J, X \in M_d(\mathbb{C})$, where $J : \mathcal{H} \to \mathcal{H} \otimes \mathcal{K}$ is an isometry, $\mathcal{K}$ a Hilbert space (an ancilla), and the vectors $(X \otimes \mathbb{1})J\psi, X \in M_d(\mathbb{C}), \psi \in \mathcal{H}$, span $\mathcal{H} \otimes \mathcal{K}$ [46]. It follows from the Radon-Nikodym theorem of completely positive maps [55] that any instrument $(\mathsf{I}_i)_{i \in \Omega}$ whose channel is Λ has the form $\mathsf{I}_i^*(X) = J^\dagger(X \otimes \mathsf{F}(i))J$ where $\mathsf{F} = (\mathsf{F}(i))_{i \in \Omega}$ is a (unique) POVM.

We now specialize to our case, with a channel Λ_C given by a PSD matrix C with unit diagonal, through Hadamard multiplication $\Lambda_C^*(X) = C * X$. Since $C \geqslant 0$, we may write $c_{nm} = \langle \eta_n | \eta_m \rangle$ where η_n are unit vectors in a Hilbert space $\mathcal{K}$ with dimension equal to the rank of C, that is, $\mathcal{K} = \mathrm{span}\{\eta_n \mid n = 1, \ldots, d\}$ (see, e.g., [39]). These vectors constitute the minimal Stinespring dilation $\Lambda_C^*(X) = J^\dagger(X \otimes \mathbb{1})J$ of Λ_C, where the isometry is defined by $J|n\rangle = |n\rangle \otimes \eta_n$ (note that $|m\rangle \otimes \eta_n = (X \otimes \mathbb{1})J|n\rangle$ where $X = |m\rangle\langle n|$). Then any GII $(\mathsf{I}_j)_{j \in \Omega}$ with channel Λ_C has the form

$$\mathsf{I}_j^*(X) = J^\dagger(X \otimes \mathsf{F}(j))J = \sum_{n,m} \langle n|X|m\rangle \langle \eta_n|\mathsf{F}(j)\eta_m\rangle |n\rangle\langle m|,$$

where $\mathsf{F} = (\mathsf{F}(j))_{j \in \Omega}$ is a POVM of $\mathcal{K}$. This gives us the Hadamard form $\mathsf{I}_j^*(X) = C(j) * X$ used in the main text, with the matrix $C(j)$ given by

$$c_{nm}(j) = \langle \eta_n | \mathsf{F}(j)\eta_m \rangle. \tag{B1}$$

We stress that *every* instrument with channel Λ_C has this form. In particular, if $\{C(j)\}$ is any collection of PSD matrices with $\sum_j C(j) = C$, then $C(j)$ can be written as (B1) for some (unique) F.

APPENDIX C: PROOFS OF THEOREMS 1 AND 2

Recall that in Theorem 1 we let Q_0 be any fixed maximally coherent observable, with outcome set Ω_0 (assumed to be minimal). By Proposition 7, we can write

$$\mathsf{Q}_0(i) = p(i)d|\psi_i\rangle\langle\psi_i|, \tag{C1}$$

where $i \mapsto p(i)$ is a probability distribution on Ω_0, and ψ_i are unit vectors such that $|\langle\psi_i|n\rangle|^2 = d^{-1}$ for all n, i. Let $\mathcal{M}$ be a copy of $\mathbb{C}^{|\Omega_0|}$, and note that $\langle n|\mathsf{Q}_0(i)|n\rangle = p(i)$ for all $n = 1, \ldots, d$.

The proofs are based on the dilation theory described above; let η_n be vectors such that $c_{nm} = \langle \eta_n|\eta_m\rangle$ as in Appendix B.

Proof of Theorem 1. Fix a basis $\{|i\rangle \mid i \in \Omega_0\}$ of $\mathcal{M}$, and define an isometry $V : \mathcal{H} \to \mathcal{M} \otimes \mathcal{K}$ via

$$V|n\rangle = \sum_{i \in \Omega_{\mathsf{Q}_0}} \sqrt{p(i)d} \langle\psi_i|n\rangle |i\rangle \otimes \eta_n.$$

Then $C * \mathsf{Q}_0(i) = V^*(|i\rangle\langle i| \otimes \mathbb{1}_\mathcal{K})V$. Hence, this is a Naimark dilation of the observable $C * \mathsf{Q}_0$. Since $\mathrm{span}\{(|i\rangle\langle i| \otimes \mathbb{1})V|n\rangle \mid n \in \{1, \ldots, d\}, i \in \Omega_0\} = \mathrm{span}\{|i\rangle \otimes \eta_n \mid n \in \{1, \ldots, d\}, i \in \Omega_0\} = \mathcal{M} \otimes \mathcal{K} (= \mathcal{H}_\oplus)$, the dilation is minimal.

Now assume that $C * \mathsf{Q}_0$ is jointly measurable with an incoherent observable P. Since the above dilation is minimal, Theorem 3 applies: P must be of the form $\mathsf{P}(j) = V^\dagger \mathsf{F}(j)V$, $j \in \Omega_\mathsf{P}$, where $[\mathsf{F}(j), |i\rangle\langle i| \otimes \mathbb{1}_\mathcal{K}] = 0$ for all i, j. This implies that for each i there is a POVM $\mathsf{F}_i = (\mathsf{F}_i(j))_{j \in \Omega_\mathsf{P}}$ on $\mathcal{K}$, such that $\mathsf{F}(j) = \sum_i |i\rangle\langle i| \otimes \mathsf{F}_i(j)$. Furthermore, according to Theorem 3, P and $C * \mathsf{Q}_0$ have a joint observable

$$\tilde{\mathsf{G}}(i, j) = V^\dagger \mathsf{F}(j)(|i\rangle\langle i| \otimes \mathbb{1})V = V^\dagger(|i\rangle\langle i| \otimes \mathsf{F}_i(j))V$$
$$= \sum_{n,m} \langle n|\mathsf{Q}_0(i)|m\rangle \langle \eta_n|\mathsf{F}_i(j)\eta_m\rangle |n\rangle\langle m|$$

and hence P must have the form

$$\mathsf{P}(j) = \sum_i \tilde{\mathsf{G}}(i, j) = \sum_{n,m} \sum_i \langle \eta_n|\mathsf{F}_i(j)\eta_m\rangle \langle n|\mathsf{Q}_0(i)|m\rangle |n\rangle\langle m|$$
$$= \sum_n \sum_i \langle \eta_n|\mathsf{F}_i(j)\eta_n\rangle \langle n|\mathsf{Q}_0(i)|n\rangle |n\rangle\langle n|$$
$$= \sum_n \langle \eta_n| \sum_i p(i)\mathsf{F}_i(j)\eta_n\rangle |n\rangle\langle n|. \tag{C2}$$

In the third step we have used the assumption that P is incoherent (so there are no off-diagonal elements), and in the fourth step the maximal coherence condition $\langle n|\mathsf{Q}_0(i)|n\rangle = p(i)$. We now define, for each j, a matrix $C(j)$ by $c_{nm}(j) := \langle \eta_n|\mathsf{A}(j)|\eta_m\rangle$, where $\mathsf{A} := \sum_i p(i)\mathsf{F}_i$ is a POVM by convexity. Therefore we have $C(j) \geqslant 0$ and $\sum_j c_{nm}(j) = \langle \eta_n|\eta_m\rangle = c_{nm}$; that is, $C(j)$ form a GII whose channel is Λ_C. Finally, by the computation (C2), $\mathsf{P}(j) = \sum_n \langle \eta_n|\mathsf{A}(j)\eta_n\rangle |n\rangle\langle n| = \sum_n c_{nn}(j)|n\rangle\langle n|$, showing that the observable of this GII is precisely P. Applying the GII to any observable Q we get

a joint observable $\mathsf{G}(i, j) = C(j) * \mathsf{Q}(i)$ for $C * \mathsf{Q}$ and P, as $\sum_i \mathsf{G}(i, j) = C(j) * \mathbb{1} = \mathsf{P}(j)$ and $\sum_j \mathsf{G}(i, j) = C * \mathsf{Q}(i)$. Hence $C * \mathsf{Q}$ and P are jointly measurable. This completes the proof of Theorem 1.

The crucial point of the proof is the computation (C2); one can readily see how the two strong assumptions, P incoherent and Q_0 maximally coherent, fit together rather neatly to form the *single* dilation POVM A.

Proof of Theorem 2. If (i) holds then $C * \mathsf{Q}$ is jointly measurable with P for all Q, so in particular for Q_0. By the above proof we obtain matrices $C(j)$ satisfying (5), so (ii) holds. Conversely, if such matrices exist [that is, (ii) holds], the observable $\mathsf{G}(i, j) = C(j) * \mathsf{Q}(i)$ defined in the above proof is a joint observable for P and $C * \mathsf{Q}$ for any observable Q, hence $\mathsf{P} \in \mathcal{C}_C$, i.e., (i) holds.

APPENDIX D: REDUCTION BY SYMMETRY

Here we develop in detail the theory of covariance systems for a $d \times d$ coherence matrix C. Recall that the aim is to characterize the set $\mathcal{C}_C$ of incoherent observables P for which there is a GII with GIO Λ_C and observable P. The idea is that symmetries in the coherence pattern can be used to simplify the problem and single out relevant incoherent observables.

As above, we make use of the dilation $c_{nm} = \langle \eta_n | \eta_m \rangle$ (see Appendix B). For each pair (n, m) we write $n \sim_C m$ when $|c_{nm}| = 1$. This implies that $|\langle \eta_n | \eta_m \rangle| = 1 = \|\eta_n\| \|\eta_m\|$; i.e., the Cauchy-Schwarz inequality is saturated for this pair of unit vectors, and hence $\eta_n = e^{i\theta} \eta_m$ for some $\theta \in \mathbb{R}$. Now if $|c_{nm}| = 1$ and $|c_{mk}| = 1$ then $\eta_n = e^{i\theta} \eta_m$ and $\eta_m = e^{i\theta'} \eta_k$, so $\eta_n = e^{i(\theta + \theta')} \eta_k$, which implies $|c_{nk}| = 1$. Hence the relation $n \sim_C m$ is transitive, and since $|c_{nm}| = |c_{mn}|$ for each pair (n, m), it is also symmetric, so an equivalence relation on the set $\{1, \ldots, d\}$. Hence the set splits into a union $\{1, \ldots, d\} = \cup_{k=1}^{n_C} I_k^C$ of n_C equivalence classes I_k^C (unique up to ordering). We let $\Omega_C = \{1, \ldots, n_C\}$.

Now we pick from each equivalence class I_k^C one fixed representative $n_k \in I_k^C$, and let $\tilde{\eta}_k := \eta_{n_k}$ for each k; then for each $n = 1, \ldots, d$ there is a unique phase factor $e^{i\theta_n}$ so that $\eta_n = e^{i\theta_n} \tilde{\eta}_k$ where I_k^C is the class of n. Now define an $n_C \times n_C$ matrix $\tilde{C}$ by $\tilde{c}_{kk'} := \langle \tilde{\eta}_k | \tilde{\eta}_{k'} \rangle$. By construction, $\tilde{C}$ is a structure matrix, and we observe that $c_{nm} = \langle \eta_n | \eta_m \rangle = e^{-i(\theta_n - \theta_m)} \tilde{c}_{kk'}$ whenever $n \in I_k^C$ and $m \in I_{k'}^C$. Let D be the matrix $d_{nm} = e^{-i(\theta_n - \theta_m)}$; this is symmetric rank 1, hence the structure matrix of a unitary GIO $\Lambda_D^*(X) = U_D X U_D^\dagger$ where U_D is the diagonal unitary with phases $e^{-i\theta_n}$ on the diagonal. We then let $\tilde{\mathcal{H}}$ be the Hilbert space with incoherent basis $\{|k\rangle\}_{k \in \Omega_C}$ and define $L : \tilde{\mathcal{H}} \to \mathcal{H}$ by

$$L|k\rangle = \sum_{n \in I_k^C} |n\rangle.$$

We then obtain the decomposition $C = D * (L\tilde{C}L^\dagger)$, so that $C \simeq L\tilde{C}L^\dagger$, and see that the (n, m) entry of the structure matrix $L\tilde{C}L^\dagger$ is equal to $\tilde{c}_{kk'}$ for all $n \in I_k^C$, $m \in I_{k'}^C$, that is, it only depends on the classes of n and m. In other words, after the unitary GIO is factored out, the remaining channel compresses into the GIO $\Lambda_{\tilde{C}}$ on an n_C-dimensional system. By construction, this channel is unique up to diagonal unitaries, corresponding to different choices of the representatives n_k.

Assuming P is adapted, we can compress it into an incoherent observable $\tilde{\mathsf{P}}$ on the n_C-dimensional system, by setting $p_k^{\tilde{\mathsf{P}}} := p_n^{\mathsf{P}}$ for any $n \in I_k^C$, so that $\mathsf{P}(j) = \mathcal{L}(\tilde{\mathsf{P}}(j))$ where $\mathcal{L} : \text{span}\{|k\rangle\langle k| \mid k \in \Omega_C\} \to \text{span}\{|n\rangle\langle n| \mid n = 1, \ldots, d\}$ links the two diagonal algebras "incoherently":

$$\mathcal{L}(|k\rangle\langle k|) = \sum_{n \in I_k^C} |n\rangle\langle n|.$$

We can now prove our first reduction result:

Proposition 8. There is a GIO $\Lambda_{\tilde{C}}$ acting on $\tilde{\mathcal{H}}$ such that $C \simeq L\tilde{C}L^\dagger$. Then $\mathcal{C}_C = \{\mathcal{L}(\mathsf{P}(\cdot)) \mid \mathsf{P} \in \mathcal{C}_{\tilde{C}}\}$.

Proof. The decomposition $C \simeq L\tilde{C}L^\dagger$ was constructed above. To prove the second claim, assume first that $\mathsf{P}' \in \mathcal{C}_C$, and let $C(j)$ form a GII with observable P' and GIO Λ_C, so that $c_{nm}(j) = \langle \eta_n | \mathsf{F}(j) | \eta_m \rangle$ for some POVM F on the dilation space $\mathcal{K}$, with $\langle \eta_n | \mathsf{F}(j) | \eta_n \rangle = p_n^{\mathsf{P}'}(j)$ for each n. Now the $n_C \times n_C$ matrices $\tilde{C}(j)$ defined by $\tilde{c}_{kk'}(j) := \langle \tilde{\eta}_k | \mathsf{F}(j) | \tilde{\eta}_{k'} \rangle$ form a GII with channel $\Lambda_{\tilde{C}}$. In order to find the corresponding observable we compute $\tilde{c}_{kk}(j) = \langle \tilde{\eta}_k | \mathsf{F}(j) | \tilde{\eta}_k \rangle = \langle \eta_n | \mathsf{F}(j) | \eta_n \rangle = p_n^{\mathsf{P}'}(j)$ for *any* $n \in I_k^C$. Hence $p_n^{\mathsf{P}'}$ does not depend on the choice of $n \in I_k^C$, so P' is adapted to C, and $\mathsf{P}' = \mathcal{L}(\mathsf{P})$ where P is defined by $p_k^{\mathsf{P}}(j) := \tilde{c}_{kk}(j)$. This shows that the observable of this GII is P, so $\mathsf{P} \in \mathcal{C}_{\tilde{C}}$. Conversely, if $\mathsf{P}' = \mathcal{L}(\mathsf{P})$ with $\mathsf{P} \in \mathcal{C}_{\tilde{C}}$ then there is a GII $\tilde{C}(j)$ with $\sum_j \tilde{c}_{kk'}(j) = \tilde{c}_{kk'}$ and $\tilde{c}_{kk}(j) = p_k^{\mathsf{P}}(j)$. We then define $c_{nm}(j) := e^{-i(\theta_n - \theta_m)} \tilde{c}_{kk'}(j)$ whenever $(n, m) \in I_k^C \times I_{k'}^C$. This is a GII for which $\sum_j c_{nm}(j) = e^{-i(\theta_n - \theta_m)} \tilde{c}_{kk'} = c_{nm}$, and $c_{nn}(j) = \tilde{c}_{kk}(j) = p_k^{\mathsf{P}}(j) = p_n^{\mathsf{P}'}(j)$ regardless of the choice of $n \in I_k^C$. Hence $\mathsf{P}' \in \mathcal{C}_C$. This completes the proof. ∎

Now let S_d, the group of permutations of $\{1, \ldots, d\}$, act on $\mathcal{H}$ via $U_\pi |n\rangle = |\pi(n)\rangle$, and recall from the main text the symmetry group

$$G_C = \{\pi \in S_d \mid U_\pi^\dagger C U_\pi \simeq C\}.$$

By the definition of $\simeq$, G_C consists of exactly those permutations $\pi \in S_d$ for which there exists a unitary GIO with matrix D such that $U_\pi^\dagger C U_\pi = D * C$. So $\pi \in G_C$ iff there exist phase factors $u_n(\pi)$, $n = 1, \ldots, d$, such that

$$c_{\pi(n),\pi(m)} = u_n(\pi) c_{nm} \overline{u_m(\pi)} \tag{D1}$$

for each n, m. In what follows we assume for simplicity that $c_{nm} \neq 0$ for all n, m. Then for each π the coefficients $u_n(\pi)$ are uniquely determined up to an overall (π-dependent) phase factor, which we choose by setting $u_{n_0}(\pi) = 1$ for a fixed n_0. We can then construct $u_n(\pi)$ explicitly from the entries of C:

$$u_n(\pi) = c_{\pi(n),\pi(n_0)}/c_{nn_0}, \quad n = 1, \ldots, d. \tag{D2}$$

We then define, for each $\pi \in G_C$ and $n = 1, \ldots, d$, a unitary operator W_π on $\mathcal{H}$ by

$$W_\pi |n\rangle = u_n(\pi) |\pi(n)\rangle, \quad n = 1, \ldots, d,$$

so that [by (D1)] we may write

$$G_C = \{\pi \in S_d \mid W_\pi^\dagger C W_\pi = C\}.$$

The following result shows that W_π appropriately reflects the symmetries of C on the Hilbert space level:

Proposition 9. G_C is a permutation group (i.e., a subgroup of S_d), and $\pi \mapsto W_\pi$ is a projective unitary representation of

G_C with multiplier $(\pi, \pi') \mapsto u_{\pi'(n_0)}(\pi)$. If each entry of C is real positive, then $W_\pi = U_\pi$.

Proof. Let $\pi, \pi' \in G_C$. Then (D1) holds for both, so

$$c_{\pi\pi'(n),\pi\pi'(m)} = u_{\pi'(n)}(\pi) c_{\pi'(n),\pi'(m)} \overline{u_{\pi'(m)}(\pi)}$$
$$= u_{\pi'(n)}(\pi) u_n(\pi') c_{nm} \overline{u_m(\pi') u_{\pi'(m)}(\pi)}$$

for all n, m, showing that (D1) holds also for $\pi\pi'$. Hence $\pi\pi' \in G_C$, and since G_C is finite, this implies that G_C is a subgroup. Taking $m = n_0$ and using (D2) we find

$$u_n(\pi\pi') = u_{\pi'(n)}(\pi) u_n(\pi') \overline{u_{\pi'(n_0)}(\pi)},$$

which reads $W_\pi W_{\pi'} = u_{\pi'(n_0)}(\pi) W_{\pi\pi'}$. Since clearly $W_e = \mathbb{1}$, the second claim follows. Finally, if each entry of C is real positive, then $u_n(\pi) = 1$ for all π and n, and we have simply $W_\pi = U_\pi$. ∎

It is clear that $\{I_k^C\}$ forms a block system for the group G_C: for each $\pi \in G_C$ we have $|c_{nm}| = 1$ iff $|c_{\pi(n),\pi(m)}| = 1$, so π moves each class as a whole, $\pi(I_k^C) = I_{\phi(\pi)(k)}^C$ for a unique $\phi(\pi) \in G_{\tilde{C}}$, where $\tilde{C}$ is the reduced $n_C \times n_C$ GIO matrix. The map $\phi : G_C \to G_{\tilde{C}}$ is a homomorphism with $\phi(G_C) \leqslant G_{\tilde{C}}$ consisting of permutations between classes of the same size. This structure is unique up to an irrelevant overall permutation of $\{1, \ldots, n_C\}$, fixed by the labeling of I_k^C.

Next, recall that given any subgroup $G \leqslant G_C$, a G-covariant incoherent observable P is one with outcome set Ω_C satisfying $p_{\pi^{-1}(n)}^{\mathsf{P}}(j) = p_n^{\mathsf{P}}(\phi(\pi)(j))$ for each $\pi \in G$, $j \in \Omega_C$ and $n \in \{1, \ldots d\}$. It is convenient to write this condition equivalently using the representation W_π as

$$W_\pi \mathsf{P}(j) W_\pi^\dagger = \mathsf{P}(\phi(\pi)(j)), \; \pi \in G, \; j \in \Omega_C. \qquad \text{(D3)}$$

Note that the reduced matrix $\tilde{C}$ obviously does not reduce further, i.e., $n_{\tilde{C}} = n_C$ (each equivalence class is a singleton). Hence for any subgroup $\tilde{G} \leqslant G_{\tilde{C}} \leqslant S_{n_C}$, the $\tilde{G}$-covariant observables P are given by (D3) with d replaced by n_C and $\phi = \text{Id}$.

We recall that $\mathcal{C}_C[G]$ is the set of all G-covariant incoherent observables in $\mathcal{C}_C$, and $\mathcal{C}_C^{\text{sym}} = \mathcal{C}_C[G_C]$. The symmetry constraint (D3) can be naturally formulated in the GII level: we call a GII $C(j)$ G covariant if

$$W_\pi C(j) W_\pi^\dagger = C(\phi(\pi)(j)), \; \pi \in G, \; j \in \Omega_C. \qquad \text{(D4)}$$

Notice that here the matrices $C(j)$ are not diagonal, so we need to state the condition using the representation W_π. The following result shows that the SDP (5) in the main text can be supplemented by an extra symmetry constraint if P is G covariant:

Proposition 10. Any $\mathsf{P} \in \mathcal{C}_C[G]$ has a G-covariant GII.

Proof. To prove the claim, let $\mathsf{P} \in \mathcal{C}_C[G]$. Then there is a GII $C(j)$ with $\sum_j C(j) = C$ and $c_{nn}(j) = p_n^{\mathsf{P}}(j)$ for all n. We define

$$C'(j) := \frac{1}{|G|} \sum_{\pi \in G} W_\pi^\dagger C(\phi(\pi)(j)) W_\pi.$$

This is essentially the "averaging argument" often used in the context of symmetry constraints for joint measurability [27,56,57], except that now we apply it at the level of structure matrices as opposed to POVM elements. Now $C'(j) \geqslant 0$, so it

defines a GII, which is G covariant, as

$$W_{\pi_0} C'(j) W_{\pi_0}^\dagger = \frac{1}{|G|} \sum_{\pi \in G} W_{\pi\pi_0^{-1}}^\dagger C(\phi(\pi)(j)) W_{\pi\pi_0^{-1}}$$
$$= \frac{1}{|G|} \sum_{\pi \in G} W_\pi^\dagger C(\phi(\pi\pi_0)(j)) W_\pi$$
$$= \frac{1}{|G|} \sum_{\pi \in G} W_\pi^\dagger C(\phi(\pi)\phi(\pi_0)(j)) W_\pi$$
$$= C'(\phi(\pi_0)(j))$$

for each $\pi_0 \in G$. Here we used the fact that $\pi \mapsto W_\pi$ is a (projective) representation, and ϕ is a homomorphism. Furthermore,

$$\sum_j C'(j) = \frac{1}{|G|} \sum_{\pi \in G} W_\pi^\dagger \sum_j C(\phi(\pi)(j)) W_\pi$$
$$= \frac{1}{|G|} \sum_{\pi \in G} W_\pi^\dagger C W_\pi = \frac{1}{|G|} \sum_{\pi \in G} C = C,$$

as G is a subgroup of $G_C = \{\pi \in S_d \mid W_\pi C W_\pi^\dagger = C\}$. Finally,

$$c'_{nn}(j) = \frac{1}{|G|} \sum_{\pi \in G} \langle n| W_\pi^\dagger C(\phi(\pi)(j)) W_\pi |n\rangle$$
$$= \frac{1}{|G|} \sum_{\pi \in G} c_{\pi(n),\pi(n)}(\phi(\pi)(j))$$
$$= \frac{1}{|G|} \sum_{\pi \in G} p_{\pi(n)}^{\mathsf{P}}(\phi(\pi)(j))$$
$$= \frac{1}{|G|} \sum_{\pi \in G} p_n^{\mathsf{P}}(j) = p_n^{\mathsf{P}}(j),$$

because P is G covariant. Therefore, $C'(j)$ satisfies Eq. (5) in the main text, and is G covariant. ∎

We also remark that the GII matrices can always be chosen real if C is a real matrix (independently of permutation symmetry). In fact, if Eq. (5) holds for matrices $C(j)$, we can define $C^{\text{re}}(j) = \frac{1}{2}(C(j) + C(j)^T)$; then $C^{\text{re}}(j) \geqslant 0$ since transpose preserves positivity, and $C^{\text{re}}(j)$ is a real symmetric matrix since $c_{nm}^{\text{re}}(j) = \text{Re} \, c_{nm}(j)$ (as $C(j) = C(j)^*$). Since C is real we therefore still have $\sum_j C^{\text{re}}(j) = C$, and since the diagonal of $C(j)$ is real in any case, it coincides with the diagonal of $C^{\text{re}}(j)$. Hence the matrices $C^{\text{re}}(j)$ fulfill Eq. (5) as well.

We now prove the main reduction result, which in the main text was stated in Eq. (6):

Proposition 11. $\mathcal{C}_C^{\text{sym}} = \{\mathcal{L}(\mathsf{P}(\cdot)) \mid \mathsf{P} \in \mathcal{C}_{\tilde{C}}[\phi(G_C)]\}$.

Proof. Let $\mathsf{P} \in \mathcal{C}_{\tilde{C}}[\phi(G_C)]$. Hence P is $\phi(G_C)$ covariant and $\mathsf{P} \in \mathcal{C}_{\tilde{C}}$. Now define $\mathsf{P}' := \mathcal{L}(\mathsf{P})$. Then $\mathsf{P}' \in \mathcal{C}_C$ by Proposition 8. Note that P' still has n_C outcomes, but lives in dimension d; explicitly, $\mathsf{P}'(j) = \sum_{k=1}^{n_C} p_k^{\mathsf{P}}(j) \sum_{n \in I_k^C} |n\rangle\langle n|$. The following rearrangement now shows that P' is G_C

covariant:

$$W_\pi \mathsf{P}'(j) W_\pi^\dagger = \sum_{k=1}^{n_C} p_k^{\mathsf{P}}(j) \sum_{n \in I_k^C} |\pi(n)\rangle\langle\pi(n)|$$

$$= \sum_{k=1}^{n_C} p_k^{\mathsf{P}}(j) \sum_{\pi^{-1}(n) \in I_k^C} |n\rangle\langle n|$$

$$= \sum_{k=1}^{n_C} p_k^{\mathsf{P}}(j) \sum_{n \in I_{\phi(\pi)(k)}^C} |n\rangle\langle n|$$

$$= \sum_{k=1}^{n_C} p_{\phi(\pi)^{-1}(k)}^{\mathsf{P}}(j) \sum_{n \in I_k^C} |n\rangle\langle n|$$

$$= \sum_{k=1}^{n_C} p_k^{\mathsf{P}}(\phi(\pi)(j)) \sum_{n \in I_k^C} |n\rangle\langle n| = \mathsf{P}'(\phi(\pi)(j)).$$

Hence $\mathsf{P}' \in \mathcal{C}_C^{\text{sym}}$. Conversely, if we pick a $\mathsf{P}' \in \mathcal{C}_C^{\text{sym}}$ then by Proposition 8 we can write it as $\mathsf{P}' := \mathcal{L}(\mathsf{P})$ for some $\mathsf{P} \in \mathcal{C}_{\tilde{C}}$, and reverse the rearrangement to show that $p_{\phi(\pi)^{-1}(k)}^{\mathsf{P}}(j) = p_k^{\mathsf{P}}(\phi(\pi)(j))$, i.e., P is $\phi(G_C)$ covariant and hence $\mathsf{P} \in \mathcal{C}_{\tilde{C}}[\phi(G_C)]$. This completes the proof. ∎

Finally, we modify the robustness idea described above to account for symmetry: instead of Eq. (2) we use the "canonical" G_C-covariant observable $\mathsf{P}^C(j) := \mathcal{L}(|j\rangle\langle j|)$, $j \in \Omega_C$, and the line $\mathsf{P}_\alpha^C = \alpha \mathsf{P}^C + (1-\alpha)\mathsf{P}_{\text{dep}}^C$, where $\mathsf{P}_{\text{dep}}^C(j) = d^{-1} \text{tr}[\mathsf{P}^C(j)]\mathbb{1} = d^{-1}|I_j^C|\mathbb{1}$. Noting that $\mathsf{P}^C \notin \mathcal{C}_C^{\text{sym}}$, we use Proposition 11 to set

$$\alpha_C := \max\left\{\alpha > 0 \mid \mathsf{P}_\alpha^C \in \mathcal{C}_C\right\}$$
$$= \max\left\{\alpha > 0 \mid \mathsf{P}_\alpha^C \in \mathcal{C}_C^{\text{sym}}\right\}$$
$$= \max\left\{\alpha > 0 \mid \alpha|j\rangle\langle j| + (1-\alpha)d^{-1}|I_j^C|\mathbb{1} \in \mathcal{C}_{\tilde{C}}^{\text{sym}}\right\},$$
$$\text{(D5)}$$

so α_C is the proportion of the line where coherence does *not* sustain incompatibility. Note that in the nondegenerate case ($|c_{nm}| < 1$ for all $n \neq m$) we have $\mathsf{P}_\alpha^C = \mathsf{P}_\alpha$, so Eq. (D5) is (by Theorem 1) consistent with α_{M} defined after Eq. (2) in the main text, when $\mathsf{M} = C * \mathsf{Q}_0$ where Q_0 is maximally coherent.

APPENDIX E: UNIFORM COHERENCE WITH NEGATIVE ENTRIES

Let C be a coherence matrix with full symmetry, i.e., $G_C = S_d$. Then $c_{nm} = \lambda$ for all $n \neq m$, for some $\lambda \in \mathbb{R}$; i.e., all coherences are equal. From its eigenvalues one sees that C defines a GIO iff $-(d-1)^{-1} \leqslant \lambda \leqslant 1$. Any G_C-covariant P has $p_n^{\mathsf{P}}(j) = q$ for all n, j, $j \neq n$, for a fixed q; writing $q = (1-\alpha)/d$ we see that $\mathsf{P} = \mathsf{P}_\alpha^C = \mathsf{P}_\alpha$ for some $-(d-1)^{-1} \leqslant \alpha \leqslant 1$. Hence these families are naturally motivated by symmetry considerations. Recall from the main text (Proposition 3) that for $\lambda, \alpha > 0$ we have $\mathsf{P}_\alpha \in \mathcal{C}_C^{\text{sym}}$ if and only if $g_d(\alpha) \geqslant \lambda$ where $g_d(\alpha) = \frac{1}{d}((d-2)(1-\alpha) + 2\sqrt{1-\alpha}\sqrt{1+(d-1)\alpha})$, and we now note that the same argument clearly applies also for $\alpha < 0$. If $\alpha > 0$ we can write this equivalently as $\alpha \leqslant g_d(\lambda)$; the func-

tion $\alpha \mapsto g_d(\alpha)$ is decreasing for $\alpha \in [0, 1]$ and is its own inverse. If $\alpha < 0$ the result still holds, but the inequality cannot be inverted using g_d, as $\alpha \mapsto g_d(\alpha)$ is increasing for $\alpha \in [-(d-1)^{-1}, 0]$ with inverse $u \mapsto \frac{1}{d}((d-2)(1-u) - 2\sqrt{1-u}\sqrt{1+(d-1)u})$. To summarize the $\lambda > 0$ case:

$$\mathcal{C}_C^{\text{sym}} = \left\{\mathsf{P}_\alpha^C \mid g_d(\alpha) \geqslant \lambda\right\} \quad \text{when } \lambda \in [0, 1].$$

Now if $\lambda < 0$, the Corollaries 1 and 2 do not completely determine $\mathcal{C}_C^{\text{sym}}$. Indeed, Corollary 1 gives the necessary condition $\lambda \geqslant -g_d(\alpha)$ for $\mathsf{P}_\alpha^C \in \mathcal{C}_C^{\text{sym}}$, and Corollary 2 the sufficient condition $\lambda \geqslant -g_d(\alpha)(d-1)^{-1}$, which only coincide in the qubit case. However, since $C * \mathsf{Q}_0$ and P_α have the exact same form, we can interchange α and λ above to conclude that for $\alpha > 0$ and $\lambda \in [-(d-1)^{-1}, 1]$ we have $\mathsf{P}_\alpha^C \in \mathcal{C}_C^{\text{sym}}$ if and only if $g_d(\lambda) \geqslant \alpha$. This already gives $\alpha_C = g_d(\lambda)$ in Eq. (D5). In order to fully characterize $\mathcal{C}_C^{\text{sym}}$ we need to show that $\mathsf{P}_\alpha^C \in \mathcal{C}_C^{\text{sym}}$ for all $(\alpha, \lambda) \in [-(d-1)^{-1}, 0] \times [-(d-1)^{-1}, 0]$; this then gives

$$\mathcal{C}_C^{\text{sym}} = \left\{\mathsf{P}_\alpha^C \mid -(d-1)^{-1} \leqslant \alpha \leqslant g_d(\lambda)\right\},$$
$$\text{when } \lambda \in [-(d-1)^{-1}, 0].$$

To prove the remaining bit it suffices (by convexity) to show that $\mathsf{P}_\alpha^C \in \mathcal{C}_C^{\text{sym}}$ for the "corner" $\alpha = \lambda = -(d-1)^{-1}$, which was done in the main text.

APPENDIX F: EXAMPLE: CENTROSYMMETRIC CASE IN DIMENSION 3

Here we give a nontrivial example of the theory developed in the main text (and the Appendixes above). This example is relevant for the $N = 2$ case of the spin-boson model but we work it out slightly more generally.

Let C be any 3×3 GIO matrix with real positive entries such that $(13) \in G_C$; that is, the symmetry group contains the permutation which exchanges 1 and 3 and leaves 2 unchanged. Then C must be centrosymmetric, i.e., (also) symmetric about the counterdiagonal, so

$$C = \begin{pmatrix} 1 & \lambda & \gamma \\ \lambda & 1 & \lambda \\ \gamma & \lambda & 1 \end{pmatrix},$$

for some $\lambda, \gamma \in [0, 1]$ and $D := \frac{1}{2}(1+\gamma) - \lambda^2 \geqslant 0$. The conditions ensure that $C \geqslant 0$. This covers both the uniform coherence in dimension 3 ($\gamma = \lambda$ with $G_C = S_3$), and the reduction $\tilde{C}$ of the spin-boson model for $N = 2$ ($\gamma = \lambda^4$ with $G_C = \{e, (13)\}$). In the former case $D = (\lambda + \frac{1}{2})(1 - \lambda)$, and in the latter case $D = \frac{1}{2}(1 - \lambda^2)^2$, which are indeed both positive for all $\lambda \in [0, 1]$.

If $G_C = S_3$ (i.e., $\gamma = \lambda$) we know from the main text that $\mathcal{C}_C^{\text{sym}} = \{\mathsf{P}_\alpha^C \mid \lambda \leqslant g_3(\alpha)\}$, i.e., has affine dimension one. We now proceed to characterize $\mathcal{C}_C^{\text{sym}}$ assuming $G_C = \{e, (13)\}$ (i.e., $\gamma \neq \lambda$). Denote $\pi_0 = (13)$ (as in the main text). We first note that each $\{e, (13)\}$-covariant incoherent observable P has $\mathsf{P}(2) = U_{\pi_0}^\dagger \mathsf{P}(0) U_{\pi_0}$ and $\mathsf{P}(1) = U_{\pi_0}^\dagger \mathsf{P}(1) U_{\pi_0}$. Therefore, it is of the form $\mathsf{P} = \mathsf{P}_\mathbf{q}$ for some $\mathbf{q} = (q, p, r) \in \mathcal{M} := \Delta \times$

$[0, \frac{1}{2}]$ where $\Delta := \{(q, p) \in [0, 1]^2 \mid p + q \leqslant 1\}$, and

$$\mathsf{P_q}(0) = \begin{pmatrix} p & 0 & 0 \\ 0 & r & 0 \\ 0 & 0 & q \end{pmatrix}, \quad \mathsf{P_q}(1) = \begin{pmatrix} s & 0 & 0 \\ 0 & 1-2r & 0 \\ 0 & 0 & s \end{pmatrix},$$

$$\mathsf{P_q}(2) = \begin{pmatrix} q & 0 & 0 \\ 0 & r & 0 \\ 0 & 0 & p \end{pmatrix},$$

with $s = 1 - p - q$. Since the map $\mathbf{q} \mapsto \mathsf{P_q}$ is convex, the convex structure of the set of incoherent observables (including the shape of $\mathcal{C}_C^{\mathrm{sym}}$ inside it) is faithfully represented inside $\mathcal{M}$. In particular, the incoherent basis observable $\mathsf{P}_0(j) = |j\rangle\langle j|$ and its permutation $\mathsf{P}_0(\pi_0(j))$ are represented by the extremal points $(1,0,0)$ and $(0,1,0)$, while the trivial observables $\mathsf{P}(j) = \mu(j)\mathbb{1}$ (where μ is π invariant) form the line from the origin [with $\mathsf{P}(1) = \mathbb{1}$] to $\frac{1}{2}(1, 1, 1)$ [with $\mathsf{P}(0) = \mathsf{P}(2) = \frac{1}{2}\mathbb{1}$]. In particular, the centroid $\frac{1}{4}(1, 1, 1)$ of $\mathcal{M}$ is the "coin toss" observable $\mathsf{P}(j) = \binom{2}{j}\frac{1}{4}\mathbb{1}$, while the uniform trivial observable $\mathsf{P}(j) = \frac{1}{3}\mathbb{1}$ is $\frac{1}{3}(1, 1, 1)$. The former appears in the spin-boson model as the depolarization of the spectral measure of the Hamiltonian (see the main text).

In order to state the result, we define the functions $w_+ : \Delta \to [0, 2]$, $w_- : \Delta \to [0, 1]$, $w_0 : \Delta \to [\gamma - 1, \gamma + 1]$, and $w_0^- : \Delta \to [0, 1 + \gamma]$ by

$$w_\pm(p, q) = (\sqrt{q} \pm \sqrt{p})^2, \quad w_0(p, q) = \gamma - 1 + 2(q + p),$$

$$w_0^-(p, q) = \begin{cases} w_-, & w_+ \leqslant 1 - \gamma \\ w_0, & w_+ \geqslant 1 - \gamma. \end{cases}$$

Clearly, $w_- \leqslant w_+$ (for any p, q). Moreover, $w_0 \leqslant w_-$ when $w_+ \leqslant 1 - \gamma$, with $w_0 = w_-$ when $w_+ = 1 - \gamma$. Correspondingly, $w_0 \leqslant w_+$ when $w_- \leqslant 1 - \gamma$, with $w_0 = w_+$ when $w_- = 1 - \gamma$. In particular, $0 \leqslant w_0^- \leqslant w_+$, and w_0^- is a continuous function.

Since $D \geqslant 0$ we have $0 \leqslant 2D \leqslant 1 + \gamma$ and $2\lambda^2 \leqslant 1 + \gamma$. Therefore, we can define the functions

$$h_- : [0, 1 + \gamma] \to [0, \lambda^2/(1 + \gamma)],$$

$$h_-(w) = \begin{cases} 0, & w \in [0, 2D] \\ \left(\frac{\lambda\sqrt{w} - \sqrt{1+\gamma-w}\sqrt{D}}{1+\gamma}\right)^2, & w \in [2D, 1 + \gamma], \end{cases}$$

$$h_+ : [0, 1 + \gamma] \to \left[D/(1 + \gamma), \tfrac{1}{2}\right],$$

$$h_+(w) = \begin{cases} \left(\frac{\lambda\sqrt{w} + \sqrt{1+\gamma-w}\sqrt{D}}{1+\gamma}\right)^2, & w \in [0, 2\lambda^2] \\ \frac{1}{2}, & w \in [2\lambda^2, 2]. \end{cases}$$

One can readily check that these functions are continuous. The following result characterizes $\mathcal{C}_C^{\mathrm{sym}}$ explicitly:

Proposition 12.

$$\mathcal{C}_C^{\mathrm{sym}} = \{\mathbf{q} \in \mathcal{M} \mid w_- \leqslant 1 - \gamma, \ r \in [h_-(w_0^-), h_+(w_+)]\}.$$

Before giving a proof, we apply Proposition 12 to a convex line P_α of the form $\mathsf{P}_\alpha(j) = \alpha|j\rangle\langle j| + (1 - \alpha)\mu(j)\mathbb{1}$, where $\mu = (\mu(0), \mu(1), \mu(2))$ is a probability distribution, which must satisfy $\mu(0) = \mu(2) = t \in [0, \frac{1}{2}]$ and $\mu(1) = 1 - 2t$ for P_α to be $\{e, (13)\}$ covariant. Fixing t we then have P_α represented by the line

$$p = \alpha + (1 - \alpha)t, \quad q = r = (1 - \alpha)t,$$

inside $\mathcal{M}$. The goal is to find to value of α at which it intersects the boundary of $\mathcal{C}_C^{\mathrm{sym}}$. The reason for not restricting to the canonical line P_α^C (i.e., $t = \frac{1}{3}$) is that we can cover also the cases where C is obtained as a reduction from some higher dimension as described in Appendix D. In particular, the case of the spin-boson model for $N = 2$ corresponds to $t = \frac{1}{4}$.

Since r decreases as α increases, the intersection point must lie on the lower boundary surface $h_-(w_0^-)$. We restrict to the case $t \geqslant \frac{1}{4}(1 - \gamma)$ for simplicity, because then $w_+(t, t) = 4t \geqslant 1 - \gamma$, and hence $w_+ \geqslant 1 - \gamma$ on the whole line. Therefore $w_0^- = w_0 = \gamma + 1 - 2(1 - \alpha)(1 - 2t)$ on the line, and so $\mathsf{P}_\alpha^C \in \mathcal{C}_C$ iff $h_-(w_0) \leqslant (1 - \alpha)t$, which reads

$$\lambda\sqrt{w_0} - \sqrt{1 + \gamma - w_0}\sqrt{D} \leqslant (1 + \gamma)\sqrt{(1 - \alpha)t}.$$

Rearranging this yields

$$\lambda^2 w_0 \leqslant (1 - \alpha)(\sqrt{2(1 - 2t)}\sqrt{D} + (1 + \gamma)\sqrt{t})^2,$$

from which one can conveniently solve α as

$$\alpha \leqslant 1 - \frac{\lambda^2}{1 - t(1 - \gamma) + 2\sqrt{2t(1 - 2t)D}}.$$

In particular, for $t = \frac{1}{4}$ [the centroid of $\mathcal{M}$ corresponding to $\mathsf{P}(j) = \binom{2}{j}4^{-1}\mathbb{1}$] we get

$$\alpha \leqslant 1 - \frac{4\lambda^2}{3 + \gamma + 4\sqrt{D}}, \tag{F1}$$

while the case $t = \frac{1}{3}$ (the uniform trivial observable) gives instead

$$\alpha \leqslant 1 - \frac{3\lambda^2}{2 + \gamma + 2\sqrt{2D}},$$

which for uniform decoherence, $\gamma = \lambda$, reduces to

$$\alpha \leqslant 1 - \frac{3\lambda^2}{2 + \lambda + 2\sqrt{(1 + 2\lambda)(1 - \lambda)}}.$$

One can easily check that the right-hand side is equal to $g_3(\lambda)$ appearing in the main text. Since $\alpha \leqslant g_3(\lambda)$ is equivalent to $\lambda \leqslant g_3(\alpha)$ (as $\alpha, \lambda > 0$), the results are consistent.

Proof of Proposition 12. As per the reduction method in the main text (proved in Appendix D), $P_\mathbf{q} \in \mathcal{C}_C^{\mathrm{sym}}$ if and only if there exist real matrices $C(j)$ satisfying Eqs. (D4) and (5). This forces the matrices to have the following form, where $a, b, c \in \mathbb{R}$:

$$C(0) = \begin{pmatrix} p & a & c \\ a & r & b \\ c & b & q \end{pmatrix},$$

$$C(1) = \begin{pmatrix} s & \lambda - a - b & \gamma - 2c \\ \lambda - a - b & 1 - 2r & \lambda - a - b \\ \gamma - 2c & \lambda - a - b & s \end{pmatrix},$$

$$C(2) = \begin{pmatrix} q & b & c \\ b & r & a \\ c & a & p \end{pmatrix}.$$

The problem is, then, whether we can find $a, b, c \in \mathbb{R}$ so that the *first two* of these three matrices are positive semidefinite.

[Note that $C(2) = U_{\pi_0} C(0) U_{\pi_0}^\dagger$ is then automatically positive semidefinite.]

In order to further simplify the positivity condition for $C(1)$ (which is easier of the two), we note that all *centrosymmetric* matrices (i.e., ones commuting with U_{π_0}) can be brought to a block form by a specific orthogonal matrix Q only depending on U_{π_0} [58]; in our case,

$$Q = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 & 1 \\ 0 & \sqrt{2} & 0 \\ -1 & 0 & 1 \end{pmatrix},$$

and letting $x = a + b$, $y = a - b$ we obtain

$$Q^T C(0) Q = \begin{pmatrix} \frac{p+q}{2} - c & \frac{y}{\sqrt{2}} & \frac{p-q}{2} \\ \frac{y}{\sqrt{2}} & r & \frac{x}{\sqrt{2}} \\ \frac{p-q}{2} & \frac{x}{\sqrt{2}} & \frac{p+q}{2} + c \end{pmatrix},$$

$$Q^T C(1) Q = \begin{pmatrix} s - \gamma + 2c & 0 & 0 \\ 0 & 1 - 2r & \sqrt{2}(\lambda - x) \\ 0 & \sqrt{2}(\lambda - x) & s + \gamma - 2c \end{pmatrix}.$$

Since orthogonal transformations preserve positivity (and determinants), we can extract the conditions for $C(j) \geqslant 0$ from these matrices. First of all, $\frac{p+q}{2} + c \geqslant 0$ is clearly necessary for $C(0) \geqslant 0$. The 2×2 principal minors of $Q^T C(0) Q$ are

$$d_{(0)} := r\left(\frac{p+q}{2} + c\right) - \frac{x^2}{2},$$

$$d_{(1)} := \left(\frac{p+q}{2} - c\right)\left(\frac{p+q}{2} + c\right) - \left(\frac{p-q}{2}\right)^2 = qp - c^2,$$

$$d_{(2)} := r\left(\frac{p+q}{2} - c\right) - \frac{y^2}{2}.$$

Assuming $\frac{p+q}{2} + c > 0$, we can write

$$\det C(0) = r d_{(1)} - \frac{1}{2}\left(\frac{p+q}{2} - c\right)x^2 - \frac{1}{2}\left(\frac{p+q}{2} + c\right)y^2$$
$$+ xy \frac{p-q}{2}$$
$$= d_{(0)} d_{(1)} / \left(\frac{p+q}{2} + c\right) - \frac{1}{2}\left(\frac{p+q}{2} + c\right)(y - y_0)^2,$$

where $y_0 = \frac{1}{2} x(p-q)/(\frac{p+q}{2} + c)$. Hence, $C(0) \geqslant 0$ is equivalent to $\det C(0) \geqslant 0$ and $d_{(i)} \geqslant 0$ for $i = 1, 2, 3$. Since $d_{(0)}, d_{(1)}$ do not depend on y and imply $d_{(2)} \geqslant 0$ when $y = y_0$, it follows that if $C(0) \geqslant 0$ for some choices of x, y, c, it also holds if we take $y = y_0$ (as the determinant can only increase). As $C(1)$ does not depend on y, we may therefore always take $y = y_0$. With this choice, $C(0) \geqslant 0$ if and only if

$$\frac{p+q}{2} + c \geqslant 0, \quad |x| \leqslant \sqrt{2r\left(\frac{p+q}{2} + c\right)}, \quad c^2 \leqslant qp. \quad \text{(F2)}$$

[In the special case $\frac{p+q}{2} + c = 0$, we have $C(0) \geqslant 0$ only if $p = q$ and $x = 0$, so $C(0) \geqslant 0$ iff $y^2 \leqslant 4rp$. Hence we can take $y = y_0 = 0$, and this case is covered by (F2)].

Next we observe that $C(1) \geqslant 0$ if and only if

$$\left| c - \frac{\gamma}{2}\right| \leqslant \frac{s}{2}, \quad |\lambda - x| \leqslant \sqrt{(1 - 2r)\left(\frac{s + \gamma}{2} - c\right)}. \quad \text{(F3)}$$

For fixed c, the inequalities (F2) and (F3) force x into an intersection of two intervals. By the triangle inequality, (F2) and (F3) hold for *some* x, if and only if $\lambda \leqslant g(c)$ where

$$g(c) := \sqrt{2r\left(\frac{p+q}{2} + c\right)} + \sqrt{(1 - 2r)\left(\frac{s + \gamma}{2} - c\right)},$$

and the remaining constraints hold for c. These constraints are given by the following set:

$$\mathcal{D} := \left\{ c \in \mathbb{R} \,\middle|\, \left| c - \frac{\gamma}{2}\right| \leqslant \frac{s}{2}, \; |c| \leqslant \sqrt{pq} \right\}.$$

Hence, $\mathbf{q} \in \mathcal{C}_C$ if and only if $\lambda \leqslant g(c)$ for some $c \in \mathcal{D}$. Clearly, this is in turn equivalent to the following:

$$\mathcal{D} \neq \emptyset \text{ and } \lambda \leqslant \max_{c \in \mathcal{D}} g(c). \quad \text{(F4)}$$

By the triangle inequality, $\mathcal{D} \neq \emptyset$ if and only if

$$\frac{\gamma - s}{2} \leqslant \sqrt{qp}, \quad \text{(F5)}$$

in which case $\mathcal{D}$ is the interval

$$\mathcal{D} := \left[\max\left\{ -\sqrt{qp}, \frac{\gamma - s}{2}\right\}, \min\left\{\sqrt{qp}, \frac{\gamma + s}{2}\right\}\right] \quad \text{(F6)}$$

(where the left boundary does not exceed the right). Hence, (F5) is a *necessary* (but not sufficient) condition for $\mathbf{q} \in \mathcal{C}_C$. In fact, it is one of the two Hellinger distance conditions given by Corollary 1 of the main text. We note that (F5) does not depend on r, and let $\mathcal{R}$ denote the set of those $(p, q) \in \Delta$ for which it holds. Then

$$\mathcal{R} = \{(p, q) \in \Delta \mid w_- \leqslant 1 - \gamma\},$$

where the function $w_- = w_-(p, q)$ was defined above. Next we note that the maximal domain of g (where the square roots are defined) is

$$\mathcal{D}_{\max} := \left[-\tfrac{1}{2}(p + q), \tfrac{1}{2}(s + \gamma)\right],$$

which clearly contains $\mathcal{D}$ because $\sqrt{qp} \leqslant \frac{1}{2}(q + p)$. We readily find the global maximum point of g within $\mathcal{D}_{\max}$:

$$2\frac{dg}{dc} = \sqrt{\frac{2r}{c + (p+q)/2}} - \sqrt{\frac{1 - 2r}{(s + \gamma)/2 - c}},$$

and hence $\frac{dg}{dc} \geqslant 0$ iff $c \leqslant c_0$ where $c_0 = r(1 + \gamma) - \frac{1}{2}(p + q)$. Note that indeed $c_0 \in \mathcal{D}_{\max}$, as

$$c_0 + \frac{p+q}{2} = r(1 + \gamma) \geqslant 0,$$

$$\frac{s + \gamma}{2} - c_0 = \left(\frac{1}{2} - r\right)(1 + \gamma) \geqslant 0.$$

It follows that $g(c_0) = \sqrt{\frac{1}{2}(1 + \gamma)}$, so that $g(c_0) \geqslant \lambda$ automatically by the positivity of C, and hence $c_0 \in \mathcal{D}$ is a *sufficient* condition for $\mathbf{q} \in \mathcal{C}_C$. However, it is not a necessary condition, as c_0 may fall on either side of $\mathcal{D}$; in those cases, the maximum is attained at the boundary, and we obtain a constraint in terms of λ. In order to find it we consider the three possible cases

for $\mathcal{D}$:

(1) $\mathcal{D}_1 = [-\sqrt{qp}, \sqrt{qp}]$.

(2) $\mathcal{D}_2 = [\frac{\gamma-s}{2}, \sqrt{qp}]$.

(3) $\mathcal{D}_3 = [\frac{\gamma-s}{2}, \frac{\gamma+s}{2}]$.

(The case $\mathcal{D} = [-\sqrt{qp}, \frac{\gamma+s}{2}]$ cannot occur as $\gamma \geqslant 0$.) Since $\mathcal{D}$ does not depend on r, these cases set up a unique partition of $\mathcal{R}$; we have $\mathcal{R} = \mathcal{R}_1 \cup \mathcal{R}_2 \cup \mathcal{R}_3$ where $\mathcal{R}_i := \{(p, q) \in \mathcal{R} \mid \mathcal{D} = \mathcal{D}_i\}$. It is then easy to check that

$$\mathcal{R}_1 = \{(p, q) \in \Delta \mid w_+ < 1 - \gamma\},$$

$$\mathcal{R}_2 = \{(p, q) \in \Delta \mid 1 - \gamma \leqslant w_+ < 1 + \gamma\} \cap \mathcal{R},$$

$$\mathcal{R}_3 = \{(p, q) \in \Delta \mid w_+ \geqslant 1 + \gamma\},$$

where we have used the function $w_+ = w_+(p, q)$ defined above. Each of these cases then has three subcases (a)–(c) according to whether $c_0 \leqslant \min \mathcal{D}$, $c_0 \in \mathcal{D}$, or $c_0 \geqslant \max \mathcal{D}$, respectively. In order to describe them we also need the functions $w_0 = w_0(p, q)$, and $l(w) := \frac{1}{2}w/(1 + \gamma)$. We observe that $\mathbf{q} \in \mathcal{C}_C$ if and only if (q, p) falls into one of the following eight categories:

(1) $(p, q) \in \mathcal{R}_1$ [implying $0 \leqslant l(w_-) \leqslant l(w_+) \leqslant \frac{1}{2}$], and

    (a) $0 \leqslant r \leqslant l(w_-)$ and $\lambda \leqslant g(-\sqrt{qp})$, or

    (b) $l(w_-) \leqslant r \leqslant l(w_+)$, or

    (c) $l(w_+) \leqslant r \leqslant \frac{1}{2}$ and $\lambda \leqslant g(\sqrt{qp})$.

(2) $(p, q) \in \mathcal{R}_2$ [implying $0 \leqslant l(w_0) \leqslant l(w_+) \leqslant \frac{1}{2}$] and

    (a) $0 \leqslant r \leqslant l(w_0)$ and $\lambda \leqslant g(\frac{\gamma-s}{2})$, or

    (b) $l(w_0) \leqslant r \leqslant l(w_+)$ or

    (c) $l(w_+) \leqslant r \leqslant \frac{1}{2}$ and $\lambda \leqslant g(\sqrt{qp})$.

(3) $(p, q) \in \mathcal{R}_3$ [implying $0 \leqslant l(w_0) \leqslant \frac{1}{2}$], and

    (a) $0 \leqslant r \leqslant l(w_0)$ and $\lambda \leqslant g(\frac{\gamma-s}{2})$, or

    (b) $l(w_0) \leqslant r \leqslant \frac{1}{2}$.

(In this case (c) does not occur.) We then notice that

$$g(\pm\sqrt{qp}) = \sqrt{rw_\pm} + \sqrt{(\tfrac{1}{2} - r)(1 + \gamma - w_\pm)},$$

$$g\left(\tfrac{1}{2}(\gamma - s)\right) = \sqrt{rw_0} + \sqrt{(\tfrac{1}{2} - r)(1 + \gamma - w_0)}; \quad \text{(F7)}$$

hence in each case the condition involving λ is of the form

$$\lambda \leqslant \sqrt{rw} + \sqrt{(\tfrac{1}{2} - r)(1 + \gamma - w)}, \quad \text{(F8)}$$

for $(r, w) \in [0, \frac{1}{2}] \times [0, 1 + \gamma]$. Equivalently,

$$h_-(w) \leqslant r \leqslant h_+(w), \quad \text{(F9)}$$

where $h_\pm$ were introduced above. We observe that

$$h_-(w) \leqslant l(w) \leqslant h_+(w) \quad \text{(F10)}$$

for all $(r, w) \in [0, \frac{1}{2}] \times [0, 1 + \gamma]$. (In fact, the region defined by (F8) is symmetric about the line $r = l(w)$.) Using (F7), (F9), and (F10) we can put together subcases (a)–(c) in the above three cases: $\mathbf{q} \in \mathcal{C}_C$ if and only if one of the following conditions hold:

(1) $(p, q) \in \mathcal{R}_1$ and $h_-(w_-) \leqslant r \leqslant h_+(w_+)$.

(2) $(p, q) \in \mathcal{R}_2$ and $h_-(w_0) \leqslant r \leqslant h_+(w_+)$.

(3) $(p, q) \in \mathcal{R}_3$ and $h_-(w_0) \leqslant r \leqslant \frac{1}{2}$.

Noting that $w_+ \geqslant 1 + \gamma \geqslant 2\lambda^2$ when $(p, q) \in \mathcal{R}_3$, we have $h_+(w_+) = \frac{1}{2}$ when $(p, q) \in \mathcal{R}_3$, and hence the upper bound for r is always $h_+(w_+)$. By the definition of w_0^-, the lower bound is $h_-(w_0^-)$, and the proof of the proposition is complete.

APPENDIX G: SPIN-BOSON MODEL WITH $N = 2$

Here we present in detail the analytical solution of $\mathcal{C}_C^{\text{sym}}$ for $N = 2$ in the spin-boson model. We order the two-qubit incoherent basis in the usual way as $\{|00\rangle, |01\rangle, |10\rangle, |11\rangle\}$, with respective label set $\{1, 2, 3, 4\}$, on which the symmetric group S_4 acts. In this basis our matrix $C[\lambda]$ of the dynamical GIO reads

$$C[\lambda] = \begin{pmatrix} 1 & \lambda & \lambda & \lambda^4 \\ \lambda & 1 & 1 & \lambda \\ \lambda & 1 & 1 & \lambda \\ \lambda^4 & \lambda & \lambda & 1 \end{pmatrix}.$$

The equivalence classes of maximal coherence are given by $I_0^C = \{1\}$, $I_1^C = \{2, 3\}$, $I_2^C = \{4\}$, so $n_C = 3$. These correspond to the eigenspaces of S_z given by $\mathcal{S}_0 = \text{span}\{|00\rangle\}$, $\mathcal{S}_1 = \text{span}\{|01\rangle, |10\rangle\}$, and $\mathcal{S}_2 = \text{span}\{|11\rangle\}$. Note that $\mathcal{S}_1$ is a nontrivial two-dimensional decoherence-free subspace, as we can see from the matrix. Now the canonical incoherent observable P^C has three outcomes $\{0, 1, 2\}$, and is given by $\mathsf{P}^C(0) = |00\rangle\langle00|$, $\mathsf{P}^C(1) = |10\rangle\langle01| + |10\rangle\langle01|$, $\mathsf{P}^C(2) = |11\rangle\langle11|$, which is just the spectral decomposition of S_z as mentioned in the main text. The line P_α^C used to define the quantity α_C is given by $\mathsf{P}_\alpha^C(j) = \alpha\mathsf{P}^C(j) + (1 - \alpha)\text{tr}[\mathsf{P}^C(j)]\frac{1}{4}\mathbb{1} = \alpha\mathsf{P}^C(j) + (1 - \alpha)\binom{2}{j}\frac{1}{4}\mathbb{1}$. Finally, the symmetry group G_C leaving C unchanged is the subgroup of S_4 generated by the within-class permutation (23) (exchanging 2 and 3), and the order reversal $(14)(23)$, that is, $G_C = \{e, (23), (14)(23), (14)\}$. The task is to characterize the set $\mathcal{C}_C^{\text{sym}}$.

We now carry out the reduction to dimension $n_C = 3$. First, we have

$$\tilde{C}[\lambda] = \begin{pmatrix} 1 & \lambda & \lambda^4 \\ \lambda & 1 & \lambda \\ \lambda^4 & \lambda & 1 \end{pmatrix},$$

with $G_{\tilde{C}} = \{e, (13)\}$. The homomorphism $\phi : G_C \to G_{\tilde{C}}$ defined by $\pi(I_k^C) = I_{\phi(\pi)(k)}^C$ maps as follows: $\phi((23)) = \phi(e) = e$, $\phi((14)) = \phi((14)(23)) = (13)$, so that $\phi(G_C) = \{e, (13)\} = G_{\tilde{C}}$, i.e., the within-class permutation is mapped to the identity, and the reversal carries over to the reduction. In this way we end up with the case considered above in Appendix F with $\gamma = \lambda^4$, so Proposition 12 gives the three-dimensional convex set $\mathcal{C}_C[\phi(G_C)] = \mathcal{C}_C^{\text{sym}}$. Hence every $\mathsf{P} \in \mathcal{C}_C^{\text{sym}}$ is of the form

$$\mathsf{P}(0) = \begin{pmatrix} p & 0 & 0 & 0 \\ 0 & r & 0 & 0 \\ 0 & 0 & r & 0 \\ 0 & 0 & 0 & q \end{pmatrix},$$

$$\mathsf{P}(1) = \begin{pmatrix} s & 0 & 0 & 0 \\ 0 & 1-2r & 0 & 0 \\ 0 & 0 & 1-2r & 0 \\ 0 & 0 & 0 & s \end{pmatrix},$$

$$\mathsf{P}(2) = \begin{pmatrix} q & 0 & 0 & 0 \\ 0 & r & 0 & 0 \\ 0 & 0 & r & 0 \\ 0 & 0 & 0 & p \end{pmatrix},$$

where $(p, q, r) \in [0, 1]$, $r \in [0, \frac{1}{2}]$ are such that $w_-(p, q) \leqslant 1 - \lambda^4$, $r \in [h_-(w_0^-(p, q)), h_+(w_+(p, q))]$ (see Appendix F). As noted in the main text, $\mathcal{C}_C^{\text{sym}}$ is therefore a convex set of affine dimension 3 only depending on λ, and can conveniently be plotted in the parametrization (p, q, r), as shown in Fig. 1 in the main text. Furthermore, by substituting $\gamma = \lambda^4$ into Eq. (F1) in Appendix F we immediately deduce that

$$\alpha_2(\lambda) = 1 - \frac{4\lambda^2}{3 + \lambda^4 + 2\sqrt{2}(1 - \lambda^2)},$$

as claimed in the main text.

APPENDIX H: SMALL COHERENCE LIMIT IN THE SPIN-BOSON MODEL

Here we prove the asymptotic behavior of the curve $\alpha = \alpha_N(\lambda)$ stated in Proposition 5. We first consider the upper bound $\alpha = U_N(\lambda)$, or, equivalently, $\lambda = \beta_{01}(\alpha)$, which is an explicit algebraic curve given by the Hellinger distance $d_{01}^2(\mathsf{P}_\alpha^C)$ corresponding to the dominant coherence λ in $C[\lambda]$, as explained in the main text. Hence the asymptotic form is easily obtained: $\beta_{01}(\alpha) = k_N\sqrt{1 - \alpha} + O(1 - \alpha)$, where $k_N = 2^{-N/2}(1 + \sqrt{N})$. Here we have used the customary notation where $g(\alpha) = O((1 - \alpha)^k)$ means that the function $\alpha \mapsto |g(\alpha)|/(1 - \alpha)^k$ is bounded on some neighborhood of $\alpha = 1$. Note that this does not require a convergent series expansion for g at $\alpha = 1$. Indeed, while such an expansion exists for $\beta_{01}(\alpha)$, the same is not clear for the exact curve $\alpha = \alpha_N(\lambda)$, which nevertheless turns out to have the same behavior. In order to see this we find a lower bound with the same asymptotic behavior. We denote $q_k(\alpha) = \binom{N}{k}\frac{1-\alpha}{2^N}$, for each $k = 0, \ldots, N$, and $u_k(\alpha) = \sqrt{q_k(\alpha)(\alpha + q_k(\alpha))}$ for $k = 0, 1$. Then the upper bound reads $\beta_{01}(\alpha) = u_0(\alpha) + u_1(\alpha) + (1 - \alpha)(1 - \frac{1}{2^N}(1 + N))$. It turns out that the first two terms form a lower bound:

Lemma 1. $u_0(\alpha) + u_1(\alpha) \leqslant \alpha_N^{-1}(\alpha)$ for all $\alpha \in [0, 1]$, where $\alpha_N^{-1} : [0, 1] \to [0, 1]$ is the inverse of the monotone function α_N.

As a consequence, we obtain the following result, the first part of which is Proposition 5 in the main text:

Proposition 13. For any fixed N,

$$\alpha_N^{-1}(\alpha) = k_N\sqrt{1 - \alpha} + O(1 - \alpha) \text{ as } \alpha \to 1.$$

For each $\alpha \in [0, 1]$ and N, we have the error bound

$$\left|\alpha_N^{-1}(\alpha) - k_N\sqrt{1 - \alpha}\right| \leqslant 1 - \alpha + \frac{3}{2}k_N\left(\frac{1 - \alpha}{\alpha}\right)^{\frac{3}{2}}.$$

First define

Proof. Using the bijection $\alpha \mapsto v = \sqrt{1 - \alpha}$ we define

$$
\begin{aligned}
f(v) &:= u_0(\alpha) + u_1(\alpha) \\
&= v\sqrt{1 - r}\sqrt{1 - rv^2} + v\sqrt{1 - s}\sqrt{1 - sv^2},
\end{aligned}
$$

where $r = 1 - 2^{-N}$ and $s = 1 - N2^{-N}$. Now $\beta_{01}(\alpha) = f(v) + v^2(1 - \frac{1}{2^N}(1 + N)) \leqslant f(v) + v^2$. Combined with Lemma 1, this gives $f(v) \leqslant \alpha_N^{-1}(\alpha) \leqslant f(v) + v^2$, that is, $|\alpha_N^{-1}(\alpha) - f(v)| \leqslant v^2$ for all $v \in [0, 1]$. Since $f(0) = 0$, Taylor's theorem gives $f(v) = k_N v + z(v)$, where $|z(v)| \leqslant \frac{1}{2}v^2 \max_{0 \leqslant \tilde{v} \leqslant v} |\frac{d^2 f}{dv^2}(\tilde{v})|$. Now

$$
\begin{aligned}
\left|\frac{d^2 f}{dv^2}(\tilde{v})\right| &= \frac{r\sqrt{1 - r}(3 - 2r\tilde{v}^2)\tilde{v}}{(1 - r\tilde{v}^2)^{\frac{3}{2}}} + \frac{s\sqrt{1 - s}(3 - 2s\tilde{v}^2)\tilde{v}}{(1 - s\tilde{v}^2)^{\frac{3}{2}}} \\
&\leqslant \frac{3vr\sqrt{1 - r}}{(1 - rv^2)^{\frac{3}{2}}} + \frac{3vs\sqrt{1 - s}}{(1 - sv^2)^{\frac{3}{2}}} \leqslant \frac{3(1 + \sqrt{N})v}{2^{N/2}(1 - v^2)^{\frac{3}{2}}},
\end{aligned}
$$

and hence $|z(v)| \leqslant \frac{3}{2}k_N v^3(1 - v^2)^{-\frac{3}{2}}$. Therefore,

$$
\begin{aligned}
|\alpha_N^{-1}(\alpha) - k_N v| &= |\alpha_N^{-1}(\alpha) - f(v) + z(v)| \\
&\leqslant |\alpha_N^{-1}(\alpha) - f(v)| + |z(v)| \\
&\leqslant v^2 + \frac{3}{2}k_N v^3(1 - v^2)^{-\frac{3}{2}}.
\end{aligned}
$$

Substituting $v = \sqrt{1 - \alpha}$ yields the claim. ∎

Since $\alpha_N^{-1}(1) = 0$, the validity of the approximation can be quantified by the relative error $\epsilon = |\alpha_N^{-1}(\alpha) - k_N v|/\alpha_N^{-1}(\alpha)$. Assuming that the second term in the error bound of the proposition is negligible for this consideration, we get the maximum relative error $\epsilon_{\max} \approx (k_N/\sqrt{1 - \alpha} - 1)^{-1}$. This suggests that the asymptotic form becomes valid around $\alpha \approx 1 - ck_N^2$ where c is a constant. For instance, $\alpha \approx 1 - (k_N/24)^2$ corresponds to a maximum error of 4–5 %.

We now prove Lemma 1 by constructing explicitly a GII satisfying Eqs. (D4) and (5), for $\lambda = u_0(\alpha) + u_1(\alpha)$ and all $\alpha \in [0, 1]$. [This then shows that $\mathsf{P}_\alpha^C \in \mathcal{C}_C$ whenever α satisfies $\lambda \leqslant u_0(\alpha) + u_1(\alpha)$, and therefore the transition point $\alpha = \alpha_N(\lambda)$ must satisfy $\lambda \geqslant u_0(\alpha) + u_1(\alpha)$, giving the claimed inequality.] For simplicity, we show the construction for $N \geqslant 5$ (for smaller N it needs a few modifications).

$$
C(0) = \left(
\begin{array}{ccc|ccc|ccc}
\alpha + q_0 & u_0 & 0 & & & & & & \\
u_0 & q_0 & 0 & & \mathbf{0} & & & \mathbf{0} & \\
0 & 0 & q_0 & & & & & & \\
\hline
 & & & q_0 & & & & & \\
 & \mathbf{0} & & & \ddots & & & \mathbf{0} & \\
 & & & & & q_0 & & & \\
\hline
 & & & & & & q_0 & 0 & 0 \\
 & \mathbf{0} & & & \mathbf{0} & & 0 & q_0 & 0 \\
 & & & & & & 0 & 0 & q_0
\end{array}
\right)
$$

and

$$C(1) = \left(\begin{array}{ccc|ccc|ccc} q_1 & u_1 & q_1 & & & & & & \\ u_1 & \alpha + q_1 & u_1 & & \mathbf{0} & & & \mathbf{0} & \\ q_1 & u_1 & q_1 & & & & & & \\ \hline & & & q_1 & & & & & \\ & \mathbf{0} & & & \ddots & & & \mathbf{0} & \\ & & & & & q_1 & & & \\ \hline & & & & & & q_1 & 0 & -q_1 \\ & \mathbf{0} & & & \mathbf{0} & & 0 & q_1 & 0 \\ & & & & & & -q_1 & 0 & q_1 \end{array} \right).$$

These matrices are clearly positive semidefinite. (If $N = 5$ the central block is empty.) We then set $C(N) := U_{\pi_0}^\dagger C(0) U_{\pi_0}$, $C(N-1) := U_{\pi_0}^\dagger C(1) U_{\pi_0}$, where U_{π_0} is the permutation matrix for the order reversal π_0. Recalling that $A \mapsto U_{\pi_0}^\dagger A U_{\pi_0}$ transposes the matrix along the counterdiagonal, we can easily check that $C(0) + C(1) + C(N-1) + C(N)$ reads

$$\left(\begin{array}{ccc|ccc|ccc} \alpha + r_1 & \lambda & 0 & & & & & & \\ \lambda & \alpha + r_1 & u_1 & & \mathbf{0} & & & \mathbf{0} & \\ 0 & u_1 & r_1 & & & & & & \\ \hline & & & r_1 & & & & & \\ & \mathbf{0} & & & \ddots & & & \mathbf{0} & \\ & & & & & r_1 & & & \\ \hline & & & & & & r_1 & u_1 & 0 \\ & \mathbf{0} & & & \mathbf{0} & & u_1 & \alpha + r_1 & \lambda \\ & & & & & & 0 & \lambda & \alpha + r_1 \end{array} \right)$$

where $r_k = 2 \sum_{j=0}^{k} q_j$. Note that $-q_1$ on the lower right block of $C(1)$ cancels out the q_1 on the upper left block, and the overlap between $C(0)$ and $C(1)$ produces λ on both ends of the diagonal $(n, n+1)$.

Next, let $j_0 = N/2$ if N is even, and $j_0 = (N-1)/2$ if N is odd, and define

$$M_j(w) = \begin{pmatrix} q_j & w & 0 \\ w & \alpha + q_j & w \\ 0 & w & q_j \end{pmatrix}$$

for $j = 2, \ldots, j_0$ and $w \in [0, 1]$. Now $M_j(w) \geqslant 0$ if and only if $2w^2 \leqslant q_j(q_j + \alpha)$, which is clearly the case for $w = u_0$ when $j \geqslant 2$, and for $w = u_1$ when $j \geqslant 3$, because q_j is increasing in j (up to j_0), and $q_2 \geqslant 2q_0$, $q_3 \geqslant 2q_1$. [Note that the same is not true for $j = 0, 1$, which is why we defined $C(0)$ and $C(1)$ differently above.] Then let

$$V_j(w) = \begin{pmatrix} q_k \mathbb{1}_{j-1} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & M_j(w) & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & q_k \mathbb{1}_{N-j-1} \end{pmatrix}$$

for each $j = 2, \ldots, j_0$.

We now consider even and odd N separately.

If N is even, j_0 is the "middle" point of $\{0, \ldots, N\}$, and we can set up $C(2), \ldots, C(j_0 - 1)$ as follows: $C(j) := V_j(u_1)$ if j is odd, and $C(j) := V_j(u_0)$ if j is even. Notice that the block $M_j(w)$ moves down the diagonal as j increases, with w alternating between u_1 and u_0. These blocks only overlap between neighboring matrices $C(j)$, $C(j+1)$, and hence the sum $\sum_j C(j)$ has $\lambda = u_0 + u_1$ on each $(k, k-1)$ entry for $k = 0, \ldots, j_0 - 1$. We then set $C(j_0 + j) := U_{\pi_0}^\dagger C(j_0 - j) U_{\pi_0}$ for $j = 1, \ldots, j_0 - 2$, to satisfy the symmetry. Finally, we define the middle element by $C(j_0) := D + G$ where D

follows the above pattern, that is, $D := V_{j_0}(u_1)$ ($V_{j_0}(u_0)$) if j_0 is odd (even), $G := C[\lambda] - \tilde{C}$, and $\tilde{C}$ denotes the truncation of $C[\lambda]$ to second order in λ, so that $\tilde{C}$ is a tridiagonal matrix. Now $\sum_{j \neq j_0} C(j) + D = \tilde{C}$, and the remainder G is included in $C(j_0)$ so that $\sum_j C(j) = C[\lambda]$. Note also that $C(j_0)$ satisfies $U_{\pi_0}^\dagger C(j_0) U_{\pi_0} = C(j_0)$ as D has the block $M_{j_0}(w)$ exactly at the center. We are left to prove that $C(j_0) \geqslant 0$. To do this we write

$$C(j_0) = D + G = (D - \epsilon \mathbb{1}) + (\epsilon \mathbb{1} + G),$$

where we pick $\epsilon > 0$ small enough so that $D - \epsilon \mathbb{1} \geqslant 0$, but large enough to make $\epsilon \mathbb{1} + G \geqslant 0$. We can take, for instance, $\epsilon = \frac{2}{3} q_1$. In fact, first note that $\lambda = u_0 + u_1 \leqslant k_N \sqrt{1 - \alpha}$, and $\lambda \leqslant 0.305$ for all $\alpha \in [0, 1]$, $N \geqslant 5$. Also, $k_N^2 \leqslant 2.1 N / 2^N$ for $N \geqslant 5$ so

$$\frac{1}{2} \sum_{j \neq i} G_{ij} \leqslant \sum_{k=2}^{\infty} \lambda^k \cdot 2 \leqslant \lambda^4 \sum_{k=0}^{\infty} \lambda^k = \frac{\lambda^4}{1 - \lambda} \leqslant 0.14 \lambda^2$$

$$\leqslant 0.14 k_N^2 (1 - \alpha) \leqslant 0.14 * 2.1 q_1 \leqslant \frac{1}{3} q_1,$$

and hence $\epsilon \mathbb{1} + G \geqslant 0$ when $N \geqslant 5$ by diagonal dominance. Moreover, $M_{j_0}(w) - \epsilon \mathbb{1} \geqslant 0$ since for $N \geqslant 6$,

$$(q_{j_0} - \epsilon)(\alpha + q_{j_0} - \epsilon) - 2w^2$$
$$\geqslant (q_3 - \epsilon)(\alpha + q_3 - \epsilon) - 2q_1(\alpha + q_1)$$
$$\geqslant (q_3 - 2q_1 - \epsilon)(\alpha + q_3) + 2q_1(q_3 - q_1) - q_3 \epsilon$$
$$= (q_3 - \frac{8}{3} q_1)(\alpha + q_3) + \frac{4}{3} q_1(q_3 - \frac{3}{2} q_1) \geqslant 0,$$

where $q_3 - \frac{8}{3} q_1 = \frac{N}{6}((N-1)(N-2) - 16)\frac{1-\alpha}{2^N} \geqslant 0$ as $N \geqslant 6$. [Note that the 2×2 principal minors of $M_{j_0}(w)$ are then

automatically positive.] Hence $D - \epsilon \mathbb{1} \geqslant 0$. This completes the construction for even N.

If N is odd, we have two middle points j_0 and $j_0 + 1$. We now define $C(2), \ldots, C(j_0 - 1)$ as above, and again set $C(j_0 + 1 + j) := U_{\pi_0}^\dagger C(j_0 - j) U_{\pi_0}$, for $j = 1, \ldots, j_0 - 2$. The sum of these matrices coincides with $\tilde{C}$ everywhere except in the 4×4 block at the center of the matrix, and on the main diagonal. The two remaining matrices have to be set up separately. Let $w = u_1$ if j_0 is odd, and $w = u_0$ if it is even. We first define D as the $(N + 1) \times (N + 1)$ matrix having q_{j_0} on the main diagonal outside the central 4×4 block,

$$
\begin{pmatrix}
q_{j_0} & w & 0 & 0 \\
w & \alpha + q_{j_0} & \frac{\lambda}{2} & 0 \\
0 & \frac{\lambda}{2} & q_{j_0} & 0 \\
0 & 0 & 0 & q_{j_0}
\end{pmatrix}, \tag{H1}
$$

and the remaining elements zero. Now $D \geqslant 0$ due to $q_{j_0} \geqslant q_2 \geqslant 2q_1$, which holds as $N \geqslant 5$. Clearly, the sum $D + U_{\pi_0}^\dagger D U_{\pi_0}$ has $2q_{j_0} = q_{j_0} + q_{j_0+1}$ on the main diagonal outside the central block, which reads

$$
\begin{pmatrix}
2q_{j_0} & w & 0 & 0 \\
w & \alpha + 2q_{j_0} & \lambda & 0 \\
0 & \lambda & \alpha + 2q_{j_0} & w \\
0 & 0 & w & 2q_{j_0}
\end{pmatrix}.
$$

Added to the previously constructed $C(j)$, this produces $\tilde{C}$. Now define $C(j_0) := D + \frac{1}{2} G$ and $C(j_0 + 1) = U_{\pi_0}^\dagger D U_{\pi_0} + \frac{1}{2} G$, where G is as before. Then $C(j_0 + 1) = U_{\pi_0}^\dagger C(j_0) U_{\pi_0}$

and $\sum_{j=0}^{N} C(j) = C[\lambda]$. As in the even case, we establish that $C(j_0) \geqslant 0$; we write

$$
C(j_0) = \left(D - \frac{\epsilon}{2} \mathbb{1} \right) + \frac{1}{2} (\epsilon \mathbb{1} + G),
$$

with the same ϵ as before, so the second term is positive for $N \geqslant 5$. Using $\frac{1}{4} \lambda^2 \leqslant \frac{1}{2} (u_0^2 + u_1^2)$ we get

$$
\left(q_{j_0} - \frac{\epsilon}{2} \right) \left(\alpha + q_{j_0} - \frac{\epsilon}{2} \right) - (\lambda/2)^2 - w^2
$$

$$
\geqslant \left(q_2 - \frac{\epsilon}{2} \right) \left(\alpha + q_2 - \frac{\epsilon}{2} \right) - \frac{1}{2} (u_0^2 + u_1^2) - q_1(\alpha + q_1)
$$

$$
= \left(q_2 - \frac{1}{3} q_1 \right) \left(\alpha + q_2 - \frac{1}{3} q_1 \right)
$$

$$
- \frac{1}{2} q_0 (\alpha + q_0) - \frac{3}{2} q_1 (\alpha + q_1)
$$

$$
= \left(q_2 - \frac{11}{6} q_1 - \frac{1}{2} q_0 \right) \alpha + \left(q_2 - \frac{1}{3} q_1 \right)^2 - \frac{1}{2} q_0^2 - \frac{3}{2} q_1^2
$$

$$
= \left(\frac{N^2 - 1}{2} - \frac{11N}{6} \right) \frac{\alpha(1 - \alpha)}{2^N}
$$

$$
+ \left(\left(\frac{N^2}{2} - \frac{5N}{6} \right)^2 - \frac{1 + 3N^2}{2} \right) \frac{(1 - \alpha)^2}{2^{2N}}
$$

$$
\geqslant 0 \quad \text{for } N \geqslant 5,
$$

which implies that $D - \frac{\epsilon}{2} \mathbb{1} \geqslant 0$. This completes the proof for the odd case, and the proof of Lemma 1 is complete.

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