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Estimation of correlations and non-separability in quantum channels via unitarity benchmarking

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The ability to transfer coherent quantum information between systems is a fundamental component of quantum technologies and leads to coherent correlations within the global quantum process. However correlation structures in quantum channels are less studied than those in quantum states. Motivated by recent techniques in randomized benchmarking, we develop a range of results for efficient estimation of correlations within a bipartite quantum channel. We introduce sub-unitarity measures that are invariant under local changes of basis, generalize the unitarity of a channel, and allow for the analysis of coherent information exchange within channels. Using these, we show that unitarity is monogamous, and provide a novel information-disturbance relation. We then define a notion of correlated unitarity that quantifies the correlations within a given channel. Crucially, we show that this measure is strictly bounded on the set of separable channels and therefore provides a witness of non-separability. Finally, we describe how such measures for effective noise channels can be efficiently estimated within different randomized benchmarking protocols. We find that the correlated unitarity can be estimated in a SPAM-robust manner for any separable quantum channel, and show that a benchmarking/tomography protocol with mid-circuit resets can reliably witness non-separability for sufficiently small reset errors. The tools we develop provide information beyond that obtained via simultaneous randomized benchmarking and so could find application in the analysis of cross-talk and coherent errors in quantum devices.

I. INTRODUCTION

Efficient certification and benchmarking of non-classical features in quantum theory are pressing questions with wide importance to the development of quantum technologies [1–7], which require precise control and manipulation of quantum systems. High fidelity quantum gates and circuits are essential for scalable quantum computing so it is important to benchmark the effects of physical noise on how accurately a target unitary is realized on the quantum device.

Direct process tomography [8, 9] of noisy gates and circuits faces two non-trivial obstacles: firstly the complexity of full tomography is known to scale exponentially, and secondly there is the problem of characterizing errors in the presence of other types of errors such as those arising from state-preparation and measurement (SPAM). To circumvent these obstacles techniques have been developed such as gate-set tomography and randomized benchmarking, which allow for efficient estimation of measures that is robust against SPAM errors.

In the simplest instance, randomized benchmarking (RB) returns an estimate of the average gate infidelity $r(\mathcal{E})$ over a quantum computational gate-set. However this only provides a blunt estimate of the performance of the device. Firstly, the average gate infidelity for coherent errors [10] is known to only weakly constrain the worst-case error rate, defined in terms of the dia-

mond norm, which is the relevant quantity in the context of fault-tolerance [11, 12]. Unitarity benchmarking [13–15] provides additional information to the average gate infidelity. In particular the unitarity $u(\mathcal{E})$ provides a measure of how coherent the noise channel is in the device, and witnesses the poor scaling between $r(\mathcal{E})$ and the diamond norm.

Secondly, RB gives average, coarse grained noise characterization that largely ignores the effect of errors that depend on circuit structures. Correlated, context or time dependent noise can have a more detrimental effect on the accumulation of errors in a circuit – features that may persist even when considering quantum error correction codes, that largely have been designed to exponentially suppress noise for specific models [16–18]. Therefore, detection and quantification of noise correlations in quantum devices not only impacts NISQ era devices [19] by improving circuit fidelities and error mitigation methods but goes beyond it in providing necessary tools to test physical assumptions of quantum error correction. To remedy these obstacles, techniques such as simultaneous randomized benchmarking [20] have been developed as a means to quantify the *addressability* of a subsystem in a device and thus provide a basic assessment of the presence of cross-talk errors.

Recent work has sought to deepen the core benchmarking toolkit, for example by considering higher-order moment analysis [21], character benchmarking techniques [22], the extension to benchmarking of logical qubits [23] and analogue regimes [24]. In this work we first consider general structural questions on quantum channels, and then address their relationship to

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benchmarking scenarios.

Quantum channels are the fundamental building blocks of quantum information theory. They allow for the description of general state preparation, restriction to subsystems, reversible and irreversible dynamics and general quantum measurements. There is increasing interest in both delineating and efficiently certifying non-classicalities in quantum theory, with concrete motivations coming from the development of Quantum Technologies. Therefore we ask the following structural question:

How can correlations in a multipartite quantum channel be quantified through measures that are efficiently and robustly estimatable in practice?

Motivated by the observation that the unitarity $u(\mathcal{E}_A)$ can be viewed as a variance of quantum channel we construct a ‘‘correlated unitarity’’ measure $u_c(\mathcal{E}_{AB})$ for a bipartite quantum channel that parallels the covariance of two random variables. Our approach takes into account the exponential complexity of full channel tomography [25–27], and provides a basic measure of channel correlations that can be estimated in an efficient and robust manner. Additionally, it satisfies a range of operational properties (such as invariance under local changes of bases, vanishing on product channels, and taking a value 1 on the *SWAP* channel), and is directly relevant to the benchmarking of quantum technologies.

The measure $u_c(\mathcal{E}_{AB})$ is also of use for certifying non-classical features of a channel. In particular, over the set of separable quantum channels (i.e. convex mixtures of product channels) it is strictly bounded away from the global maximum, and thus provides a witness of non-separability for quantum channels.

The correlation measure $u_c(\mathcal{E}_{AB})$ is built from simpler ‘‘sub-unitarities’’, which are of interest in their own right. In particular we describe some of their properties and show that the unitarity of a quantum channel is monogamous, and obeys a form of information-disturbance trade-off relation that is accessible to efficient experimental verification.

We then address the problem of efficiently estimating the correlated unitarity of effective noise channels in a benchmarking scenario. For this we follow a similar approach to simultaneous randomized benchmarking in which one employs local 2-designs on each subsystem. This is of relevance for cross-talk errors in quantum devices. We show that for bipartite separable channels the correlated unitarity can be obtained efficiently in a SPAM-robust protocol. For more general non-separable channels, we show that for weak reset errors that this can still be estimated and within a natural model demonstrate explicitly that the protocols can witness non-separability over a substantial range of reset errors. Finally, we discuss the relation between our work and simultaneous randomized benchmarking and show that our protocols provide additional,

independent information on cross-talk and correlative errors.

II. DEFINING A TRACTABLE MEASURE OF CORRELATION FOR BIPARTITE QUANTUM CHANNELS

Quantum entanglement allows for violations of Bell inequalities, generically appears in models of quantum computing, and leads to quantum advantages in quantum metrology. We now have a very well-developed theory of quantum entanglement through the resource theory of Local Operations and Classical Communications [28], which provides a detailed means to quantify non-separable correlations in multipartite states and describes the interconversion structure of such states. However there is far less work studying the correlations in quantum channels. Recent research on this line takes a resource-theoretic perspective [29, 30] or investigates information-theoretic features of Local Operations and Shared Randomness [31, 32].

In this work, we aim to formulate an experimentally accessible measure of coherent correlations in a general bipartite quantum channel. It is useful to first compare with the corresponding problem for classical random variables. Given two classical random variables X and Y there are many correlation measures that one could formulate, however the simplest and most direct method is to compute the covariance of X and Y . This is given simply as $\text{cov}(X, Y) := \langle XY \rangle - \langle X \rangle \langle Y \rangle$, where the angle brackets denote taking the expectation value of the random variable. Moreover, we have that $\text{cov}(X, X) = \text{var}(X)$, the variance of the random variable X , which in turn quantifies the noisiness of X .

Our starting point in this work is to first note that in the context of quantum channels there exists a measure that parallels the variance that arose in the randomized benchmarking schemes, namely the unitarity of a quantum channel [13]. The *unitarity* $u(\mathcal{E})$ of any quantum channel \mathcal{E} from a quantum system A to some other quantum system A' is defined as

$$u(\mathcal{E}) := \frac{d_A}{d_A - 1} \int d\psi \text{tr} \left[\mathcal{E}(\psi - \frac{\mathbb{1}}{d_A})^2 \right], \quad (1)$$

where the integration is with respect to the Haar measure over pure states of the input system A . However, as was noted in [33], this can be expressed more abstractly as

$$u(\mathcal{E}) = \text{tr}[\text{var}(\mathcal{E})], \quad (2)$$

where $\text{var}(\mathcal{E}) := \langle \mathcal{E}(\psi)^2 \rangle - \langle \mathcal{E}(\psi) \rangle^2$ and the angle brackets denote taking the expectation of an operator-valued random variable with respect to the Haar measure. This variance provides a simple measure of the degree to which the quantum channel preserves quantum coherence.

Given this, we can ask if one can construct a correlation measure related to the unitarity similar to the covariance of two random variables. However, while there is a clear notion of a marginal distribution for a joint probability distribution the situation is more complex for a bipartite quantum channel where the reduction to ‘marginal channels’ depends on the structure of the initial state considered [34].

Here we instead take the basic structure of covariance of two random variables as a guide and construct a unitarity-based correlation measure $u_c(\mathcal{E}_{AB})$ for a bipartite quantum channel with certain desirable features. Specifically, we require a measure such that $u_c(\mathcal{E}_{AB}) = 0$ for product channels $\mathcal{E}_{AB} = \mathcal{E}_A \otimes \mathcal{E}_B$, and that $u_c(\mathcal{E}_{AB})$ is invariant under local changes of bases on both the input and output systems. To connect with unitarity we shall construct a quantity $u_{AB \rightarrow AB}(\mathcal{E}_{AB})$ for a bipartite channel such that on product channels we have

$$u_{AB \rightarrow AB}(\mathcal{E}_A \otimes \mathcal{E}_B) = u(\mathcal{E}_A)u(\mathcal{E}_B). \quad (3)$$

To define the correlation measure using $u_{AB \rightarrow AB}$ we then require ‘marginal unitarity’ terms for the quantum channel. We refer to these as *sub-unitarities* $u_{A \rightarrow A}$ and $u_{B \rightarrow B}$ for the bipartite quantum channel that have the property that when restricted to product channels give

$$\begin{aligned} u_{A \rightarrow A}(\mathcal{E}_A \otimes \mathcal{E}_B) &= u(\mathcal{E}_A) \\ u_{B \rightarrow B}(\mathcal{E}_A \otimes \mathcal{E}_B) &= u(\mathcal{E}_B). \end{aligned} \quad (4)$$

More generally, when evaluated on a general quantum channel these sub-unitarities are marginal quantities describing the unitarity for particular outputs of the quantum channel and are of interest in their own right, as we explain in the next section.

Once these quantities are properly defined, our correlation measure then takes the following form.

Definition II.1. *The correlated-unitarity of a bipartite channel \mathcal{E}_{AB} is defined as:*

$$u_c(\mathcal{E}_{AB}) := u_{AB \rightarrow AB}(\mathcal{E}_{AB}) - u_{A \rightarrow A}(\mathcal{E}_{AB}) u_{B \rightarrow B}(\mathcal{E}_{AB}) \quad (5)$$

where $u_{i \rightarrow i}(\mathcal{E}_{AB})$ are sub-unitarities of the channel.

It remains to provide exact specification of these sub-unitarity terms. Given this high-level account, in the next section we describe how these individual terms are explicitly defined and their operational significance. In Section III we then discuss how the correlated unitarity relates to randomized benchmarking and how this measure can be used in SPAM-robust protocols for the diagnosis of cross-talk errors.

A. Sub-unitarities of a quantum channel and quantum incompatibility

We now give specific details on the terms discussed in the previous section. From a bipartite channel \mathcal{E}_{AB}

we define distinguished marginal channels that are natural in the context of unitarity. Specifically, we obtain marginal channels when the state of one of the input subsystems is taken to be the maximally mixed state. From this we then compute the unitarity of the resultant channel. More precisely we make the following definition.

Definition II.2. *The sub-unitarity $u_{A \rightarrow A}$ of a bipartite channel \mathcal{E}_{AB} is defined as*

$$u_{A \rightarrow A}(\mathcal{E}_{AB}) := u(\mathcal{E}_A), \quad (6)$$

where $\mathcal{E}_A(\rho) := \text{tr}_B[\mathcal{E}_{AB}(\rho \otimes \frac{\mathbb{1}_B}{d_B})]$ for any state ρ of A .

Exactly the same construction is used for subsystem B with the associated channel $\mathcal{E}_B(\rho) := \text{tr}_A[\mathcal{E}(\frac{\mathbb{1}_A}{d_A} \otimes \rho)]$ giving $u_{B \rightarrow B}(\mathcal{E}_{AB}) := u(\mathcal{E}_B)$. These measures quantify the degree to which coherent quantum information is maintained in either the A subsystem or B subsystem under the bipartite channel.

However, we can equally define two other sub-unitarities $u_{A \rightarrow B}$ and $u_{B \rightarrow A}$, where we consider the flow of quantum information from A to B or from B to A respectively. These are obtained simply as

$$u_{A \rightarrow B}(\mathcal{E}_{AB}) = u_{A \rightarrow A}(SWAP \circ \mathcal{E}_{AB}), \quad (7)$$

and similarly for $B \rightarrow A$, where $SWAP$ is the unitary that swaps the two subsystems A and B .

Note that we have assumed that the input and output systems are identical, but the above definitions can be extended to a channel from arbitrary input systems AB to output systems $A'B'$. Given this in Appendix B.2 we show the following result that demonstrates a basic constraint on sub-unitarities that relates directly to quantum incompatibility [35, 36].

Theorem II.1 (Monogamy of unitarity). *For any bipartite channel \mathcal{E} from input systems A_1B_1 to output systems A_2B_2 the local sub-unitarities are bounded by*

$$u_{A_1 \rightarrow A_2}(\mathcal{E}) + u_{A_1 \rightarrow B_2}(\mathcal{E}) \leq 1. \quad (8)$$

Consequently, if \mathcal{E}_{AB} is a channel from a single input system X to a bipartite quantum system AB then

$$u(\mathcal{E}_A) + u(\mathcal{E}_B) \leq 1, \quad (9)$$

where $\mathcal{E}_A = \text{tr}_B \circ \mathcal{E}_{AB}$ and $\mathcal{E}_B = \text{tr}_A \circ \mathcal{E}_{AB}$.

For a general bipartite channel this bound places a basic constraint on coherent quantum information flowing from a system X into two output systems A and B .

The theorem provides a compact form of the information-disturbance theorem [36], which in turn implies the no-cloning and no-broadcasting theorems [37–40]. More precisely, we can consider leakage of quantum information from a system into its environment, which is of relevance to, for example, quantum

computing in a noisy environment when one wishes to approximate a unitary channel as accurately as possible. We can consider a quantum channel $\mathcal{E}_{X \rightarrow AB}$ from a system X to a composite system AB such that $\mathcal{E}_{X \rightarrow A} \approx \mathcal{U}_{X \rightarrow A}$, for some target isometry $\mathcal{U}_{X \rightarrow A}$. We now quantify this in terms of unitarity as $u(\mathcal{E}_{X \rightarrow A}) = u(\mathcal{U}_{X \rightarrow A}) - \epsilon$ for some $\epsilon \geq 0$ quantifying the approximation. However the unitarity of a channel equals 1 if and only if it is an isometry [13, 41] and so the above monogamy relation implies that $u_{X \rightarrow B}(\mathcal{E}) \leq \epsilon$. Since we only have one input system, $u_{X \rightarrow B}(\mathcal{E})$ is simply the unitarity of the marginal channel from X to B , however it is easily shown (see Lemma B.1) that the unitarity vanishes if and only if the channel is a completely depolarizing channel. This in turn implies that the channel from X to the environment B must be ϵ -close (in terms of unitarity) to a completely depolarizing channel. Put another way, the information leaking into the environment necessarily decreases to zero as the channel into A approaches an isometry channel.

The remaining sub-unitarity term $u_{AB \rightarrow AB}$ in the correlated unitarity is slightly more awkward, and is best defined via the Liouville representation of a quantum channel, which we now introduce.

B. The Liouville representation of quantum channels

Consider quantum channels $\mathcal{E}: \mathcal{B}(\mathcal{H}_A) \rightarrow \mathcal{B}(\mathcal{H}_A)$, where $\mathcal{B}(\mathcal{H}_A)$ denotes the space of linear operators on the Hilbert space \mathcal{H}_A for a d -dimensional quantum system A . We choose an orthonormal basis of operators $X_0, X_1, \dots, X_{d^2-1}$ for $\mathcal{B}(\mathcal{H}_A)$ with $X_0 = \mathbb{1}/\sqrt{d}$ and with respect to the Hilbert Schmidt inner product $\langle X_\mu, X_\nu \rangle := \text{tr}[X_\mu^\dagger X_\nu] = \delta_{\mu,\nu}$. In particular, this means that X_1, \dots, X_{d^2-1} are all traceless operators.

We define vectorisation of operators via $|\text{vec}(|a\rangle\langle b|)\rangle := |a\rangle \otimes |b\rangle$ for any computational basis states [42]. This definition can be extended by linearity to get the mapping $M \rightarrow |\text{vec}(M)\rangle$ for any operator $M \in \mathcal{B}(\mathcal{H}_A)$. Then for any quantum channel $\mathcal{E}: \mathcal{B}(\mathcal{H}_A) \rightarrow \mathcal{B}(\mathcal{H}_A)$ we define its Liouville representation $\mathcal{L}(\mathcal{E})$ through the relation

$$\mathcal{L}(\mathcal{E})|\text{vec}(M)\rangle = |\text{vec}(\mathcal{E}(M))\rangle, \quad (10)$$

for all M . To simplify things going forward, we shall adopt the notation that we denote all vectorized quantities in boldface (this is similar to how a vector is sometimes represented in boldface as $\mathbf{v} = (v_1, v_2, \dots, v_n)$), and so write $|\mathbf{M}\rangle := |\text{vec}(M)\rangle$ and $\mathcal{E} := \mathcal{L}(\mathcal{E})$. Using this boldface notation we can re-express equation (10) in the more compact form

$$\mathcal{E}|\boldsymbol{\rho}\rangle = |\mathcal{E}(\boldsymbol{\rho})\rangle, \quad (11)$$

for any state ρ , and any channel \mathcal{E} . Using equation (11) we can therefore decompose any channel in the or-

thonormal basis $\{X_\mu\}$ as

$$\mathcal{E} = \sum_{\mu=0}^{d^2-1} |\mathcal{E}(X_\mu)\rangle\langle X_\mu|, \quad (12)$$

More explicitly, in terms of matrix components we have that

$$\mathcal{E} = \begin{matrix} & |\mathbf{X}_0\rangle & |\mathbf{X}_j\rangle \\ \langle \mathbf{X}_0| & \begin{pmatrix} 1 & \mathbf{0} \\ \mathbf{x} & T \end{pmatrix} \end{matrix}, \quad (13)$$

where $\mathcal{E}_{00} = 1$ and $\mathcal{E}_{0j} = \mathbf{0}$ follow from the fact that the channel is a completely positive trace-preserving operation. The $d^2 - 1$ component vector \mathbf{x} corresponds to the generalized Bloch vector of $\mathcal{E}(\mathbb{1}/d)$, which characterizes the degree to which the channel breaks unitarity. The matrix block T encodes the remaining features of the channel. In this notation, the unitarity of a channel is then given by the simple relation [13]

$$u(\mathcal{E}) = \frac{1}{d^2 - 1} \text{tr}[T^\dagger T]. \quad (14)$$

This core form is the one we use to define sub-unitarities in the next subsection.

C. Liouville decomposition of bipartite quantum channels and general sub-unitarities

We can also compute Liouville representations of bipartite channels, $\mathcal{E}_{AB}: \mathcal{B}(\mathcal{H}_A \otimes \mathcal{H}_B) \rightarrow \mathcal{B}(\mathcal{H}_A \otimes \mathcal{H}_B)$, where we assume for simplicity that the input and output systems are identical.

For subsystem A , we choose an orthonormal basis of operators $X_\mu = (X_0 = \frac{1}{\sqrt{d_A}} \mathbb{1}_A, X_i)$, where d_A is dimension of the subsystem A , and similarly for B a basis $Y_\mu = (Y_0 = \frac{1}{\sqrt{d_B}} \mathbb{1}_B, Y_i)$. Together these provide a basis for the full system which is given in the Liouville representation as [43]

$$|\mathbf{X}_a \otimes \mathbf{Y}_b\rangle := |\mathbf{X}_a\rangle \otimes |\mathbf{Y}_b\rangle. \quad (15)$$

This in turn provides the following matrix decomposition of \mathcal{E}_{AB} ,

$$\mathcal{E}_{AB} = \begin{matrix} & |\mathbf{X}_0 \otimes \mathbf{Y}_0\rangle & |\mathbf{X}_{j_1} \otimes \mathbf{Y}_0\rangle & |\mathbf{X}_{j_1} \otimes \mathbf{Y}_{j_2}\rangle & |\mathbf{X}_0 \otimes \mathbf{Y}_{j_2}\rangle \\ \langle \mathbf{X}_0 \otimes \mathbf{Y}_0| & \begin{pmatrix} 1 & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{x}_{A \rightarrow A} & T_{A \rightarrow A} & T_{AB \rightarrow A} & T_{B \rightarrow A} \\ \langle \mathbf{X}_{i_1} \otimes \mathbf{Y}_{i_2}| & \mathbf{x}_{AB \rightarrow AB} & T_{A \rightarrow AB} & T_{AB \rightarrow AB} & T_{B \rightarrow AB} \\ \langle \mathbf{X}_0 \otimes \mathbf{Y}_{i_2}| & \mathbf{x}_{B \rightarrow B} & T_{A \rightarrow B} & T_{AB \rightarrow B} & T_{B \rightarrow B} \end{pmatrix} \end{matrix}$$

where $i_1 = \{1, 2, \dots, (d_A^2 - 1)\}$, $i_2 = \{1, 2, \dots, (d_B^2 - 1)\}$ and similarly for j . Here we break the entire T matrix of the channel up according to the subsystem contributions where, for example, the term $T_{AB \rightarrow B}$ denotes the mapping of joint degrees of freedom of the input system AB into the B output subsystem.

With this notation in place, we can now define the general sub-unitarities of the bipartite channel.

Definition II.3. For any quantum channel \mathcal{E}_{AB} on a bipartite quantum system AB the sub-unitarity $u_{i \rightarrow j}$ of the channel is defined as:

$$u_{X \rightarrow Y}(\mathcal{E}_{AB}) := \alpha_X \text{tr} \left[T_{X \rightarrow Y}^\dagger T_{X \rightarrow Y} \right], \quad (16)$$

for any $X, Y \in \{A, B, AB\}$ and with $\alpha_A = 1/(d_A^2 - 1)$, $\alpha_B = 1/(d_B^2 - 1)$ and $\alpha_{AB} = \alpha_A \alpha_B$.

This coincides with our previous definitions for the single subsystem sub-unitarities, and also provides the form for the remaining other choices. Also note that under a local change of bases on the input and output subsystems we have

$$\mathcal{E}_{AB} \rightarrow (\mathcal{V}_A \otimes \mathcal{V}_B) \circ \mathcal{E}_{AB} \circ (\mathcal{U}_A^\dagger \otimes \mathcal{U}_B^\dagger), \quad (17)$$

for local unitary channels denoted with \mathcal{V} and \mathcal{U} . These changes of bases transform the sub-matrices $T_{X \rightarrow Y}$ under multiplication by orthogonal matrices. For example

$$T_{A \rightarrow A} \rightarrow \mathcal{O}_1 T_{A \rightarrow A} \mathcal{O}_2^T, \quad (18)$$

for orthogonal matrices $\mathcal{O}_1, \mathcal{O}_2$, with e.g. \mathcal{O}_2 arising from the $\mathcal{U}_A(X_i) = \sum_{m=1}^{d_A^2-1} \mathcal{O}_{2;i,m} X_m$ (see Appendix C). This implies that all the sub-unitarity terms are invariant under local changes of bases.

It is straightforward to show (see Appendix B 1) that these sub-unitarities relate to the total unitarity of the quantum channel \mathcal{E}_{AB} as follows.

Theorem II.2. The unitarity of a bipartite channel \mathcal{E}_{AB} is obtained from the weighted sum of its sub-unitarities:

$$u(\mathcal{E}_{AB}) = \frac{1}{d^2 - 1} \sum_{X, Y \in \{A, B, AB\}} \frac{u_{X \rightarrow Y}(\mathcal{E}_{AB})}{\alpha_X}, \quad (19)$$

where $d = d_A d_B$ is the dimension of the total system.

We shall make use of this decomposition of unitarity for our benchmarking protocol to estimate the correlated unitarity. But before discussing the protocol, we first give core properties of this measure that demonstrate its usefulness for assessing the correlation structure of a given channel.

D. Properties of the correlated unitarity for a bipartite quantum channel

The correlated unitarity u_c is given in terms of sub-unitarities as $u_c(\mathcal{E}) = u_{AB \rightarrow AB}(\mathcal{E}) - u_{A \rightarrow A}(\mathcal{E}) u_{B \rightarrow B}(\mathcal{E})$, and we now address the core properties of this measure. The following result shows that it obeys natural conditions.

Theorem II.3. For any bipartite quantum channel \mathcal{E}_{AB} , we have $u_c(\mathcal{E}_{AB}) \leq 1$, and is invariant under local unitary transformations on either the input or output systems. Moreover $u_c(\mathcal{E}_{AB}) = 0$ for product channels and $u_c(\mathcal{E}_{AB}) = 1$ when \mathcal{E}_{AB} is the SWAP channel modulo local unitary changes of bases.

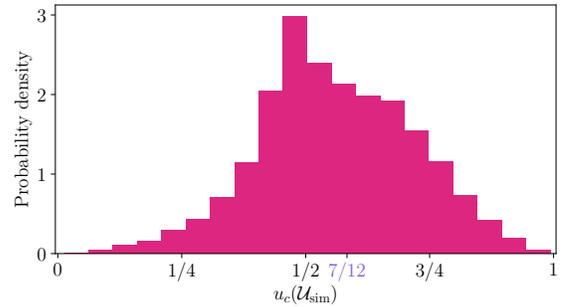


FIG. 1. **Distribution of u_c for 2-qubit unitaries.** We plot the histogram of values of $u_c(\mathcal{U}_{\text{sim}})$ for 20,000 random 2 qubit unitaries, \mathcal{U}_{sim} . These correlated unitarities lie between 0 and 1, and take the value $u_c(\mathcal{E}_A \otimes \mathcal{E}_B) = 0$ for product channels, and $u_c(\text{SWAP}) = 1$ for the SWAP channel. The value of u_c is invariant under local unitary changes of basis. The upper bound for separable channels is $u_c^{\text{sep}} \leq 7/12$, and is also shown on the plot. We sampled using the methods of [44] and simulated using QuTip [45].

A proof of this can be found in Appendices B 2 & C 4. Therefore, under this measure the SWAP channel is the farthest from being a product channel, which is consistent with the fact that it perfectly transfers coherent quantum information from one subsystem to the other. However we can also consider intermediate regimes in which the bipartite channel is *separable*, namely it can be written as

$$\mathcal{E}_{AB} = \sum_k p_k \mathcal{E}_k \otimes \mathcal{F}_k, \quad (20)$$

for some probability distribution (p_k) , and local channels \mathcal{E}_k and \mathcal{F}_k on A and B respectively. This class of channels are also known as Local Operations with Shared Randomness [31, 32]. The above definition generalizes that of separable states, and defines a convex subset of channels. A bipartite channel that is not separable is called *non-separable*. It turns out that the correlated unitarity is strictly bounded over separable channels as the following establishes.

Theorem II.4 (Witness of non-separability). Given a bipartite quantum system AB with subsystems A, B of dimensions d_A and d_B respectively we have that

$$u_c(\mathcal{E}_{AB}) \leq C(d_A, d_B) < 1, \quad (21)$$

with the upper bound $C(d_A, d_B) \leq \frac{23}{32}$ if $\max(d_A, d_B) = 3$ and $C(d_A, d_B) \leq \frac{7}{12}$ otherwise.

The proof of this bound is non-trivial, and we provide it in Appendix C 5. This bound is not tight in general, and we provide sharper bounds in terms of the subsystem dimensions. The $d = 3$ qutrit case is singled out from dimensional scaling in our specific analysis, and could be improved, albeit via a non-trivial analysis of qutrit channels.

The consequence of the result is that if the correlated unitarity can be efficiently estimated, then obtaining values above the upper bound witnesses non-separability in the quantum channel and so provides a practical way to certify that coherent information flows between A and B .

It is straightforward to compute u_c for a range of channels. For example, consider the channel

$$\mathcal{E}_{AB} = \sum_k p_k \mathcal{U}_k \otimes \mathcal{V}_k, \quad (22)$$

where $\{\mathcal{U}_i\}_{i=1}^{d_A^2}$ and $\{\mathcal{V}_j\}_{j=1}^{d_B^2}$ are local unitary error bases [46] on A and B respectively, namely unitaries on each subsystem that also form an orthonormal basis with respect to the Hilbert-Schmidt inner product. For this channel, $u_c(\mathcal{E}_{AB})$ then takes the form

$$u_c(\mathcal{E}_{AB}) = \sum_k p_k^2 - \left(\sum_k p_k\right)^2. \quad (23)$$

Further insight into $u_c(\mathcal{E})$ can be obtained by formulating it in terms of two-point correlation measures. Suppose we have local observables O_A and O_B for system A and B respectively. We define the following correlation function

$$\begin{aligned} F_{O_A, O_B}(\mathcal{E}, \psi_{AB}) &:= |\langle O_A \otimes O_B \rangle_{\mathcal{E}_{AB}(\psi_{AB})}|^2 \\ &\quad - |\langle O_A \rangle_{\mathcal{E}_A(\psi_A)}|^2 |\langle O_B \rangle_{\mathcal{E}_B(\psi_B)}|^2 \end{aligned} \quad (24)$$

where the channels \mathcal{E}_A and \mathcal{E}_B are local channels on A respectively B defined in Defn. (II.2) and the input states ψ_A and ψ_B are marginals of ψ_{AB} .

The correlation function above becomes related to the covariance of classical random variables when considering classical states embedded in a quantum system

$$\begin{aligned} F_{O_A, O_B}(id, \rho_{AB}) &= \text{cov}(O_A, O_B) [\langle O_A \otimes O_B \rangle_{\rho_{AB}} \\ &\quad + \langle O_A \rangle_{\rho_A} \langle O_B \rangle_{\rho_B}], \end{aligned} \quad (25)$$

where $\rho_{AB} = \sum_{x,y} p(x,y) |x\rangle\langle y| \langle x| \langle y|$ for $|x\rangle, |y\rangle$ computational basis states that diagonalize the hermitian operators O_A and O_B and $p(x,y)$ is a joint probability distribution with marginals $p(x)$ and $p(y)$. In this case $\text{cov}(O_A, O_B) = \langle O_A \otimes O_B \rangle_{\rho_{AB}} - \langle O_A \rangle_{\rho_A} \langle O_B \rangle_{\rho_B}$ and matches the covariance of classical random variables X, Y .

Then the correlated unitarity can be expressed as

$$u_c(\mathcal{E}) = \alpha_{AB} d_{AB}^2 \sum_{i,j,k,k'} F_{P_i, P_j}(\mathcal{E}, \psi_{k,k'}) \quad (26)$$

where P_i are the traceless Pauli operators on each subsystem, and $\psi_{k,k'} = \frac{\mathbf{1}_{AB} + P_k \otimes P_{k'}}{d_{AB}}$.

Overall, the correlated unitarity amounts to a working notion of correlation in a bipartite quantum channel, and we do not delve any further into its theoretical

properties. In Appendix C 1 we also compare $u_c(\mathcal{E}_{AB})$ to a norm measure of correlation. While norm-based measures are mathematically more natural, our aim is to connect to benchmarking protocols, and so ultimately the utility of this measure should be judged by how useful it is in practice. We find that sub-unitarities arise very naturally in benchmarking protocols.

III. ESTIMATION OF CORRELATED UNITARITY VIA BENCHMARKING PROTOCOLS

In the previous section we developed a collection of tools, based around unitarity, to address sub-system features of a quantum channel. The introduction of sub-unitarities and the correlated unitarity allow us to quantify structures specific to bipartite quantum channels in a simple and direct manner. We now turn to the question of how such quantities may be estimated in practice in a protocol that is both efficient in the number of operations required and robust against SPAM errors.

These quantities are generalizations of the unitarity, which can be efficiently estimated in benchmarking protocols, and it turns out similar methods work for sub-unitarities, however some complications do arise as we shall discuss.

A. Randomized Benchmarking Protocols

The certification of quantum devices is a fundamental problem of quantum technologies, so as to verify that a physical device is actually performing with a sufficiently high fidelity. In the context of quantum computing it is desirable to provide a greater abstraction from the underlying physical implementation and talk of benchmarking a logical gate-set $\Gamma = \{\mathcal{U}_1, \mathcal{U}_2, \dots, \mathcal{U}_n\}$ of target unitary gates.

The worst-case error rate is given by the diamond norm [42] distances $\|\tilde{\mathcal{U}}_i - \mathcal{U}_i\|_{\diamond}$, which is the relevant physical parameter for the fault tolerance theorem [47]. However the diamond norm is a difficult quantity to measure, and so one must instead consider weaker measures, such as the average gate infidelity, given by

$$r(\mathcal{E}) := 1 - \int d\psi \langle \psi | \mathcal{E}(|\psi\rangle\langle\psi|) | \psi \rangle, \quad (27)$$

measuring the Haar-average deviation from the identity channel of a given channel \mathcal{E} . The average gate infidelity then provides bounds on the diamond distance of the form [48],

$$O(r(\mathcal{E})) \leq \frac{1}{2} \|id - \mathcal{E}\|_{\diamond} \leq O(d\sqrt{r(\mathcal{E})}). \quad (28)$$

The problem with this route is that the bounds cannot be tightened, and for \mathcal{E} corresponding to a coherent error there is a weak link between $r(\mathcal{E})$ and the diamond norm [48–50].

Randomized benchmarking techniques can be used to estimate $r(\mathcal{E})$ and circumvent the exponential complexity of tomography, and the unavoidable SPAM errors. The core components of a randomized benchmarking protocol generally involves the noisy preparation of some initial quantum state ρ , which is then subject to a number k of physical gates \tilde{U}_i that approximate target unitaries $U_i \in \Gamma$, before a final imperfect measurement is performed for some binary outcome measurement $\{M, \mathbb{1} - M\}$. If the gates applied correspond to a (noisy) 2-design, such as Γ being the Clifford group, then it can be shown that [1] the resulting statistics are exponentially decreasing in k , namely $\mathbb{E}[m(k)] = c_1 + c_2 \lambda^k$, for constants c_1 and c_2 that contain the state preparation and measurement details. The decay constant λ is then a measure of the noisiness of the physical gate-set $\tilde{\Gamma} := \{\tilde{U}_i\}$ employed.

In the simplified model of *gate-independent* noise, in which each channel can be decomposed as $\tilde{U}_i = \mathcal{E} \circ U_i$ for some \mathcal{E} that is independent of i , then it can be shown that $\lambda \propto 1 - r(\mathcal{E})$, where $r(\mathcal{E})$ is the average gate infidelity of the noise channel \mathcal{E} . In the more realistic case of *gate-dependent* noise the relationship between the decay parameter λ and the physics of the set $\tilde{\Gamma}$ is subtle, due to gauge degrees of freedom in the representation of the physical components [51]. However, despite these details the decay parameter can still be related to the physical gate-set and essentially corresponds to the average gate-set infidelity [52].

At a more abstract level, a randomized benchmarking scheme admits a compact description in terms of convolutions of channels \tilde{U}_i with respect to the Clifford group [53]. The decay law is then viewed in a Fourier-transformed basis where the channel compositions become matrix multiplication over different irreps [2]. The resultant protocol then provides a benchmark for the degree to which the physically realized channels $\{\tilde{U}_i\}$ form an approximate representation of the Clifford group [54, 55].

In the next section we expand on the components of the benchmarking scheme for the case of unitarity benchmarking.

B. Unitary 2-designs & Unitarity Benchmarking Protocols

We now provide an outline of how the unitarity of a quantum channel can be estimated in a benchmarking protocol.

Recall that by \mathcal{U} we denote the Liouville representation of a unitary channel $\mathcal{U}(X) = UXU^\dagger$, and therefore it takes the explicit form, $\mathcal{U} = U \otimes U^*$. A probability measure μ over the set of unitaries $U(d)$ is called a *unitary 2-design* if we have that

$$\int d\mu(U) \mathcal{U}^{\otimes 2} = \int d\mu_{\text{Haar}}(U) \mathcal{U}^{\otimes 2}, \quad (29)$$

where μ_{Haar} is the Haar measure over the group $U(d)$. In practice we are interested in unitary 2-designs which are finite, discrete distributions of unitaries. In particular the uniform distribution over the Clifford group \mathcal{C} of unitaries is a 2-design (in fact it is a 3-design [56]), and therefore

$$\frac{1}{|\mathcal{C}|} \sum_{U \in \mathcal{C}} \mathcal{U}^{\otimes 2} = \int d\mu_{\text{Haar}}(U) \mathcal{U}^{\otimes 2} =: P \quad (30)$$

where $|\mathcal{C}|$ is the number of elements in the Clifford group and we denote the resultant operator by P . This operator acts on the vectorized form of $\mathcal{B}(\mathcal{H}) \otimes \mathcal{B}(\mathcal{H})$, and using Schur-Weyl duality, it can be shown that P is the projector onto the subspace

$$S := \text{span}\{|\mathbf{1}^{\otimes 2}\rangle, |\mathbb{F}\rangle\}, \quad (31)$$

where \mathbb{F} is the unitary that transposes vectors in the two subsystems, $|\phi_1\rangle \otimes |\phi_2\rangle \rightarrow |\phi_2\rangle \otimes |\phi_1\rangle$.

We can define an effective noise channel \mathcal{E} via $\mathcal{E} := \mathcal{U}^\dagger \circ \tilde{\mathcal{U}}$, and moreover in what follows we shall assume for simplicity that each gate $U \in \Gamma$ is subject to the same effective noise channel (but again this assumption can be weakened and gate-dependent noise can be assessed via interleaved benchmarking [57]).

The unitarity of this noise channel can then be estimated in the following way. We prepare a quantum state ρ of the system and choose the Clifford group as the gate-set. We now define

$$\mathcal{U}_s := \mathcal{U}_{(s_1, s_2, \dots, s_k)} := \mathcal{U}_{s_1} \circ \mathcal{U}_{s_2} \circ \dots \circ \mathcal{U}_{s_k}, \quad (32)$$

where $\mathcal{U}_{s_i} \in \Gamma$ for all i , and s_i labels the particular choice of unitary in the gate-set. We also denote by $\tilde{\mathcal{U}}_s$ the corresponding noisy implementation of the above sequence $s = (s_1, s_2, \dots, s_k)$ of unitaries. For any sequence s and some hermitian observable M we estimate the quantity

$$m(s) := \text{tr}\left[M\tilde{\mathcal{U}}_s(\rho)\right], \quad (33)$$

and then by randomly sampling over the Clifford group for each step in the sequence estimate $\mathbb{E}_s[m(s)^2] := \frac{1}{|\Gamma|^k} \sum_s m(s)^2$. By exploiting the fact that the Clifford group is a 2-design, and specifically equations (30) and (31), it was shown in [13] that

$$\mathbb{E}_s[m(s)^2] = c_1 + c_2 u(\mathcal{E})^{k-1}, \quad (34)$$

for constants c_1 and c_2 that contain any errors due to state-preparation or measurement. Therefore, by repeating this estimation for sequences of varying length we may extract an estimation of $u(\mathcal{E})$ as a decay constant for the quantity in an efficient and SPAM-robust manner.

C. Estimation of channel sub-unitarities via local & global twirls

The unitarity arose from considering a global twirl using a 2-design, it turns out that the sub-unitarities

arise in a similar fashion, but now by considering local twirls for a bipartite quantum system. Specifically, we now have a bipartite quantum system AB with local gate-sets Γ_A and Γ_B , which we assume are 2-designs, and a global gate-set Γ_{AB} . Then, we may consider the independent twirls

$$\frac{1}{|\Gamma_A||\Gamma_B|} \sum_{U_A \in \Gamma_A, U_B \in \Gamma_B} \mathbf{u}_A^{\otimes 2} \otimes \mathbf{u}_B^{\otimes 2} = P_A \otimes P_B, \quad (35)$$

where we now have local projections of channels at A and B onto subspaces S_A and S_B , where

$$S_A = \text{span}\{|\mathbf{1}_A \otimes \mathbf{1}_{A'}\rangle, |\mathbb{F}_{AA'}\rangle\}, \quad (36)$$

where A' is isomorphic to A , and we have a similar expression for S_B .

In the context of benchmarking we have the problem of determining the *addressability* of qubits and the existence of *crosstalk* between qubits. For example, we want to implement some target unitary $U_i \otimes id$ on one qubit, while leaving all others unaffected. However, in reality the physical channel performed \tilde{U}_i will involve an effective noise channel \mathcal{E} that does not factorize neatly with noise only on the target qubit. Instead, the noise channel will act non-trivially on each subsystem of the bipartite split and could involve correlations that include coherent leakage of the quantum information.

In what follows we again consider the averaged noise channel over the gate-set, and so at the simplest level of analysis assume that we have gate-independent noise. A more general analysis involving gate-dependent noise should be possible by following perturbative approaches such as in [52] and by making use of interleaved benchmarking [57]. We also note that the channel under consideration need not be a noise channel in such a scheme, but could be a target channel on which we wish to do robust tomography. For this context it would be possible to exploit recent methods that make use of randomized benchmarking to do tomography of quantum channels such as in [58]. We leave this kind of analysis for later investigation.

Under this average noise model assumption, we now perform a unitarity benchmarking scheme by randomly sampling from $\Gamma_A \otimes \Gamma_B$ and obtain a circuit of depth k , with sequence indexed via $s = (s_A, s_B)$ with $s_A = (a_1, a_2, \dots, a_k)$ and $s_B = (b_1, b_2, \dots, b_k)$ specifying the particular target unitary in the local gate-sets. As before, we estimate the quantity $m(s) := \text{tr}[M\tilde{U}_s(\rho)]$ and also $\mathbb{E}_s[m(s)^2]$ for circuits of depth k . However, for these local twirls, this quantity now has a different decay profile. As we show in Appendix D this quantity behaves as

$$\mathbb{E}_s[m(s)^2] = c_{00} + c_{01}\lambda_1^{k-1} + c_{10}\lambda_2^{k-1} + c_{11}\lambda_3^{k-1}, \quad (37)$$

where $(\lambda_1, \lambda_2, \lambda_3)$ are the singular values [59] of the ma-

trix of sub-unitarities

$$\mathcal{S} = \begin{pmatrix} u_{A \rightarrow A}(\mathcal{E}) & \frac{1}{\sqrt{\alpha_B}} u_{AB \rightarrow A}(\mathcal{E}) & \sqrt{\frac{\alpha_A}{\alpha_B}} u_{B \rightarrow A}(\mathcal{E}) \\ \sqrt{\alpha_B} u_{A \rightarrow AB}(\mathcal{E}) & u_{AB \rightarrow AB}(\mathcal{E}) & \sqrt{\alpha_A} u_{B \rightarrow AB}(\mathcal{E}) \\ \sqrt{\frac{\alpha_B}{\alpha_A}} u_{A \rightarrow B}(\mathcal{E}) & \frac{1}{\sqrt{\alpha_A}} u_{AB \rightarrow B}(\mathcal{E}) & u_{B \rightarrow B}(\mathcal{E}) \end{pmatrix}, \quad (38)$$

with $\alpha_X = \frac{1}{d_X^2 - 1}$, and the constants c_{00}, \dots, c_{11} contain the SPAM-errors. Therefore, the sub-unitarities arise in the context of this benchmarking, albeit in a more non-trivial form to the global protocol. For example, we have that

$$\text{tr}(\mathcal{S}) = \sum_i \lambda_i = u_{A \rightarrow A}(\mathcal{E}) + u_{AB \rightarrow AB}(\mathcal{E}) + u_{B \rightarrow B}(\mathcal{E}), \quad (39)$$

with similar relations existing for the other coefficients of the characteristic polynomial of \mathcal{S} [60]. Note that $\sum_i \lambda_i = 3$ if and only if \mathcal{E} is a product of unitaries, and so this sum of eigenvalues gives a blunt handle on how much \mathcal{E} deviates from this regime.

By estimating the decay constants in equation (37) it is possible to obtain an estimate of channel correlations that coincides with the correlated unitarity for a family of channels. It is easily checked that for a product noise channel $\mathcal{E} = \mathcal{E}_A \otimes \mathcal{E}_B$ we have the matrix of sub-unitarities given by

$$\mathcal{S} = \begin{pmatrix} u(\mathcal{E}_A) & 0 & 0 \\ \sqrt{\alpha_B} u(\mathcal{E}_A) x_B & u(\mathcal{E}_A) u(\mathcal{E}_B) & \sqrt{\alpha_A} u(\mathcal{E}_B) x_A \\ 0 & 0 & u(\mathcal{E}_B) \end{pmatrix}, \quad (40)$$

where x_A and x_B are constants related to deviations from unitality (see Appendix D3). This implies that eigenvalues of \mathcal{S} are given by

$$\{\lambda_i\} = \{u(\mathcal{E}_A), u(\mathcal{E}_B), u(\mathcal{E}_A)u(\mathcal{E}_B)\}. \quad (41)$$

It can be checked that this simple link with sub-unitarities extends to arbitrary *separable* channels, for which $\lambda_1, \lambda_2, \lambda_3$ are exactly equal to the sub-unitarities $u_{A \rightarrow A}, u_{B \rightarrow B}, u_{AB \rightarrow AB}$. This provides a way to compute the correlated unitarity. More precisely, given $\lambda_1 \geq \lambda_2 \geq \lambda_3$, we may compute the quantity

$$C = |\lambda_3 - \lambda_1 \cdot \lambda_2|, \quad (42)$$

where we use the fact that sub-unitarities are upper bounded by one to distinguish λ_3 from the other two.

For non-separable channels the deviation of the eigenvalues from each of the subunitarities can be bounded by using the Girshgorin Circle Theorem or Brauer's Theorem [60]. For example, we obtain the bounds

$$|\lambda_1 - u_{A \rightarrow A}(\mathcal{E})| \leq \frac{1}{\sqrt{\alpha_B}} u_{AB \rightarrow A}(\mathcal{E}) + \sqrt{\frac{\alpha_A}{\alpha_B}} u_{B \rightarrow A}(\mathcal{E}). \quad (43)$$

Using identities for sub-unitarities, we can further show that

$$|\lambda_1 - u_{A \rightarrow A}(\mathcal{E})| \leq \frac{1}{\sqrt{\alpha_B}} [1 - u_{A \rightarrow A}(\mathcal{E})]. \quad (44)$$

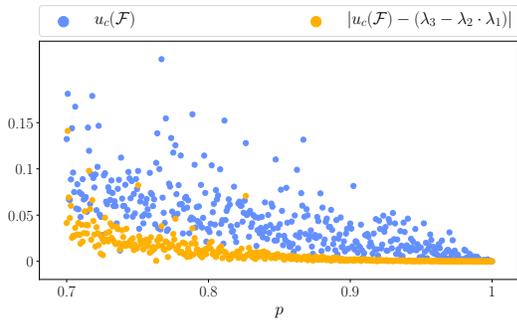


FIG. 2. **SPAM error robust estimation of u_c for generic quantum channels.** The convergence of the values of correlated unitarity and C as gate noise takes a product form, for a 2 qubit simulation. We show $|u_c - C|$ over p , where $\mathcal{F} = p\mathcal{E}_A \otimes \mathcal{E}_B + (1-p)\mathcal{G}$. The channels \mathcal{E}_A , \mathcal{E}_B and \mathcal{G} are sampled using the methods of [44] and simulated using QuTip [45].

These two inequalities are generally weak, due to the factors of α_B and α_A , but they do imply that the approximation is very good when either the off-diagonal elements are small or when the local unitarities are large. In such regimes this protocol will return a good estimate of the correlated unitarity, as shown in Figure 2.

Estimation of the three decay constants requires fitting noisy multi-exponential data which is non-trivial, but a range of methods have been developed to tackle this problem [2]. To assist with fitting, and moreover identify the sub-unitarity $u_{AB \rightarrow AB}$, we may supplement the local twirling with a global estimate of unitarity, and then make use of the decomposition of unitarity into sub-unitarities. Specifically, for the case of *unital* separable channels, with $d_A = d_B = d$, we have that

$$u(\mathcal{E}) = \frac{u_{A \rightarrow A}(\mathcal{E}) + u_{B \rightarrow B}(\mathcal{E}) + (d^2 - 1)u_{AB \rightarrow AB}(\mathcal{E})}{d^2 + 1}, \quad (45)$$

and therefore we have the relation

$$u_{AB \rightarrow AB}(\mathcal{E}) = \frac{(d^2 + 1)u(\mathcal{E}) - \sum_i \lambda_i}{d^2 - 2}. \quad (46)$$

This means that separate estimations of $u(\mathcal{E})$ and the decay constants (λ_i) provide an estimate of $u_{AB \rightarrow AB}(\mathcal{E})$, and so provides additional independent information on the terms entering the correlated unitarity. In practice, this will require careful consideration as the average noise channel associated with Γ_{AB} (employed in the estimation of unitarity) might be different than that associated with $\Gamma_A \otimes \Gamma_B$.

We note that by using *randomized compiling* [61, 62] for the implementation of a quantum circuit we may reduce the noise channel to being a Pauli channel. Since a general noise channel will not have λ_i coinciding precisely with the sub-unitarities, by running the local twirling protocol with and without randomized

compiling one could witness the presence of non-Pauli noise.

Protocol 1: SPAM error robust, $\mathcal{C} \times \mathcal{C}$

1. **Prepare** the system in a state ρ .
 2. **Select** a sequence of length k of simultaneous random noisy Clifford gates locally on subsystems A and B , starting with $k = 1$. E.g. for each gate $\mathcal{U}_{AB,i} = \mathcal{U}_{A,i_1} \otimes \mathcal{U}_{B,i_2}$.
 3. **Estimate** the square $(m)^2$ of an expectation value of an observable M , for this particular sequence of gates.
 4. **Repeat 1, 2 & 3** for many random sequences of the same length, finding the average estimation $\mathbb{E}[(m)^2]$ of $(m)^2$.
 5. **Repeat 1, 2, 3 & 4** increasing the length of the sequence k by 1.
 6. **Fit** the data $\mathbb{E}[(m)^2]$ against k and obtain decay parameters as in Equation (37).
-

D. Estimation of sub-unitarities for non-separable channels with low re-setting errors

While the local twirling protocol provides a means to estimate the correlated unitarity in the case of any separable channel, we would like to be able to estimate such correlations for general non-separable channels. The obstacle here is to determine sub-unitarities such as $u_{A \rightarrow A}(\mathcal{E}_{AB})$. However, this requires preparing the maximally mixed state on subsystem B and benchmarking the unitarity of the effective channel output on A . This presents a problem of how accurately such a re-set can be performed. Current devices, including ion-traps [63] and IBM's superconducting qubits [64], allow for mid-circuit measurements and resets. These dynamical circuits capabilities can be accessed through hardware-agnostic SDKs [65, 66].

This is challenging to do in a fully SPAM-robust way, however from the form of Equation (II.2) we see that if it is possible to do a resetting of sub-system close to the maximally mixed state then one can obtain an estimate of the sub-unitarity $u_{A \rightarrow A}(\mathcal{E}_{AB})$, and similarly for other single-subsystem cases, by estimating the unitarity of the marginal channel $\mathcal{E}_A = \text{tr}_B \circ \mathcal{E}_{AB} \circ \mathcal{R}_B$, where $\mathcal{R}_B(\rho) = \frac{1}{d} \mathbb{1}_B$. Within the benchmarking circuit this would mean performing a noisy re-set $\tilde{\mathcal{R}}_B$ on B after each $\tilde{\mathcal{U}}_i$ on A , with the aim of having $\tilde{\mathcal{R}}_B \approx \mathcal{R}_B$. This is a non-trivial assumption, and so in general the protocol will not be fully robust against re-set errors. However, if these errors are substantially smaller than the addressability errors one wishes to estimate then the protocol returns an approximate estimate.

We can summarize this sub-unitarity protocol as follows:

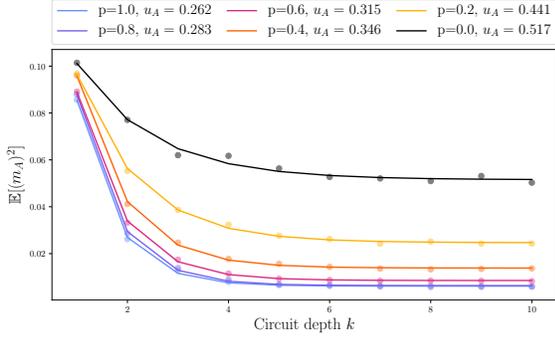


FIG. 3. **Sub-unity estimation with re-set error.** Shown is a simulation of Protocol 2 to estimate the sub-unity $u_A \equiv u_{A \rightarrow A}(\mathcal{E}_{AB})$, modelling the re-set error associated B as in Equation (47). This re-set error is shown for different levels of depolarization p , including $p = 0$ i.e. no re-set. The channel \mathcal{E}_{AB} in this case has a theoretical value of $u_{A \rightarrow A}(\mathcal{E}_{AB}) = 0.263$. The protocol returns an estimate of the sub-unity accurate to $\sim 90\%$ for re-set errors up to $\sim 20\%$.

Protocol 2: **SPAM error effected**, $\mathcal{C} \times 1$

1. **Prepare** the system in the state ρ .
 2. **Select** a sequence of length k of random noisy Clifford gates on subsystem A , starting with $k = 1$. E.g. for each gate $\mathcal{U}_{A,i} \otimes id_B$
 3. **Estimate** the square $(m_A)^2$, of the expectation value of an observable M_A on subsystem A for this particular sequence of gates, while performing a **reset** \mathcal{R}_B of the B subsystem after every gate.
 4. **Repeat 1, 2 & 3** for many random sequences of the same length, finding the average estimation $\mathbb{E}[(m_A)^2]$ of $(m_A)^2$.
 5. **Repeat 1, 2, 3 & 4** increasing the length of the sequence k by 1.
 6. **Fit** the data $\mathbb{E}[(m_A)^2]$ against k and obtain decay parameters as in Equation (34).
-

Given approximate estimates of $u_{A \rightarrow A}(\mathcal{E}_{AB})$ and $u_{B \rightarrow B}(\mathcal{E}_{AB})$ we may then exploit the fact that $\sum_i \lambda_i = u_{A \rightarrow A}(\mathcal{E}_{AB}) + u_{B \rightarrow B}(\mathcal{E}_{AB}) + u_{AB \rightarrow AB}(\mathcal{E}_{AB})$ to infer the value of $u_{AB \rightarrow AB}(\mathcal{E}_{AB})$ and thus compute the correlated unitarity for the channel \mathcal{E}_{AB} . Therefore, under the assumption of sufficiently small re-setting errors we may estimate the correlated unitarity for an arbitrary channel. Note that in the context of the local Clifford gate-sets the effective channel need not be the same in each protocol since Protocol 2 uses a different gate-set. However, we can use the same gate-set in Protocol 2 as in 1, since the application of non-trivial Clifford gates on B does not change matters if $\tilde{\mathcal{R}}_B \approx \mathcal{R}_B$.

It is straightforward to numerically test how sensitive the above protocol is to re-setting errors. For exam-

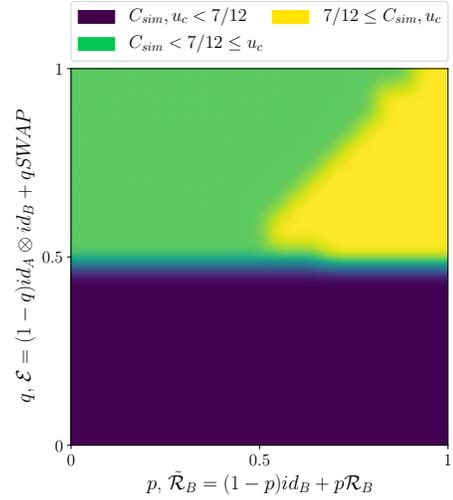


FIG. 4. **Witnessing channel non-separability.** Given a quantum channel \mathcal{E}_{AB} we consider the ability to efficiently witness its non-separability via correlated unitarity in the presence of re-setting noise. This could be realized, for example, in the context of robust tomography using randomized benchmarking [58]. We consider a 1-parameter family of 2-qubit channels obtained from a convex mixture of the maximally non-separable *SWAP* channel and the identity channel (a product channel). The contour plot compares the true value of correlated unitarity $u_c(\mathcal{E}_{AB})$ with the correlation measure $C_{sim} \approx C$ estimating Equation (42) in the presence of re-set errors. For two qubits, non-separability occurs if $u_c(\mathcal{E}_{AB}) > 7/12$. We simulate both Protocol 1 and 2, and we find that for a wide range of re-set errors we may witness non-separability for $p, q \gtrsim 0.5$. The region of green where $p, q \geq 1/2$ is an artifact of our particular method, and with a more refined algorithm we expect detection of non-separability also in this region.

ple, one can model such re-set errors as depolarizing

$$\tilde{\mathcal{R}}_B = id_A \otimes (p\mathcal{R}_B + (1-p)id_B), \quad (47)$$

where $p \in [0, 1]$. In Figure 3 we plot the benchmarking decay curves and find that for re-setting errors up to $\sim 20\%$ the protocol returns an estimate of the sub-unity $u_{A \rightarrow A}(\mathcal{E})$ accurate to $\sim 90\%$. Note that such a channel will not in general destroy correlations between A and B , in contrast to a stronger, more simplistic error model of

$$\tilde{\mathcal{R}}_B(\rho_{AB}) = \rho_A \otimes \left(\frac{1}{2}(\mathbb{1} + \mathbf{b} \cdot \boldsymbol{\sigma}) \right), \quad (48)$$

where one assumes a re-set to a local qubit state with non-zero Bloch vector \mathbf{b} . Under this stronger model assumption a simulation shows that such a scenario returns a good estimate for the sub-unity for $|\mathbf{b}| \leq 0.2$.

There are further variants around the above protocol. For example, if re-setting to non-maximally mixed states have very low errors then this provides another means to estimate $u_{A \rightarrow A}(\mathcal{E}_{AB})$. For example, if a low-error re-set to the pair of states $\frac{1}{2}(\mathbb{1} \pm \mathbf{b} \cdot \boldsymbol{\sigma})$ is possible

for some \mathbf{b} then it can be shown that the average unitarity of the output on A over the pair is always an upper bound on $u_{A \rightarrow A}(\mathcal{E}_{AB})$ (see Appendix E for details), and so would provide a lower bound on the correlated unitarity. Therefore, this would allow witnessing of non-separability under the preceding assumptions.

In theory, another source of information that could be exploited is the unitarity of the channel from AB to A , given by

$$\mathcal{E}_{AB \rightarrow A}(\rho) = \text{tr}_B \circ \mathcal{E}_{AB}(\rho). \quad (49)$$

In terms of sub-unitarities this quantity can be decomposed as

$$u(\mathcal{E}_{AB \rightarrow A}) = \frac{1}{(d_A d_B)^2 - 1} \left(\frac{1}{\alpha_A} u_{A \rightarrow A}(\mathcal{E}_{AB}) + \frac{1}{\alpha_B} u_{B \rightarrow A}(\mathcal{E}_{AB}) + \frac{1}{\alpha_A \alpha_B} u_{AB \rightarrow A}(\mathcal{E}_{AB}) \right). \quad (50)$$

However, while this provides an expression in terms of sub-unitarities without requiring re-setting, the standard benchmarking protocol will not work here due to the input and output systems being of different dimensions, and therefore a more involved protocol would be required.

E. Addressability of qubits and sub-unitarities

Several methods have recently been developed for detection [67], characterization [20, 68] and mitigation [69] of unwanted correlations between subsystems (specifically cross-talk) in a quantum device from a hardware-agnostic and model independent perspective. Our work adds to this toolkit new methods to characterize coherent correlations and provides information about noise channels that is independent from features captured by previous works.

Simultaneous randomized benchmarking (SimRB) [20] compares the increase in error rates when both subsystems are simultaneously and independently driven vs when one subsystem is driven and the other is kept idle. This quantifies the amount of new errors experienced by a subsystem as a result of simultaneously applying Clifford gates on the other. As it is the case for Protocol 2, due to the local independent Clifford twirl on one subsystem, SimRB is also affected by SPAM, and strong errors may be detected by deviations from exponential decay [20].

To compare with the information obtained from sub-unitarities, a quantity to detect correlations can be determined from the simultaneous Clifford twirl as in [20]. We denote this quantity by

$$a(\mathcal{E}_{AB}) := e_{AB} - e_A \cdot e_B. \quad (51)$$

where \mathcal{E}_{AB} is an effective noise channel associated to the Clifford gate-set acting locally on each subsystem

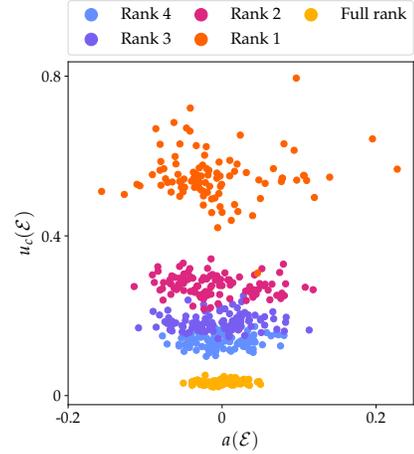


FIG. 5. **Correlated unitarity vs. addressability.** Correlated unitarity is largely independent from existing addressability measures, while Kraus rank is a better indicator of the value of u_c , which is consistent with it capturing the coherent correlations between subsystems. This suggests the measure might be suitable for benchmarking 2-qubit gates where large coherence transfer is required. The above plot is for random channels of different ranks from the distributions of Bruzda *et al.* and simulated using QuTip [44, 45].

A and B . The three decay parameters e_{AB} , e_A and e_B are extracted from the randomized benchmarking protocol that applies simultaneous local Clifford gates to subsystems A and B and are given in terms of the Liouville data for the channel as

$$\begin{aligned} e_A &= \alpha_A \text{tr}[T_{A \rightarrow A}], \\ e_B &= \alpha_B \text{tr}[T_{B \rightarrow B}], \\ e_{AB} &= \alpha_A \alpha_B \text{tr}[T_{AB \rightarrow AB}], \end{aligned} \quad (52)$$

with the coefficients α_X as defined earlier.

For a product channel, $T_{AB \rightarrow AB} = T_{A \rightarrow A} \otimes T_{B \rightarrow B}$ and therefore $a(\mathcal{E}_A \otimes \mathcal{E}_B) = 0$. In this manner, any deviation of $a(\mathcal{E})$ from zero is taken as detection of correlated behaviour. Note that in contrast to sub-unitarities, these measures are not invariant under local basis changes which makes it more problematic to interpret as a strict correlation measure.

It is easy to verify that the correlated unitarity provides independent information to a SimRB protocol, for example the CNOT gate is undetected by the addressability correlation measure; however it is detected by correlated unitarity. Figure 5 shows this is generic for bipartite channels, and we find that there are regions where the addressability correlation measure is zero or close to it, but the correlated unitarity varies greatly.

IV. OUTLOOK

Our starting point in this work was to develop simple, yet effective measures of correlations in quantum

channels and means to assess coherent sub-structures of such channels. The approach was motivated and guided by the idea of introducing measures that can be both efficiently estimated through RB-type of techniques and interpreted operationally as to quantify coherent correlations.

Certain sub-unitarities of a general bipartite channel can be interpreted as unitarities of locally acting channels induced by state preparation and discarding on one subsystem. Furthermore, we showed that they satisfy a set of inequalities that express an information-disturbance relation. This opens up new directions to analyse non-classical features of quantum channels directly from their robust tomographic description [58].

In the context of benchmarking of quantum devices, it will be of interest to develop hardware implementations of the protocols here and determine how effective and useful they are in practice. Such analysis will closely investigate the effects of re-set errors for the subsystem unaddressed by target gates. Our simulations show that our second protocol, while not fully robust can still allow small re-set errors to estimate magnitudes of correlated noise, but ultimately whether this is a reasonable assumption must be assessed for the system at hand.

Throughout this work we consider the induced error to be time-independent and gate-independent and averaged for the gate-set considered. As such, relaxing these constraints would be a natural line to develop [52, 70, 71].

Our primary protocol relies on fitting a multi-exponential decay to noisy data. In general this is a hard problem, and there will be many fits that will approximate the decay curve. The protocol could be substantially improved by exploiting recent statistical techniques [72], algorithms for multi-exponential fitting [2, 73] and other approaches such as spectral tomography [74].

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Appendix A: Quantum operations and a review of notation

1. Review of notation

Throughout these Appendices we consistently use the same notation as the main text, which we review here.

We consider an open bipartite quantum system with an associated Hilbert space $\mathcal{H}_A \otimes \mathcal{H}_B$ and dimension $d = d_A d_B$. Quantum channels act on the system such that $\mathcal{E}_{AB}: \mathcal{B}(\mathcal{H}_A \otimes \mathcal{H}_B) \rightarrow \mathcal{B}(\mathcal{H}_A \otimes \mathcal{H}_B)$, and unless otherwise stated we assume for simplicity that the input and output systems are identical. We denote all vectorized quantities in boldface, $|\mathbf{M}\rangle := |\text{vec}(M)\rangle$ for any operator $M \in \mathcal{B}(\mathcal{H}_A \otimes \mathcal{H}_B)$ and similarly, we denote the Liouville representation $\mathcal{E}_{AB} := \mathcal{L}(\mathcal{E}_{AB})$ for any channel \mathcal{E}_{AB} , as detailed in the main text.

For subsystem A , we choose an orthonormal basis of operators $X_\mu = (X_0 = \frac{1}{\sqrt{d_A}} \mathbb{1}_A, X_i)$, where d_A is dimension of the subsystem A , and $\text{tr}[X_\mu^\dagger X_\nu] = \delta_{\mu\nu}$. Similarly for B an orthonormal basis $Y_\mu = (Y_0 = \frac{1}{\sqrt{d_B}} \mathbb{1}_B, Y_i)$. Together these provide a basis for the full system which is given in the Liouville representation as

$$|\mathbf{X}_\nu \otimes \mathbf{Y}_\mu\rangle := |\mathbf{X}_\nu\rangle \otimes |\mathbf{Y}_\mu\rangle. \quad (\text{A1})$$

Furthermore $\{|\mathbf{X}_\nu \otimes \mathbf{Y}_\mu\rangle\}_{\nu,\mu}$ forms a complete orthonormal basis for $\mathcal{H}_A \otimes \mathcal{H}_A \otimes \mathcal{H}_B \otimes \mathcal{H}_B$, and with respect to this basis, the Liouville representation of \mathcal{E}_{AB} corresponds to a matrix \mathcal{E}_{AB} whose entries satisfy

$$\langle \mathbf{X}_\nu \otimes \mathbf{Y}_\mu | \mathcal{E}_{AB} | \mathbf{X}_{\nu'} \otimes \mathbf{Y}_{\mu'} \rangle = \text{tr}(X_\nu^\dagger \otimes Y_\mu^\dagger \mathcal{E}_{AB}(X_{\nu'} \otimes Y_{\mu'})). \quad (\text{A2})$$

For simplicity, where there is no ambiguity on the local labels μ and ν we will sometimes use a single-label notation $|\mathbf{Z}_\omega\rangle = |\mathbf{X}_\nu \otimes \mathbf{Y}_\mu\rangle$. In particular, we denote $|\mathbf{Z}_0\rangle = |\mathbf{X}_0\rangle \otimes |\mathbf{Y}_0\rangle$.

We highlight that we shall use the greek-labels (μ, ν, \dots) for sums that run over *all* basis operators and Latin-labels (i, j, \dots) notation to run over just the *trace-less* basis operators.

2. Quantum operations in the vectorized operator basis

Using this notation we now give some useful quantum operations in the Liouville representation that we use through out this work with proofs following. Firstly, the channel to trace out (tr) the system, and a channel we define to prepare ($\text{prep}: \text{prep}(1) = \mathbb{1}/d$) a new system in the maximally mixed state

$$\text{tr} = \sqrt{d} \langle \mathbf{Z}_0 | \quad \text{and} \quad \text{prep} = |\mathbf{Z}_0\rangle / \sqrt{d}. \quad (\text{A3})$$

A direct consequence of this is that the completely depolarizing channel $\mathcal{D}(\rho) := \mathbb{1}/d$ is given by

$$\mathcal{D} = \text{prep} \cdot \text{tr} = |\mathbf{Z}_0\rangle \langle \mathbf{Z}_0|. \quad (\text{A4})$$

The identity channel ($\text{id}(\rho) = \rho$) also allows a very simple form in the Liouville representation: $\text{id} = \mathbb{1}^{\otimes 2}$. From these definitions we can build bipartite channels, such as the partial trace of subsystem B

$$\text{id}_A \otimes \text{tr}_B = \sqrt{d_B} \text{id}_A \otimes \langle \mathbf{Y}_0|. \quad (\text{A5})$$

where id_A is the Liouville representation of the identity channel on subsystem A . Similarly, combination of this with the preparation channel on B leads to the complete depolarization channel for the B subsystem

$$\text{id}_A \otimes \mathcal{D}_B = \text{id}_A \otimes (\text{prep}_B \cdot \text{tr}_B) = \text{id}_A \otimes |\mathbf{Y}_0\rangle \langle \mathbf{Y}_0|. \quad (\text{A6})$$

Finally for $d_A = d_B$ we can express the unitary operation, *SWAP*, that swaps the states of both subsystems compactly in the Liouville representation as

$$\text{SWAP} = \sum_{\nu=0, \mu=0}^{d_A^2-1, d_B^2-1} |\mathbf{X}_\nu \otimes \mathbf{Y}_\mu\rangle \langle \mathbf{X}_\mu \otimes \mathbf{Y}_\nu|. \quad (\text{A7})$$

Proofs for the preceding Liouville operators are now given:

Proof. (of eqn. A3) For the first part we have $\text{tr}[\rho_{AB}] = \text{tr}[\mathbb{1}\rho_{AB}] = \sqrt{d}\langle \mathbf{Z}_0 | \rho_{AB} \rangle$ as $Z_0 = Z_0^\dagger$. We can then vectorize both sides and apply the definition of the Liouville representation of a channel $|\text{tr}[\rho_{AB}]\rangle = \sqrt{d}\langle \mathbf{Z}_0 | \rho_{AB} \rangle$ and $\text{tr}[\rho_{AB}] = \sqrt{d}\langle \mathbf{Z}_0 | \rho_{AB} \rangle$. Therefore $\text{tr} = \sqrt{d}\langle \mathbf{Z}_0 |$. For the second part, definitionally, $\mathbb{1}/d = Z_0/\sqrt{d}$, $\text{prep}(\mathbb{1}) = Z_0/\sqrt{d}$ and the vectorization of 1 leaves it unchanged $|\mathbb{1}\rangle = 1$. Therefore $|\text{prep}(\mathbb{1})\rangle = |\mathbf{Z}_0\rangle/\sqrt{d}$ and $\text{prep}|\mathbb{1}\rangle = |\mathbf{Z}_0\rangle/\sqrt{d}|\mathbb{1}\rangle$. As 1 is the only valid state of the trivial system, we read off $\text{prep} = |\mathbf{Z}_0\rangle/\sqrt{d}$ completing the proof. \square

Proof. (of eqn. (A4)) We have $\mathcal{D}|\rho\rangle = |\mathbb{1}/d\rangle = |\mathbf{Z}_0\rangle/\sqrt{d}$. As $\langle \mathbf{Z}_0 | \rho \rangle = 1/\sqrt{d}$ for any quantum state ρ we can write $\mathcal{D} = |\mathbf{Z}_0\rangle\langle \mathbf{Z}_0|$. \square

Proof. (of eqn. (A5)) This follows from eqn. (A3), with the identity channel on subsystem A . \square

Proof. (of $\text{prep}_B = id_A \otimes |\mathbf{Y}_0\rangle/\sqrt{d_B}$) This follows from eqn. (A3), with the identity channel on subsystem A . \square

Proof. (of eqn. (A7)) From definition, we can write any bipartite state in the form $\rho := \sum_{\nu,\mu} \lambda_{\nu\mu} X_\nu \otimes Y_\mu$. The SWAP channel then acts on this state such that $\text{SWAP}(\rho) := \sum_{\nu,\mu} \lambda_{\mu\nu} X_\nu \otimes Y_\mu$. Therefore, from inspection, the Liouville super operator of the channel is $\text{SWAP} = \sum_{\nu,\mu} |\mathbf{X}_\mu \otimes \mathbf{Y}_\nu\rangle\langle \mathbf{X}_\nu \otimes \mathbf{Y}_\mu|$. \square

Appendix B: Properties of subunitarity

1. Elementary properties of subunitarity

Lemma B.1. *Given a quantum channel \mathcal{E} , we have that $u(\mathcal{E}) = 0$ if and only if \mathcal{E} is a completely depolarizing channel.*

Proof. We have that $u(\mathcal{E}) = 0$ if and only if $\text{tr}[T^\dagger T] = \|T\|_2^2 = 0$ but this occurs if and only if $T = 0$. Therefore the only possible non-zero data in the channel's Liouville representation is the \mathbf{x} vector. This is a completely depolarizing channel to a fixed quantum state as required. \square

Theorem B.1. *For $\mathcal{E}_A(\rho) := \text{tr}_B[\mathcal{E}_{AB}(\rho \otimes \frac{\mathbb{1}_B}{d_B})]$ we have $u(\mathcal{E}_A) = u_{A \rightarrow A}(\mathcal{E}_{AB})$, the unitarity u of the local channel equal to the subunitarity $u_{A \rightarrow A}$ of the full channel.*

Proof. From definition the sub-unital block $T_{A \rightarrow A} = \langle \mathbf{X}_i \otimes \mathbf{Y}_0 | \mathcal{E}_{AB} | \mathbf{X}_j \otimes \mathbf{Y}_0 \rangle = \text{tr}\left[X_i^\dagger \otimes \frac{\mathbb{1}_B}{\sqrt{d_B}} \mathcal{E}_{AB}(X_j \otimes \frac{\mathbb{1}_B}{\sqrt{d_B}})\right] = \text{tr}_A[X_i^\dagger \text{tr}_B[\mathcal{E}_{AB}(X_j \otimes \frac{\mathbb{1}_B}{d_B})]] = \text{tr}_A[X_i^\dagger \mathcal{E}_A(X_j)]$, which gives the unital block T of \mathcal{E}_A . As $T_{A \rightarrow A, \mathcal{E}_{AB}} = T_{\mathcal{E}_A}$ from definition $u_{A \rightarrow A}(\mathcal{E}_{AB}) = u(\mathcal{E}_A)$. Similarly $u(\mathcal{E}_B) = u_{B \rightarrow B}(\mathcal{E}_{AB})$ for $\mathcal{E}_B(\rho) := \text{tr}_A[\mathcal{E}_{AB}(\frac{\mathbb{1}_A}{d_A} \otimes \rho)]$. \square

Theorem B.2. *The unitarity of a channel \mathcal{E} can be written as the weighted sum of its sub-unitarities*

$$u(\mathcal{E}) = \frac{1}{d^2 - 1} \sum_{i,j=(A,B,AB)} \frac{u_{i \rightarrow j}(\mathcal{E})}{\alpha_i}, \quad (\text{B1})$$

where $d = d_A \cdot d_B$, $\alpha_A = 1/(d_A^2 - 1)$, $\alpha_B = 1/(d_B^2 - 1)$ and $\alpha_{AB} = \alpha_A \cdot \alpha_B$.

Proof. This simply follows from block-matrix multiplication, giving $\text{tr}[T^\dagger T] = \sum_{n,m=(A,B,AB)} \text{tr}[T_{n \rightarrow m}^\dagger T_{n \rightarrow m}]$. Therefore (see eqn. (14)) the unitarity is $u(\mathcal{E}) = \frac{1}{d^2 - 1} \sum_{n,m=(A,B,AB)} \text{tr}[T_{n \rightarrow m}^\dagger T_{n \rightarrow m}]$. Rearranging the dimensional constants (see eqn. (16)) completes the proof. \square

2. Properties of subunitarity for product channels

Lemma B.2. *For a product channel, $\mathcal{E}_A \otimes \mathcal{E}_B$, the sub unital block $T_{A \rightarrow A} = T_A \otimes |\mathbf{Y}_0\rangle\langle \mathbf{Y}_0|$ where $T_A := \sum_{i,j} |\mathcal{E}_A(\mathbf{X}_j)\rangle\langle \mathbf{X}_i|$. Similarly $T_{B \rightarrow B} = |\mathbf{X}_0\rangle\langle \mathbf{X}_0| \otimes T_B$ where $T_B := \sum_{i,j} |\mathcal{E}_B(\mathbf{Y}_j)\rangle\langle \mathbf{Y}_i|$.*

Proof. From definition, $T_{A \rightarrow A, i,j} = \langle \mathbf{X}_i | \otimes \langle \mathbf{Y}_0 | \mathcal{E}_A \otimes \mathcal{E}_B | \mathbf{X}_j \rangle \otimes | \mathbf{Y}_0 \rangle = \langle \mathbf{X}_i | \mathcal{E}_A | \mathbf{X}_j \rangle \text{tr}[\mathcal{E}_B(\mathbb{1}/d_A)]$. For any trace preserving channel $\text{tr}[\mathcal{E}(\mathbb{1}/d)] = 1$ so $T_{A \rightarrow A} = \sum_{i,j} \langle \mathbf{X}_i | \mathcal{E}_A | \mathbf{X}_j \rangle |\mathbf{X}_i\rangle\langle \mathbf{X}_j| \otimes |\mathbf{Y}_0\rangle\langle \mathbf{Y}_0|$. The proof for $T_{B \rightarrow B}$ follows similarly. \square

Lemma B.3. *For a product channel, $\mathcal{E}_A \otimes \mathcal{E}_B$, we have $T_{AB \rightarrow AB} = T_A \otimes T_B$.*

Proof. From definition, $T_{AB \rightarrow AB} = \sum_{ij}^{d_A^2-1} \sum_{nm}^{d_B^2-1} \langle \mathbf{X}_i | \otimes \langle \mathbf{Y}_n | \mathcal{E}_A \otimes \mathcal{E}_B | \mathbf{X}_j \rangle \otimes | \mathbf{Y}_m \rangle | \mathbf{X}_i \rangle \langle \mathbf{X}_j | \otimes | \mathbf{Y}_n \rangle \langle \mathbf{Y}_m | = \sum_{ij}^{d_A^2-1} \sum_{nm}^{d_B^2-1} | \mathcal{E}_A(\mathbf{X}_j) \rangle \langle \mathbf{X}_i | \otimes | \mathcal{E}_B(\mathbf{Y}_m) \rangle \langle \mathbf{Y}_n | = T_A \otimes T_B.$ \square

Theorem B.3. For a product channel, $\mathcal{E} = \mathcal{E}_A \otimes \mathcal{E}_B$, $u_{AB \rightarrow AB}(\mathcal{E}) = u_{A \rightarrow A}(\mathcal{E}) \cdot u_{B \rightarrow B}(\mathcal{E})$.

Proof. From Lemma B.3 we can write $u_{AB \rightarrow AB}(\mathcal{E}) = \alpha_A \cdot \alpha_B \text{tr} \left[T_A^\dagger \otimes T_B^\dagger T_A \otimes T_B \right] = \alpha_A \cdot \alpha_B \text{tr} \left[T_A^\dagger T_A \right] \text{tr} \left[T_B^\dagger T_B \right] = u(\mathcal{E}_A)u(\mathcal{E}_B)$. As $u(\mathcal{E}_A) = u_{A \rightarrow A}(\mathcal{E})$ and $u(\mathcal{E}_B) = u_{B \rightarrow B}(\mathcal{E})$ for any channel this completes the proof. \square

Corollary B.1. The correlated unitarity u_c of a product channel $\mathcal{E}_A \otimes \mathcal{E}_B$ is $u_c(\mathcal{E}_A \otimes \mathcal{E}_B) = 0$.

Proof. This follows directly from Theorem B.3. \square

Lemma B.4. The sub-unitarity $u_{A \rightarrow AB}(\mathcal{E}_A \otimes \mathcal{E}_B)$ for a bipartite product channel $\mathcal{E}_A \otimes \mathcal{E}_B$, decomposes as

$$u_{A \rightarrow AB}(\mathcal{E}_A \otimes \mathcal{E}_B) = u_{A \rightarrow A}(\mathcal{E}_A \otimes \mathcal{E}_B)x_B, \quad (\text{B2})$$

where $x_B := \mathbf{x}_{B \rightarrow B}^\dagger \mathbf{x}_{B \rightarrow B}$ for the non-unital vector of the subsystem B of the channel \mathcal{E}_B .

Proof. From the definition of $u_{A \rightarrow AB}$ we have

$$\begin{aligned} u_{A \rightarrow AB}(\mathcal{E}_A \otimes \mathcal{E}_B) &= \alpha_A \sum_{k,j,n=1}^{(d_A^2-1)(d_B^2-1)} \langle \mathbf{X}_j \otimes \mathbf{Y}_n | \mathcal{E} | \mathbf{X}_k \otimes \mathbf{Y}_0 \rangle \langle \mathbf{X}_k \otimes \mathbf{Y}_0 | \mathcal{E}^\dagger | \mathbf{X}_j \otimes \mathbf{Y}_n \rangle, \\ &= \alpha_A \sum_{k,j,n=1}^{(d_A^2-1)(d_B^2-1)} \langle \mathbf{X}_k | \mathcal{E}_A^\dagger | \mathbf{X}_j \rangle \langle \mathbf{X}_j | \mathcal{E}_A | \mathbf{X}_k \rangle \langle \mathbf{Y}_0 | \mathcal{E}_B^\dagger | \mathbf{Y}_n \rangle \langle \mathbf{Y}_n | \mathcal{E}_B | \mathbf{Y}_0 \rangle, \\ &= u_{A \rightarrow A}(\mathcal{E}_A \otimes \mathcal{E}_B) \sum_{n=1}^{d_B^2-1} \langle \mathbf{Y}_0 | \mathcal{E}_B^\dagger | \mathbf{Y}_n \rangle \langle \mathbf{Y}_n | \mathcal{E}_B | \mathbf{Y}_0 \rangle, \\ &= u_{A \rightarrow A}(\mathcal{E}_A \otimes \mathcal{E}_B)x_B \end{aligned} \quad (\text{B3})$$

which completes the proof. \square

Swapping the subsystem labels we also have $u_{B \rightarrow AB}(\mathcal{E}_A \otimes \mathcal{E}_B) = u_{B \rightarrow B}(\mathcal{E}_A \otimes \mathcal{E}_B)x_A$, where $x_A := \mathbf{x}_{A \rightarrow A}^\dagger \mathbf{x}_{A \rightarrow A}$ for the non-unital vector of the subsystem A of the channel.

3. Properties of subunitarity for separable channels

Lemma B.5. The sub-unitarity $u_{AB \rightarrow A}(\mathcal{E})$ for a bipartite separable channel $\mathcal{E} := \sum_i^r p_i \mathcal{E}_{A,i} \otimes \mathcal{E}_{B,i}$ is zero.

Proof. From the definition of $u_{AB \rightarrow A}$ we have

$$\begin{aligned} u_{AB \rightarrow A}(\mathcal{E}) &= \alpha_A \alpha_B \text{tr} \left[T_{AB \rightarrow A}^\dagger T_{AB \rightarrow A} \right], \\ &= \alpha_A \alpha_B \sum_{k,j,n=1}^{(d_A^2-1)(d_B^2-1)} \langle \mathbf{X}_j \otimes \mathbf{Y}_n | \mathcal{E}^\dagger | \mathbf{X}_k \otimes \mathbf{Y}_0 \rangle \langle \mathbf{X}_k \otimes \mathbf{Y}_0 | \mathcal{E} | \mathbf{X}_j \otimes \mathbf{Y}_n \rangle, \\ &= \alpha_A \alpha_B \sum_{k,j,n=1}^{(d_A^2-1)(d_B^2-1)} \sum_{i,j}^r p_i p_j \langle \mathbf{X}_j | \mathcal{E}_{A,i}^\dagger | \mathbf{X}_k \rangle \langle \mathbf{X}_k | \mathcal{E}_{A,j} | \mathbf{X}_j \rangle \langle \mathbf{Y}_n | \mathcal{E}_{B,i}^\dagger | \mathbf{Y}_0 \rangle \langle \mathbf{Y}_0 | \mathcal{E}_{B,j} | \mathbf{Y}_n \rangle. \end{aligned} \quad (\text{B4})$$

For the channel to be trace preserving we must have $\langle \mathbf{Y}_0 | \mathcal{E}_{B,j} | \mathbf{Y}_n \rangle = 0$ for all n & j . Therefore $u_{AB \rightarrow A}(\mathcal{E}) = 0$. \square

Additionally, swapping the subsystem labels, $u_{AB \rightarrow B}(\mathcal{E}) = 0$ for any separable bipartite channel \mathcal{E} .

Lemma B.6. The sub-unitarity $u_{A \rightarrow B}(\mathcal{E})$ for a bipartite separable channel $\mathcal{E} := \sum_i^r p_i \mathcal{E}_{A,i} \otimes \mathcal{E}_{B,i}$ is zero.

Proof. From definition

$$\begin{aligned}
u_{A \rightarrow B}(\mathcal{E}) &= \alpha_A \text{tr} \left[T_{A \rightarrow B}^\dagger T_{A \rightarrow B} \right], \\
&= \alpha_A \sum_{k,j=1}^{(d_A^2-1)(d_B^2-1)} \langle \mathbf{X}_j \otimes \mathbf{Y}_0 | \mathcal{E}^\dagger | \mathbf{X}_0 \otimes \mathbf{Y}_k \rangle \langle \mathbf{X}_0 \otimes \mathbf{Y}_k | \mathcal{E} | \mathbf{X}_j \otimes \mathbf{Y}_0 \rangle, \\
&= \alpha_A \sum_{k,j=1}^{(d_A^2-1)(d_B^2-1)} \sum_{i,j}^r p_i p_j \langle \mathbf{X}_j | \mathcal{E}_{A,i}^\dagger | \mathbf{X}_0 \rangle \langle \mathbf{X}_0 | \mathcal{E}_{A,j} | \mathbf{X}_j \rangle \langle \mathbf{Y}_0 | \mathcal{E}_{B,i}^\dagger | \mathbf{Y}_k \rangle \langle \mathbf{Y}_k | \mathcal{E}_{B,j} | \mathbf{Y}_0 \rangle.
\end{aligned} \tag{B5}$$

For the channel to be trace preserving we must have $\langle \mathbf{X}_0 | \mathcal{E}_{A,j} | \mathbf{X}_j \rangle = 0$ for all j . Therefore $u_{A \rightarrow B}(\mathcal{E}) = 0$. \square

Additionally, swapping the subsystem labels, $u_{B \rightarrow A}(\mathcal{E}) = 0$ for any separable bipartite channel \mathcal{E} .

Lemma B.7. For a unital bipartite separable channel $\mathcal{E} := \sum_i^r p_i \mathcal{E}_{A,i} \otimes \mathcal{E}_{B,i}$ where $\mathcal{E}_{X,i}$ are local unital channels, the sub-unitarity $u_{A \rightarrow AB}(\mathcal{E})$ is zero.

Proof. From the definition of $u_{A \rightarrow AB}$ we have

$$\begin{aligned}
u_{A \rightarrow AB}(\mathcal{E}) &= \alpha_A \text{tr} \left[T_{A \rightarrow AB}^\dagger T_{A \rightarrow AB} \right], \\
&= \alpha_A \sum_{k,j,n=1}^{(d_A^2-1)(d_B^2-1)} \langle \mathbf{X}_k \otimes \mathbf{Y}_0 | \mathcal{E}^\dagger | \mathbf{X}_j \otimes \mathbf{Y}_n \rangle \langle \mathbf{X}_j \otimes \mathbf{Y}_n | \mathcal{E} | \mathbf{X}_k \otimes \mathbf{Y}_0 \rangle, \\
&= \alpha_A \sum_{k,j,n=1}^{(d_A^2-1)(d_B^2-1)} \sum_{i,j}^r p_i p_j \langle \mathbf{X}_k | \mathcal{E}_{A,i}^\dagger | \mathbf{X}_j \rangle \langle \mathbf{X}_j | \mathcal{E}_{A,i} | \mathbf{X}_k \rangle \langle \mathbf{Y}_0 | \mathcal{E}_{B,j}^\dagger | \mathbf{Y}_n \rangle \langle \mathbf{Y}_n | \mathcal{E}_{B,j} | \mathbf{Y}_0 \rangle.
\end{aligned} \tag{B6}$$

For the channel to be unital we must have $\langle \mathbf{Y}_n | \mathcal{E}_{B,i} | \mathbf{Y}_0 \rangle = 0$ for all n . Therefore $u_{A \rightarrow AB}(\mathcal{E}) = 0$. \square

Additionally, swapping the subsystem labels, $u_{B \rightarrow AB}(\mathcal{E}) = 0$ for any unital separable bipartite channel \mathcal{E} .

4. Generalized monogamy of unitarity

Lemma B.8. For any channel $\mathcal{E}: \mathcal{B}(\mathcal{H}) \rightarrow \mathcal{B}(\mathcal{H})$ with complete orthonormal operator basis $Z_\mu = (Z_0 = \mathbb{1}/\sqrt{d}, Z_i)$,

$$\sum_{j=1}^{d^2-1} |\langle \mathbf{Z}_j | \mathcal{E}(\mathbf{Z}_i) \rangle|^2 \leq 1 \text{ for all } i. \tag{B7}$$

Proof. We can directly quote Parseval's theorem for general inner product spaces that states $\sum_\mu^{d^2} |\langle \mathbf{Z}_\mu | \mathcal{E}(\mathbf{Z}_\nu) \rangle|^2 = \|\mathcal{E}(\mathbf{Z}_\nu)\|_{HS}^2$. Note that in general Hilbert-Schmidt norm is not contractive under CPTP maps (unless the map is unital, case in which result follows directly). However we can directly show that for $Z_0 = \frac{\mathbb{1}}{\sqrt{d}}$ we have $\|\mathcal{E}(Z_0)\|_{HS} = 1$ and re-write $\|\mathcal{E}(Z_\nu)\|_{HS}^2 = \text{tr}(Z_\nu^\dagger \mathcal{E}^\dagger \circ \mathcal{E}(Z_\nu)) = \langle \mathbf{Z}_\nu | \mathcal{E}^\dagger \cdot \mathcal{E} | \mathbf{Z}_\nu \rangle$. Moreover it follows that since \mathcal{E} is trace-preserving then \mathcal{E}^\dagger is unital so $T_{\mathcal{E}^\dagger \circ \mathcal{E}} = T_{\mathcal{E}^\dagger} T_{\mathcal{E}} = T_{\mathcal{E}}^\dagger T_{\mathcal{E}}$. Furthermore, since $|\mathbf{Z}_\nu\rangle$ are normalized then for the traceless elements Z_i we have the above is upper bounded by the (modulus of) the largest eigenvalue of the block $T_{\mathcal{E}^\dagger \circ \mathcal{E}}$ in the the Liouville representation $\mathcal{E}^\dagger \circ \mathcal{E}$. However, the largest eigenvalue of $T_{\mathcal{E}}$ has modulus less than 1 and thus so will the largest eigenvalue of $T_{\mathcal{E}^\dagger \circ \mathcal{E}}$ and

$$\|\mathcal{E}(Z_i)\|_{HS}^2 \leq |\lambda_{\max}(T_{\mathcal{E}^\dagger \circ \mathcal{E}})| = |\lambda_{\max}(T_{\mathcal{E}})|^2 \leq 1. \tag{B8}$$

As we have that $\|\mathcal{E}(Z_i)\|_{HS}^2 = \langle \mathbf{Z}_i | T^\dagger T | \mathbf{Z}_i \rangle = \sum_j^{d^2-1} \langle \mathbf{Z}_i | \mathcal{E}^\dagger | \mathbf{Z}_j \rangle \langle \mathbf{Z}_j | \mathcal{E} | \mathbf{Z}_i \rangle = \sum_j^{d^2-1} |\langle \mathbf{Z}_j | \mathcal{E}(\mathbf{Z}_i) \rangle|^2$ this completes the proof. \square

Theorem B.4. The subunitarities of any bipartite channel \mathcal{E} obey the following inequality:

$$0 \leq \sum_{Y=(A,B,AB)} u_{X \rightarrow Y}(\mathcal{E}) \leq 1, \tag{B9}$$

for $X = (A, B, AB)$.

Proof. The lower bound follows from the non-negativity of the H-S inner product. From Lemma B.8, $\langle \mathbf{Z}_i | T^\dagger T | \mathbf{Z}_i \rangle \leq 1$ for any traceless element of the basis. Therefore if we sum over the traceless elements of the basis any subsystem (here subsystem A) we have $\sum_i^{d_A^2-1} \langle \mathbf{X}_i \otimes \mathbf{Y}_0 | T^\dagger T | \mathbf{X}_i \otimes \mathbf{Y}_0 \rangle \leq d_A^2 - 1$. Additionally we can break up the identity matrix of $\dim(T) = (d_A^2 d_B^2 - 1)$ in terms of basis elements as

$$\mathbb{1}_T = \sum_{i=1}^{d_A^2-1} |\mathbf{X}_i \otimes \mathbf{Y}_0\rangle \langle \mathbf{X}_i \otimes \mathbf{Y}_0| + \sum_{i,j=1}^{d_A^2-1, d_B^2-1} |\mathbf{X}_i \otimes \mathbf{Y}_j\rangle \langle \mathbf{X}_i \otimes \mathbf{Y}_j| + \sum_{j=1}^{d_B^2-1} |\mathbf{X}_0 \otimes \mathbf{Y}_j\rangle \langle \mathbf{X}_0 \otimes \mathbf{Y}_j|. \quad (\text{B10})$$

We are free to insert this between the blocks $T^\dagger T = T^\dagger \mathbb{1}_T T$,

$$\begin{aligned} & \sum_m^{d_A^2-1} \sum_i^{d_A^2-1} \langle \mathbf{X}_m \otimes \mathbf{Y}_0 | T^\dagger | \mathbf{X}_i \otimes \mathbf{Y}_0 \rangle \langle \mathbf{X}_i \otimes \mathbf{Y}_0 | T | \mathbf{X}_m \otimes \mathbf{Y}_0 \rangle \\ & + \sum_m^{d_A^2-1} \sum_{ij}^{d_A^2-1, d_B^2-1} \langle \mathbf{X}_m \otimes \mathbf{Y}_0 | T^\dagger | \mathbf{X}_i \otimes \mathbf{Y}_j \rangle \langle \mathbf{X}_i \otimes \mathbf{Y}_j | T | \mathbf{X}_m \otimes \mathbf{Y}_0 \rangle \\ & + \sum_m^{d_A^2-1} \sum_j^{d_B^2-1} \langle \mathbf{X}_m \otimes \mathbf{Y}_0 | T^\dagger | \mathbf{X}_0 \otimes \mathbf{Y}_j \rangle \langle \mathbf{X}_0 \otimes \mathbf{Y}_j | T | \mathbf{X}_m \otimes \mathbf{Y}_0 \rangle \leq d_A^2 - 1, \end{aligned} \quad (\text{B11})$$

Which are definitionally the three subunitarities originating in the A subsystem, after moving the normalization:

$$\begin{aligned} \text{tr} [T_{A \rightarrow A}^\dagger T_{A \rightarrow A}] + \text{tr} [T_{A \rightarrow AB}^\dagger T_{A \rightarrow AB}] + \text{tr} [T_{A \rightarrow B}^\dagger T_{A \rightarrow B}] & \leq d_A^2 - 1, \\ u_{A \rightarrow A}(\mathcal{E}) + u_{A \rightarrow AB}(\mathcal{E}) + u_{A \rightarrow B}(\mathcal{E}) & \leq 1. \end{aligned} \quad (\text{B12})$$

Repeating the process, initially summing over subsystem B , and the traceless elements $X_i \otimes Y_j$ completes the proof for all the required cases. \square

Corollary B.2 (Monogamy of unitarity). *For a channel $\mathcal{E}_{AB}: \mathcal{B}(\mathcal{H}_{A_1} \otimes \mathcal{H}_{B_1}) \rightarrow \mathcal{B}(\mathcal{H}_{A_2} \otimes \mathcal{H}_{B_2})$, the local sub-unitarities are bounded by*

$$u_{A_1 \rightarrow A_2}(\mathcal{E}_{AB}) + u_{A_1 \rightarrow B_2}(\mathcal{E}_{AB}) \leq 1. \quad (\text{B13})$$

Further for a channel $\mathcal{E}: \mathcal{B}(\mathcal{H}_X) \rightarrow \mathcal{B}(\mathcal{H}_A \otimes \mathcal{H}_B)$, the unitarities are bounded by

$$u(\mathcal{E}_A) + u(\mathcal{E}_B) \leq 1, \quad (\text{B14})$$

where $\mathcal{E}_A = \text{tr}_B[\mathcal{E}]$ and $\mathcal{E}_B = \text{tr}_A[\mathcal{E}]$.

Proof. For the first inequality, from Theorem B.4 if $A_1 = A_2 = A$ and $B_1 = B_2 = B$ we have that

$$u_{A \rightarrow A}(\mathcal{E}_{AB}) + u_{A \rightarrow B}(\mathcal{E}_{AB}) \leq u_{A \rightarrow A}(\mathcal{E}_{AB}) + u_{A \rightarrow AB}(\mathcal{E}_{AB}) + u_{A \rightarrow B}(\mathcal{E}_{AB}) \leq 1. \quad (\text{B15})$$

The proof of Theorem B.4 is only dependent on the input subsystems and their dimension, and generalizes straightforwardly to that case when $A_1 \neq A_2$ and $B_1 \neq B_2$.

For the second inequality, if we take B_2 being trivial from Theorem B.1, the sub-unitarity $u_{A_1 \rightarrow A_2}(\mathcal{E}_{AB})$ equals the unitarity of the channel \mathcal{E}_A . Similarly for $u_{A_1 \rightarrow B_2}(\mathcal{E}_{AB})$. Relabeling A_1 to X completes the proof, and implies the monogamy of unitarity. \square

Lemma B.9. *The subunitarities of any bipartite channel (towards any either subsystem) obey the following inequality:*

$$0 \leq \sum_X u_{X \rightarrow Y}(\mathcal{E}) \leq 1, \quad (\text{B16})$$

for $X = (A, B, AB), Y = (A, B)$.

Proof. The proof follows in a similar way to Theorem B.4. The lower bound can be found from the non-negativity of the H-S inner product. To find the upper bound consider the unitarity of a channel $\mathcal{F}: \mathcal{B}(\mathcal{H}_A \otimes \mathcal{H}_B) \rightarrow \mathcal{B}(\mathcal{H}_A \otimes \mathcal{H}_B)$

that performs a bipartite channel \mathcal{E} then depolarizes subsystem B . From eqn. (A6) the Liouville representation is given by

$$\mathcal{F} = (\mathbf{id}_A \otimes \mathcal{D}_B) \mathcal{E} = \left(\sum_{\mu} |\mathbf{X}_{\mu}\rangle\langle\mathbf{X}_{\mu}| \otimes |\mathbf{Y}_0\rangle\langle\mathbf{Y}_0| \right) \mathcal{E}. \quad (\text{B17})$$

The unitarity of this channel is then

$$\begin{aligned} u(\mathcal{F}) &= \frac{1}{d^2 - 1} \text{tr} \left[T_{\mathcal{F}}^{\dagger} T_{\mathcal{F}} \right], \\ &= \frac{1}{d^2 - 1} \text{tr} \left[T_{\mathcal{E}}^{\dagger} \left(\sum_i^{d_A^2 - 1} |\mathbf{X}_i\rangle\langle\mathbf{X}_i| \otimes |\mathbf{Y}_0\rangle\langle\mathbf{Y}_0| \right) T_{\mathcal{E}} \right], \\ &= \frac{1}{d^2 - 1} \sum_X \text{tr} \left[T_{\mathcal{E}, X \rightarrow A}^{\dagger} T_{\mathcal{E}, X \rightarrow A} \right], \end{aligned} \quad (\text{B18})$$

For \mathcal{E} to be a valid quantum channel Lemma B.8 must hold for all elements of the basis. Therefore $\text{tr} \left[T_{\mathcal{E}, X \rightarrow A}^{\dagger} T_{\mathcal{E}, X \rightarrow A} \right] \leq 1/\alpha_X$ where α_X is the relevant dimensional factor for subsystem X . Rearranging the dimensional constants

$$\begin{aligned} \sum_X \alpha_X \text{tr} \left[T_{\mathcal{E}, X \rightarrow A}^{\dagger} T_{\mathcal{E}, X \rightarrow A} \right] &\leq \frac{d^2 - 1}{\sum_X \alpha_X}, \\ \sum_X u_{X \rightarrow A}(\mathcal{E}) &\leq 1, \end{aligned} \quad (\text{B19})$$

Switching the label of the initial subsystem to B completes the proof for both cases. \square

5. Properties of subunitarity for Pauli channels

Consider the Pauli operators P_{α} acting on n qubits. These will form a complete orthonormal basis (so that normalization will be included in the definition of P_{α}) so as $\text{tr}(P_{\alpha} P_{\beta}) = \delta_{\alpha, \beta}$ and $P_{\alpha}^{\dagger} = P_{\alpha}$. We will also label $P_0 := 1/\sqrt{2^n}$, the identity operator. Moreover, for simplicity we consider bipartite systems formed of A and B each of n qubits, so they have dimensions $d_A = d_B = 2^n$.

Lemma B.10. *Let $\mathcal{E}(\rho) = \sum_i p_i P_i \rho P_i$ be a Pauli channel with $\sum_i p_i = d$ where the Pauli operators are normalized so that $\text{tr}(P_i P_j) = \delta_{ij}$ with \mathcal{E} acting on a system of dimension d . Then it follows that \mathcal{E} , its Liouville matrix has entries*

$$\langle P_j | \mathcal{E} | P_k \rangle = \delta_{jk} \sum_i (-1)^{\eta(P_i, P_k)} p_i \quad (\text{B20})$$

where $\eta(P_i, P_k)$ is 0 if P_i and P_k commute and 1 if they anti-commute. The unitarity of \mathcal{E} is given by [75]

$$u(\mathcal{E}) = \frac{1}{(d^2 - 1)} \left(\left(\sum_i p_i^2 \right) - 1 \right) \quad (\text{B21})$$

Proof. Check directly $\langle P_j | \mathcal{E} | P_k \rangle = \langle P_j | \mathcal{E}(P_k) \rangle = \text{tr}(P_j \mathcal{E}(P_k)) = \sum_i p_i \text{tr}(P_j P_i P_k P_i) = \frac{1}{d} \sum_i p_i (-1)^{\eta(P_i, P_k)} \text{tr}(P_j P_k) = \frac{1}{d} \delta_{jk} \sum_i p_i (-1)^{\eta(P_i, P_k)}$. This is a diagonal Liouville matrix, and the unitarity is determined in terms of its non-unital block $T_{\mathcal{E}}$ as

$$u(\mathcal{E}) = \frac{1}{d^2 - 1} \text{tr}(T_{\mathcal{E}}^{\dagger} T_{\mathcal{E}}) \quad (\text{B22})$$

$$= \frac{1}{d^2 - 1} \sum_{j \neq 0} \langle P_j | \mathcal{E} | P_j \rangle^2. \quad (\text{B23})$$

Note that $\langle \mathbf{P}_0 | \mathcal{E} | \mathbf{P}_0 \rangle = \frac{1}{d} \sum_i p_i = 1$. Notice the orthogonality relation $\sum_j (-1)^{\eta(P_i, P_j)} (-1)^{\eta(P_{i'}, P_j)} = d^2 \delta_{ii'}$ so that

$$\sum_j \langle \mathbf{P}_j | \mathcal{E} | \mathbf{P}_j \rangle^2 = \frac{1}{d^2} \sum_{j, i, i'} p_i p_{i'} (-1)^{\eta(P_i, P_j)} (-1)^{\eta(P_{i'}, P_j)} \quad (\text{B24})$$

$$= \sum_i p_i^2. \quad (\text{B25})$$

Therefore, we have

$$u(\mathcal{E}) = \frac{1}{d^2 - 1} \sum_{j \neq 0} |\langle \mathbf{P}_j | \mathcal{E} | \mathbf{P}_j \rangle|^2 \quad (\text{B26})$$

$$= \frac{1}{(d^2 - 1)} \left(\left(\sum_i p_i^2 \right) - 1 \right). \quad (\text{B27})$$

□

A bipartite Pauli channel on two n qubits systems will take the following form

$$\mathcal{E}(\rho_{AB}) = \sum_{\alpha, \beta} p_{\alpha, \beta} P_\alpha \otimes P_\beta \rho_{AB} P_\alpha \otimes P_\beta \quad (\text{B28})$$

and trace preserving condition requires $\sum_{\alpha, \beta} p_{\alpha, \beta} = 4^n$. We denote $d = d_A = d_B = 2^n$. The Liouville representation, with respect to a Pauli basis will be a diagonal matrix. The local channel at A

$$\mathcal{E}_A(\rho_A) := \text{tr}_B \mathcal{E}(\rho_A \otimes \mathbb{1}/d) \quad (\text{B29})$$

$$= \sum_{\alpha} q_{\alpha, 0} P_\alpha \rho_A P_\alpha \quad (\text{B30})$$

where the $q_{\alpha, 0} := \frac{1}{d} \sum_{\beta} p_{\alpha, \beta}$. Similarly at B :

$$\mathcal{E}_B(\rho_B) := \text{tr}_A \mathcal{E}(\mathbb{1}/d \otimes \rho_B) \quad (\text{B31})$$

$$= \sum_{\beta} q_{0, \beta} P_\beta \rho_B P_\beta \quad (\text{B32})$$

where the $q_{0, \beta} := \frac{1}{d} \sum_{\alpha} p_{\alpha, \beta}$. The subunitarities at A and B are given by $u_{A \rightarrow A} = u(\mathcal{E}_A)$ and $u_{B \rightarrow B} = u(\mathcal{E}_B)$. Therefore we get the following result.

Lemma B.11. *Let $d = 2^n$, the dimension of system A and respectively system B , then we have that*

$$u_{A \rightarrow A} = \frac{1}{d^2 - 1} \left(\sum_{\alpha} q_{\alpha, 0}^2 - 1 \right), \quad (\text{B33})$$

$$u_{B \rightarrow B} = \frac{1}{d^2 - 1} \left(\sum_{\beta} q_{0, \beta}^2 - 1 \right), \quad (\text{B34})$$

$$u_{AB \rightarrow AB} = \frac{d^2 + 1}{d^2 - 1} u(\mathcal{E}) - \frac{1}{d^2 - 1} (u_{A \rightarrow A} + u_{B \rightarrow B}). \quad (\text{B35})$$

Proof. The relations for $u_{A \rightarrow A}$ and $u_{B \rightarrow B}$ follow directly from Lemma B.10. The relation for $u_{AB \rightarrow AB}$ follows from the fact that the Liouville representation of \mathcal{E} is diagonal so that $T_{\mathcal{E}} = T_{A \rightarrow A} \oplus T_{AB \rightarrow AB} \oplus T_{B \rightarrow B}$ and thus

$$\begin{aligned} \text{tr}(T_{\mathcal{E}}^\dagger T_{\mathcal{E}}) &= \text{tr}(T_{A \rightarrow A}^\dagger T_{A \rightarrow A}) + \text{tr}(T_{B \rightarrow B}^\dagger T_{B \rightarrow B}) + \\ &\quad + \text{tr}(T_{AB \rightarrow AB}^\dagger T_{AB \rightarrow AB}) \end{aligned}$$

In terms of the unitarities, $u(\mathcal{E}) = \frac{1}{4^{2n} - 1} \text{tr}(T_{\mathcal{E}}^\dagger T_{\mathcal{E}})$ and $u_{AB \rightarrow AB} = \frac{1}{(2^{2n} - 1)^2} \text{tr}(T_{AB \rightarrow AB}^\dagger T_{AB \rightarrow AB})$ then the above is equivalent to

$$u_{AB \rightarrow AB} = \frac{4^{2n} - 1}{(2^{2n} - 1)^2} u(\mathcal{E}) - \frac{1}{2^{2n} - 1} (u_{A \rightarrow A} + u_{B \rightarrow B}). \quad (\text{B36})$$

□

Lemma B.12. *The correlated unitarity for Pauli noise channel on a bipartite system AB with $\dim(A) = \dim(B) = d = 2^n$ is given by*

$$u_c = \frac{1}{(d^2 - 1)^2} \left(\sum_{\alpha, \beta} p_{\alpha, \beta}^2 - \left(\sum_{\alpha} q_{\alpha, 0}^2 \right) \sum_{\beta} q_{0, \beta}^2 \right). \quad (\text{B37})$$

Proof. Directly from above. \square

Appendix C: Properties of correlated unitarity

1. Comparison of correlated unitarity with norm measures

We can compare the choice of definition for correlated unitarity with a norm, which sheds light on its structure and limitations. Consider the Hilbert-Schmidt norm expression

$$\Delta^2 := \|T_{AB} - T_A \otimes T_B\|^2 \quad (\text{C1})$$

where $T_{AB} \equiv T_{AB \rightarrow AB}$ and similarly for T_A and T_B . As this is a norm we have $\Delta = 0$ if and only if $T_{AB} = T_A \otimes T_B$, namely if and only if the channel is a product channel. We can expand this expression in terms of the Hilbert-Schmidt inner product to obtain

$$\begin{aligned} \Delta^2 &= \langle T_{AB} - T_A \otimes T_B, T_{AB} - T_A \otimes T_B \rangle \\ &= \langle T_{AB}, T_{AB} \rangle + \langle T_A \otimes T_B, T_A \otimes T_B \rangle - \langle T_{AB}, T_A \otimes T_B \rangle - \langle T_A \otimes T_B, T_{AB} \rangle \\ &= \|T_{AB}\|^2 + \|T_A\|^2 \|T_B\|^2 - 2 \operatorname{Re} [\langle T_{AB}, T_A \otimes T_B \rangle] \\ &= \|T_{AB}\|^2 + \|T_A\|^2 \|T_B\|^2 - 2 \|T_{AB}\| \|T_A\| \|T_B\| \cos \theta \\ \Delta^2 &= t_{AB}^2 + t_A^2 t_B^2 - 2 t_{AB} t_A t_B \cos \theta, \end{aligned}$$

where we have defined an angular variable θ via the inner product between T_{AB} and $T_A \otimes T_B$ and replaced the norm values with t_{AB}, t_A, t_B in the obvious way. Now the correlated unitarity is given by $u_c = \alpha_{AB}(t_{AB}^2 - t_A^2 t_B^2)$, with the dimensional prefactor $\alpha_{AB} = \frac{1}{(d_A^2 - 1)(d_B^2 - 1)}$. Substituting for t_{AB} into Δ^2 we have that

$$\Delta^2 = \frac{u_c}{\alpha_{AB}} + 2(t_A t_B)^2 - 2 \sqrt{\frac{u_c}{\alpha_{AB}} + (t_A t_B)^2} (t_A t_B) \cos \theta. \quad (\text{C2})$$

This implies a few things. Firstly, for $u_c = 0$ we have

$$\Delta^2 = 2(t_A t_B)^2 (1 - \cos \theta), \quad (\text{C3})$$

and so we see that u_c vanishing does not imply a product channel unless one of the t_A, t_B vanishes or if $\theta = 0$. The expression also implies that θ is an independent parameter that will in general vary the norm distance. Note that the benchmarking protocol gives us both $(t_A t_B)$ and u_c but does not give us θ . Therefore our existing benchmarking does not return enough to determine norm distance measure.

The above highlights relevant data at quadratic order that our approach is not sensitive to, but note that the $\cos \theta$ term is bounded and so it still is the case that u_c is acting as a “distance” from being a product channel. Specifically, we have

$$\frac{u_c}{\alpha_{AB}} + 2(t_A t_B)^2 - 2 \sqrt{\frac{u_c}{\alpha_{AB}} + (t_A t_B)^2} (t_A t_B) \leq \Delta^2 \quad \text{and} \quad \Delta^2 \leq \frac{u_c}{\alpha_{AB}} + 2(t_A t_B)^2 + 2 \sqrt{\frac{u_c}{\alpha_{AB}} + (t_A t_B)^2} (t_A t_B) \quad (\text{C4})$$

This implies that estimating u_c and $t_A t_B$ allows us to estimate the norm distance Δ .

2. Operational interpretation of u_c

Proof. (Of Eqn 26) Using the definition of correlated unitarity,

$$u_c(\mathcal{E}_{AB}) = \alpha_A \alpha_B \left(\text{tr}(T_{AB \rightarrow AB}^\dagger T_{AB \rightarrow AB}) - \text{tr}(T_{A \rightarrow A}^\dagger T_{A \rightarrow A}) \text{tr}(T_{B \rightarrow B}^\dagger T_{B \rightarrow B}) \right) \quad (\text{C5})$$

$$= \alpha_A \alpha_B \left(\sum_{n,m,a,b \neq 0} |\langle \mathbf{X}_n \otimes \mathbf{Y}_m | T_{AB \rightarrow AB} | \mathbf{X}_a \otimes \mathbf{Y}_b \rangle|^2 - |\langle \mathbf{X}_n | T_{A \rightarrow A} | \mathbf{X}_a \rangle|^2 |\langle \mathbf{Y}_m | T_{B \rightarrow B} | \mathbf{Y}_b \rangle|^2 \right) \quad (\text{C6})$$

$$= \alpha_A \alpha_B \left(\sum_{n,m,a,b \neq 0} |\text{tr}(X_n \otimes Y_m \mathcal{E}_{AB}(X_a \otimes Y_b))|^2 - |\text{tr}(X_n \mathcal{E}_A(X_a))|^2 |\text{tr}(Y_m \mathcal{E}_B(Y_b))|^2 \right). \quad (\text{C7})$$

□

3. u_c is invariant under local unitaries

Corollary C.1. *The local subunitarities of any channel $u_{A \rightarrow A}(\mathcal{E})$ & $u_{B \rightarrow B}(\mathcal{E})$ are invariant under local unitaries.*

Proof. From definition $u_c := u_{AB \rightarrow AB} - u_{A \rightarrow A} \cdot u_{B \rightarrow B}$. It is easy to show that each term is invariant under local unitaries.

Firstly, the local subunitarities of any channel $u_{A \rightarrow A}(\mathcal{E})$ & $u_{B \rightarrow B}(\mathcal{E})$ are invariant under local unitaries. This is because from Theorem B.1 we have that $u_{A \rightarrow A}(\mathcal{E}) = u(\mathcal{E}_A)$, therefore sandwiching with any product unitaries $\mathcal{E}' = \mathcal{U}_{1,A} \otimes \mathcal{U}_{1,B} \circ \mathcal{E} \circ \mathcal{U}_{2,A} \otimes \mathcal{U}_{2,B}$ we have $u_{A \rightarrow A}(\mathcal{E}') = u(\mathcal{U}_{1,A} \circ \mathcal{E}_A \circ \mathcal{U}_{2,A})$. From the invariance of unitarity under unitaries [13], $u_{A \rightarrow A}(\mathcal{E}') = u(\mathcal{E}_A)$.

It remains to prove that u_{AB} is invariant. We can write the Liouville representation of any product unitary in the our basis as $\mathbf{U}_{i,A} \otimes \mathbf{U}_{i,B} = (1 \oplus \mathcal{O}_{i,A}) \otimes (1 \oplus \mathcal{O}_{i,B})$ where $\mathcal{O}_{i,X}$ are unitary matrices of dimension $(d_X^2 - 1) \times (d_X^2 - 1)$ obeying $\mathcal{O}_{i,X} \mathcal{O}_{i,X}^\dagger = \mathbb{1}_{T_X}$. Product channels have the additional property that $T_{AB, \mathcal{U}_i} = T_{A, \mathcal{U}_i} \otimes T_{B, \mathcal{U}_i} = \mathcal{O}_{i,A} \otimes \mathcal{O}_{i,B}$.

We define a channel $\mathcal{E}' = \mathcal{U}_{1,A} \otimes \mathcal{U}_{1,B} \circ \mathcal{E} \circ \mathcal{U}_{2,A} \otimes \mathcal{U}_{2,B}$: namely, the channel with product unitaries before and after. The product unitaries will have block diagonal unital blocks which can be seen from considering their only non-zero subunitarities are $u_{A \rightarrow A}$, $u_{B \rightarrow B}$, & $u_{AB \rightarrow AB}$. Because of this simple structure the sub-unital block T_{AB} of \mathcal{E}' is

$$T_{AB, \mathcal{E}'} = T_{AB, \mathcal{U}_1} T_{AB, \mathcal{E}} T_{AB, \mathcal{U}_2} = \mathcal{O}_{1,A} \otimes \mathcal{O}_{1,B} T_{AB, \mathcal{E}} \mathcal{O}_{2,A} \otimes \mathcal{O}_{2,B}. \quad (\text{C8})$$

We can now calculate the required subunitarity $u_{AB}(\mathcal{E}') = \alpha_{AB} \text{tr} \left[T_{AB, \mathcal{E}'}^\dagger T_{AB, \mathcal{E}'} \right]$, and from the cyclical properties of the trace,

$$\begin{aligned} u_{AB}(\mathcal{E}') &= \alpha_{AB} \text{tr} \left[T_{AB, \mathcal{E}}^\dagger T_{AB, \mathcal{E}} \mathcal{O}_{2,A}^\dagger \otimes \mathcal{O}_{2,B}^\dagger \mathcal{O}_{2,A} \otimes \mathcal{O}_{2,B} \right], \\ &= \alpha_{AB} \text{tr} \left[T_{AB, \mathcal{E}}^\dagger T_{AB, \mathcal{E}} \right] = u_{AB}(\mathcal{E}). \end{aligned} \quad (\text{C9})$$

This implies u_c is invariant under local unitaries. □

4. Maximal value of correlated unitarity

It is readily seen that the *SWAP* channel has correlated unitarity,

$$u_c(\text{SWAP}) = 1. \quad (\text{C10})$$

This follows since, from Equation (A7) we have $\text{SWAP} = \sum_{\nu, \mu} |\mathbf{X}_\mu \otimes \mathbf{Y}_\nu\rangle \langle \mathbf{X}_\nu \otimes \mathbf{Y}_\mu|$. In our basis, this makes the unital block T a matrix with 1 along the minor diagonal and zero everywhere else. We can then simply read off that $u_{AB \rightarrow AB} = u_{A \rightarrow B} = u_{B \rightarrow A} = 1$ and all other subunitarities are zero. Correlated unitarity is then $u_c = u_{AB \rightarrow AB} - u_{A \rightarrow A} \cdot u_{B \rightarrow B} = 1$. The following shows the converse, that if the sub-unitarities for $AB \rightarrow AB$, $A \leftrightarrow B$ are maximized then the channel must be a *SWAP* channel, modulo local changes of basis.

Lemma C.1. *Any channel \mathcal{E} with $u_{AB \rightarrow AB}(\mathcal{E}) = u_{A \rightarrow B}(\mathcal{E}) = u_{B \rightarrow A}(\mathcal{E}) = 1$ is equivalent to the *SWAP* channel up to local unitaries.*

Proof. From Theorem II.2 under the given conditions the channel is unitary, and all other subunitarities are zero. We can use that $u_{A \rightarrow B}(\mathcal{E}) = u_{A \rightarrow A}(SWAP \circ \mathcal{E}) = 1$ and similarly $u_{B \rightarrow B}(SWAP \circ \mathcal{E}) = 1$. Since the unitarity equals 1 only for a unitary we deduce that $SWAP \circ \mathcal{E}$ must be a product channel $U_A \otimes U_B$ of local unitaries on each subsystem. Since $SWAP^2 = id$, this implies that $\mathcal{E} = SWAP \circ U_A \otimes U_B$. \square

5. Proof of u_c as Witness of non-separability

The proof of the upper bound on separable channels turns out to be non-trivial, and relies on bounds on the inner product of T -matrices for quantum channels. We first establish basic ingredients we need for the analysis.

Lemma C.2. *For a channel $\mathcal{E} : \mathcal{B}(\mathcal{H}) \rightarrow \mathcal{B}(\mathcal{H}')$ the Choi–Jamiołkowski state can be expressed in the X_ν basis as*

$$\mathcal{J}(\mathcal{E}) = \frac{1}{d} \sum_{\nu=0}^{d^2} \mathcal{E}(X_\nu) \otimes X_\nu^*, \quad (\text{C11})$$

with the complete orthonormal basis of both \mathcal{H} & \mathcal{H}' as $X_\mu = (X_0 = \mathbb{1}/\sqrt{d}, X_i)$ with $\dim(\mathcal{H}) = \dim(\mathcal{H}') = d$.

Proof. $\mathcal{J}(\mathcal{E}) := \mathcal{E} \otimes id(\frac{1}{d} |\mathbf{1}_d\rangle\langle\mathbf{1}_d|)$, but one can directly show $|\mathbf{1}_d\rangle\langle\mathbf{1}_d| = \sum_\nu X_\nu \otimes X_\nu^*$. This follows from the fact that $\text{tr}(X_\nu^\dagger \otimes X_\mu^\dagger |\mathbf{1}_d\rangle\langle\mathbf{1}_d|) = \langle \mathbf{1} | \mathbf{X}_\nu^\dagger \mathbf{X}_\mu^* \rangle = \text{tr} X_\nu^\dagger X_\mu^*$ and therefore $|\mathbf{1}_d\rangle\langle\mathbf{1}_d| = \sum_{\mu,\nu} \text{tr}(X_\nu^\dagger X_\mu^*) X_\nu \otimes X_\mu$. However $\sum_\mu \text{tr}(X_\nu^\dagger X_\mu^*) X_\mu = \sum_\mu \text{tr}(X_\mu^\dagger X_\nu^*) X_\mu = X_\nu^*$ since $\text{tr}(A^T) = \text{tr}(A)$, and the result follows. \square

We now have the following estimates.

Lemma C.3. *Given two channels \mathcal{E}_1 and \mathcal{E}_2 with unital blocks in the Liouville representation T_1 and T_2 , we have*

$$-d \leq \langle T_1, T_2 \rangle \leq d^2 - 1, \quad (\text{C12})$$

where d is the dimension of the Hilbert space.

We shall use this lemma to establish the upper bound on correlated unitarity for separable channels. However, we conjecture a stronger result that for any two quantum channels $\mathcal{E}_1, \mathcal{E}_2$ that $\langle T_1, T_2 \rangle \geq -1$. This, for example implies the bound for optimal inversion of the coherence vector of a quantum state [76, 77] as a special case. The analyse to establish this sharper bound appears to be non-trivial. Since it is not essential to our work we leave it as an open problem. We do, however, establish this lower beyond for a subset of channels (see Lemma C.4 below).

Proof. In the Choi representation we have

$$\mathcal{J}(\mathcal{E}_1) = \frac{1}{d} \sum_{\mu}^{d^2} \mathcal{E}_1(X_\mu) \otimes X_\mu^* \quad \text{and} \quad \mathcal{J}(\mathcal{E}_2) = \frac{1}{d} \sum_{\mu}^{d^2} \mathcal{E}_2(X_\mu) \otimes X_\mu^* \quad (\text{C13})$$

with $X_\mu = (X_0 = \mathbb{1}/\sqrt{d}, X_i)$. Therefore we have that

$$\text{tr}(\mathcal{J}(\mathcal{E}_1)^\dagger \mathcal{J}(\mathcal{E}_2)) = \frac{1}{d^2} \sum_{\mu,\nu}^{d^2} \text{tr}(\mathcal{E}_1(X_\mu)^\dagger \mathcal{E}_2(X_\nu)) \text{tr}(X_\mu^T X_\nu^*). \quad (\text{C14})$$

Since Choi matrices are positive semidefinite, then so is the above quantity. Furthermore, $\text{tr}(X_\mu^T X_\nu^*) = \delta_{\mu\nu}$ and so

$$\text{tr}(\mathcal{J}(\mathcal{E}_1)^\dagger \mathcal{J}(\mathcal{E}_2)) = \frac{1}{d^2} \sum_{\mu}^{d^2} \text{tr}(\mathcal{E}_1(X_\mu)^\dagger \mathcal{E}_2(X_\mu)) \geq 0, \quad (\text{C15})$$

and therefore we have

$$\sum_{\mu}^{d^2} \langle \mathcal{E}_1(\mathbf{X}_\mu) | \mathcal{E}_2(\mathbf{X}_\mu) \rangle = \sum_{\mu}^{d^2} \text{tr}(\mathcal{E}_1(X_\mu)^\dagger \mathcal{E}_2(X_\mu)) \geq 0. \quad (\text{C16})$$

Now we look at $\langle T_1, T_2 \rangle = \text{tr}(T_1^\dagger T_2)$ and expand with respect to same basis.

$$\langle T_1, T_2 \rangle = \sum_{i=1}^{d^2-1} \langle \mathbf{X}_i | T_1^\dagger T_2 | \mathbf{X}_i \rangle = \sum_{i=1}^{d^2-1} \langle \mathcal{E}_1(\mathbf{X}_i) | \mathcal{E}_2(\mathbf{X}_i) \rangle = \sum_{\mu}^{d^2} \langle \mathcal{E}_1(\mathbf{X}_\mu) | \mathcal{E}_2(\mathbf{X}_\mu) \rangle - \langle \mathcal{E}_1(\mathbf{X}_0) | \mathcal{E}_2(\mathbf{X}_0) \rangle. \quad (\text{C17})$$

Then it follows that

$$\langle T_1, T_2 \rangle \geq - \langle \mathcal{E}_1(\mathbf{X}_0) | \mathcal{E}_2(\mathbf{X}_0) \rangle. \quad (\text{C18})$$

However,

$$| \langle \mathcal{E}_1(\mathbf{X}_0) | \mathcal{E}_2(\mathbf{X}_0) \rangle |^2 \leq \langle \mathcal{E}_1(\mathbf{X}_0) | \mathcal{E}_1(\mathbf{X}_0) \rangle \langle \mathcal{E}_2(\mathbf{X}_0) | \mathcal{E}_2(\mathbf{X}_0) \rangle. \quad (\text{C19})$$

and since $\langle \mathcal{E}_i(\frac{\mathbf{1}}{d}) | \mathcal{E}_i(\frac{\mathbf{1}}{d}) \rangle \leq 1$, we deduce that

$$| \left\langle \mathcal{E}_1 \left(\frac{\mathbf{1}}{\sqrt{d}} \right) \middle| \mathcal{E}_2 \left(\frac{\mathbf{1}}{\sqrt{d}} \right) \right\rangle | \leq d, \quad (\text{C20})$$

and so we obtain the lower bound of

$$-d \leq \langle T_1, T_2 \rangle. \quad (\text{C21})$$

The upper bound follows directly from Holder's inequality

$$\langle T_1, T_2 \rangle \leq \|T_1\|_\infty \|T_2\|_1 \leq (d^2 - 1) \quad (\text{C22})$$

where we have used in the above that the eigenvalues of T_1 and T_2 have modulus at most 1, and their rank is at most $d^2 - 1$. \square

We also have the following lower bound on the inner product of two T -matrices for subsets of quantum channels.

Lemma C.4. *Let \mathcal{E}_1 and \mathcal{E}_2 be two quantum channels. If we have that either*

1. *One of the channels is unital,*
2. *The channels are arbitrary $d = 2$ qubit channels,*

then it follows that $-1 \leq \langle T_1, T_2 \rangle \leq d^2 - 1$.

The proof of this is as follows.

Proof. If one of the channels, \mathcal{E}_1 say, is unital then

$$\langle T_1, T_2 \rangle \geq - \langle \mathcal{E}_1(\mathbf{X}_0) | \mathcal{E}_2(\mathbf{X}_0) \rangle = - \langle \mathbf{X}_0 | \mathcal{E}_2(\mathbf{X}_0) \rangle - \langle \mathbf{X}_0 | \mathbf{X}_0 \rangle = -1, \quad (\text{C23})$$

where we use the orthonormality $\langle \mathbf{X}_0 | \mathbf{X}_i \rangle$ for all $i = 1, \dots, d^2 - 1$ and the fact that if \mathcal{E}_1 is unital then $\mathcal{E}_1(\mathbf{X}_0) = \mathbf{X}_0$.

Now suppose that both \mathcal{E}_1 and \mathcal{E}_2 are qubit channels. Given any qubit channel \mathcal{E} , the corresponding Choi state take the form

$$\mathcal{J}(\mathcal{E}) = \frac{1}{4} (\mathbb{1} + \mathbf{x} \cdot \boldsymbol{\sigma} \otimes \mathbb{1} + \sum_{i,j} T_{ij} \sigma_i \otimes \sigma_j), \quad (\text{C24})$$

where $\{\sigma_i\}$ are the Pauli matrices. As shown in [78] it is possible to perform local unitary changes $U_A \otimes U_B$ of basis so that

$$U_A \otimes U_B [\mathcal{J}(\mathcal{E})] = \frac{1}{4} (\mathbb{1} + \mathbf{x} \cdot \boldsymbol{\sigma} \otimes \mathbb{1} + \sum_i t_i \sigma_i \otimes \sigma_i), \quad (\text{C25})$$

and so the channel is described, modulo local choices of basis, by the two vectors \mathbf{x} and $\mathbf{t} = (t_1, t_2, t_3)$. The link between T_{ij} and \mathbf{t} is that $T = O_A \text{diag}(t_1, t_2, t_3) O_B^T$ for orthogonal matrices O_A, O_B corresponding to the local unitary rotations. It can be shown that if $\mathcal{J}(\mathcal{E})$ is a valid quantum state (and so \mathcal{E} a valid quantum channel) the vector \mathbf{x} lies in the Bloch sphere, and \mathbf{t} lies in a particular tetrahedron \mathcal{T} in \mathbb{R}^3 . Moreover, if $\mathbf{x} = \mathbf{0}$ then every $\mathbf{t} \in \mathcal{T}$ corresponds to a valid quantum state. Since \mathbf{x} corresponds to the non-unitality of the quantum channel \mathcal{E} , this implies that if \mathcal{E} is a quantum channel with non-unitality vector \mathbf{x} and T -matrix T then there exists another quantum channel \mathcal{E}_u with the same T -matrix, but which is unital. This implies that for the inner product $\langle T_1, T_2 \rangle$ we can without loss of generality assume that one channel is unital, and thus from the previous part of our proof we obtain $-1 \leq \langle T_1, T_2 \rangle$. The upper bound for $\langle T_1, T_2 \rangle$ is unchanged from the previous lemma. \square

Lemma C.5. For a bipartite separable channel $\mathcal{E} := \sum_i^r p_i \mathcal{E}_{A,i} \otimes \mathcal{E}_{B,i}$ the correlated unitarity $u_c(\mathcal{E})$ can be decomposed as

$$u_c(\mathcal{E}) = \alpha_A \alpha_B \left(\sum_{i,j}^{r,r} p_i p_j \langle T_A^i, T_A^j \rangle \langle T_B^i, T_B^j \rangle - \sum_{i,j}^{r,r} p_i p_j \langle T_A^i, T_A^j \rangle \sum_{m,n}^{r,r} p_m p_n \langle T_B^m, T_B^n \rangle \right) \quad (\text{C26})$$

where T_A^i is the unital block in the Liouville representation of $\mathcal{E}_{A,i}$ and T_B^i is the unital block of $\mathcal{E}_{B,i}$.

Proof. From definition the correlated unitarity is

$$u_c(\mathcal{E}) = \alpha_A \alpha_B (\langle T_{AB \rightarrow AB}, T_{AB \rightarrow AB} \rangle - \langle T_{A \rightarrow A}, T_{A \rightarrow A} \rangle \langle T_{B \rightarrow B}, T_{B \rightarrow B} \rangle). \quad (\text{C27})$$

Since \mathcal{E} is separable, in the Liouville representation linearity implies

$$|\mathcal{E}(\rho)\rangle = \left| \sum_i^r p_i \mathcal{E}_{A,i} \otimes \mathcal{E}_{B,i}(\rho) \right\rangle = \sum_i^r p_i \mathcal{E}_{A,i} \otimes \mathcal{E}_{B,i} |\rho\rangle = \mathcal{E} |\rho\rangle \quad (\text{C28})$$

therefore it follows that the relevant subunital blocks of the channel are simply the weighted sum of the subunital blocks of each product channel:

$$T_{AB \rightarrow AB} = \sum_i^r p_i T_A^i \otimes T_B^i, \quad T_{A \rightarrow A} = \sum_i^r p_i T_A^i, \quad T_{B \rightarrow B} = \sum_i^r p_i T_B^i, \quad (\text{C29})$$

where T_A^i is the unital block in the Liouville representation of $\mathcal{E}_{A,i}$ and T_B^i is the unital block in the Liouville representation of $\mathcal{E}_{B,i}$. Thus the correlated unitarity is

$$\begin{aligned} u_c(\mathcal{E}_{AB}) &= \alpha_A \alpha_B \left(\sum_{i,j}^{r,r} p_i p_j \langle T_A^i \otimes T_B^i, T_A^j \otimes T_B^j \rangle - \sum_{i,j}^{r,r} p_i p_j \langle T_A^i, T_A^j \rangle \sum_{m,n}^{r,r} p_m p_n \langle T_B^m, T_B^n \rangle \right), \\ &= \alpha_A \alpha_B \left(\sum_{i,j}^{r,r} p_i p_j \langle T_A^i, T_A^j \rangle \langle T_B^i, T_B^j \rangle - \sum_{i,j}^{r,r} p_i p_j \langle T_A^i, T_A^j \rangle \sum_{m,n}^{r,r} p_m p_n \langle T_B^m, T_B^n \rangle \right). \end{aligned} \quad (\text{C30})$$

Which completes the proof. \square

Theorem C.1 (Correlated unitarity is a witness of non-separability). Given a bipartite quantum system AB with subsystems A, B of dimensions d_A and d_B respectively we have that

$$u_c(\mathcal{E}_{AB}) \leq C(d_A, d_B) < 1, \quad (\text{C31})$$

where $C(d_A, d_B) \leq \frac{23}{32}$ if $\max(d_A, d_B) = 3$ and $C(d_A, d_B) \leq \frac{7}{12}$ otherwise.

Proof. From Lemma C.5,

$$u_c(\mathcal{E}_{AB}) = \alpha_A \alpha_B \left(\sum_{i,j}^{r,r} p_i p_j \langle T_A^i, T_A^j \rangle \langle T_B^i, T_B^j \rangle - \sum_{i,j}^{r,r} p_i p_j \langle T_A^i, T_A^j \rangle \sum_{m,n}^{r,r} p_m p_n \langle T_B^m, T_B^n \rangle \right) \quad (\text{C32})$$

where T_A^i is the unital block in the Liouville representation of $\mathcal{E}_{A,i}$ and T_B^i is the unital block of $\mathcal{E}_{B,i}$. To simplify notation we label the normalized inner products

$$t_{ij} := \alpha_A \langle T_A^i, T_A^j \rangle \quad \text{and} \quad s_{ij} := \alpha_B \langle T_B^i, T_B^j \rangle, \quad (\text{C33})$$

and define $A := \sum_{i,j}^{r,r} p_i p_j t_{ij}$ and $B := \sum_{i,j}^{r,r} p_i p_j s_{ij}$. In this notation the correlated unitarity of the separable channel is just

$$u_c(\mathcal{E}_{AB}) = \sum_{ij}^{r,r} p_i p_j t_{ij} s_{ij} - AB. \quad (\text{C34})$$

From Lemma C.3 the range of any particular t_{ij} is

$$-\beta_A \leq t_{ij} \leq 1 \quad (\text{C35})$$

where $\beta_A = d_A \alpha_A$ applies to all channels and $\beta_A = \alpha_A$ holds for the case of qubit channels or if one of the channels is unital. Additionally from the non-negativity of the Hilbert Schmidt inner product $t_i \equiv t_{ii} \geq 0$. Similarly for the B subsystem: $-\beta_B \leq s_{ij} \leq 1$ and $s_i \equiv s_{ii} \geq 0$.

We now bound the first term in equation (C34) in relation to the second. Out of the r^2 possible terms in the first term there are r terms that are equal to $p_i^2 t_i s_i$ (namely when $i = j$). Now suppose that out of the $r^2 - r$ remaining terms there are k terms where t_{ij} is negative: t_- , and $r^2 - (r + k)$ other terms where t_{ij} is positive: t_+ . We can then write the correlated unitarity as

$$\begin{aligned} u_c(\mathcal{E}_{AB}) &= \sum_i^r p_i^2 t_i s_i + \sum_{i \neq j}^{r^2-r} p_i p_j t_{ij} s_{ij} - AB, \\ &= \sum_i^r p_i^2 t_i s_i + \sum_{m=(ij), i \neq j}^k p_i p_j t_{-,m} s_m + \sum_{n=(ij), i \neq j}^{r^2-r-k} p_i p_j t_{+,n} s_n - AB, \\ &= \sum_i^r p_i^2 t_i s_i - \sum_{m=(ij), i \neq j}^k p_i p_j |t_{-,m}| s_m + \sum_{n=(ij), i \neq j}^{r^2-r-k} p_i p_j t_{+,n} s_n - AB. \end{aligned} \quad (\text{C36})$$

We now bound the summation of positive and negative $t_{i \neq j}$ terms. As all $t_{-,m} \leq 0$ then since $|t_{-,m}| \leq \beta_A$ we can bound the summation of negative terms as

$$\sum_{m=(ij), i \neq j}^k p_i p_j |t_{-,m}| \leq \sum_{m=(ij), i \neq j}^k \beta_A p_i p_j \leq \sum_{i \neq j}^{r^2-r} \beta_A p_i p_j = \beta_A (1 - \sum_i^r p_i^2) \quad (\text{C37})$$

where we have maximized k to include all $r^2 - r$ possible terms, and used the simple relation that $\sum_i^r p_i^2 + \sum_{i \neq j}^{r^2-r} p_i p_j = 1$. From definition, $A = \sum_i^r p_i^2 t_i + \sum_{i \neq j}^{r^2-r} p_i p_j t_{ij}$ therefore the whole summation of cross terms can be written as

$$\sum_{i \neq j}^{r^2-r} p_i p_j t_{ij} = \sum_{n=(ij), i \neq j}^{r^2-r-k} p_i p_j t_{+,n} - \sum_{m=(ij), i \neq j}^k p_i p_j |t_{-,m}| = A - \sum_i^r p_i^2 t_i. \quad (\text{C38})$$

From this we can bound the summation of the positive terms using the previous bound in eqn. (C37):

$$\begin{aligned} \sum_{n=(ij), i \neq j}^{r^2-r-k} p_i p_j t_{+,n} &= A - \sum_i^r p_i^2 t_i + \sum_{m=(ij), i \neq j}^k p_i p_j |t_{-,m}|, \\ \sum_{n=(ij), i \neq j}^{r^2-r} p_i p_j t_{+,n} &\leq A - \sum_i^r p_i^2 t_i + \beta_A (1 - \sum_i^r p_i^2). \end{aligned} \quad (\text{C39})$$

Since both $t_{+,n} \geq 0$ and $|t_{-,m}| \geq 0$ and all elements $-\min(\beta_B, \sqrt{s_i s_j}) \leq s_{i \neq j} \leq \sqrt{s_i s_j} \leq 1$, then we can bound the summation containing $t_{+,n} s_n$ elements as

$$\sum_{n=(ij), i \neq j}^{r^2-r-k} p_i p_j t_{+,n} s_n \leq \sum_{n=(ij), i \neq j}^{r^2-r-k} p_i p_j t_{+,n} \leq A - \sum_i^r p_i^2 t_i + \beta_A (1 - \sum_i^r p_i^2) \quad (\text{C40})$$

and the summation containing $t_{-,m} s_m$ elements (assuming $\sqrt{s_i s_j} \geq \beta_B$)

$$- \sum_{m=(ij), i \neq j}^k p_i p_j |t_{-,m}| s_m \leq \beta_B \sum_{m=(ij), i \neq j}^k p_i p_j |t_{-,m}| \leq \beta_B (\beta_A (1 - \sum_i^r p_i^2)). \quad (\text{C41})$$

Putting all this together we get a bound on the correlated unitarity of

$$\begin{aligned} u_c(\mathcal{E}_{AB}) &\leq \sum_i^r p_i^2 t_i s_i + \beta_B (\beta_A (1 - \sum_i^r p_i^2)) + A - \sum_i^r p_i^2 t_i + \beta_A (1 - \sum_i^r p_i^2) - AB, \\ &\leq \sum_i^r p_i^2 t_i (s_i - 1) + \beta_A (1 + \beta_B) (1 - \sum_i^r p_i^2) + A(1 - B). \end{aligned} \quad (\text{C42})$$

With no loss of generality we can set $A \leq B$ as A and B are interchangeable. Therefore we have that $A(1 - B) \leq B(1 - B)$. As $0 \leq B \leq 1$, this is maximized when $B = 1/2$. Additionally as $s_i \leq 1$ then $s_i - 1 \leq 0$ and the whole first term is negative. Therefore

$$u_c(\mathcal{E}_{AB}) \leq \beta_A(1 + \beta_B)(1 - \sum_i^r p_i^2) + \frac{1}{4}. \quad (\text{C43})$$

Further from the Cauchy-Schwartz inequality $\sum_i^r p_i^2 \geq \frac{1}{r} \geq \frac{1}{\min(d_A^2, d_B^2)}$ so expanding the dimensional constants we get that

$$u_c(\mathcal{E}_{AB}) \leq \frac{d_A}{d_A^2 - 1} \left(1 + \frac{d_B}{d_B^2 - 1}\right) \left(1 - \frac{1}{\min(d_A^2, d_B^2)}\right) + \frac{1}{4}. \quad (\text{C44})$$

Without loss of generality we can take $d_A \geq d_B$, reducing the inequality to:

$$u_c(\mathcal{E}_{AB}) \leq \frac{d_A}{d_A^2 - 1} \left(\frac{d_B^2 - 1 + d_B}{d_B^2}\right) + \frac{1}{4}. \quad (\text{C45})$$

If $d_A \geq 4$ then we find an upper bound of

$$u_c(\mathcal{E}_{AB}) \leq \frac{4}{15} \left(\frac{d_B^2 - 1 + d_B}{d_B^2}\right) + \frac{1}{4} \leq \frac{4}{15} \cdot \frac{5}{4} + \frac{1}{4} = \frac{1}{3} + \frac{1}{4} = \frac{7}{12}. \quad (\text{C46})$$

For $d_A = 3$, we have

$$u_c(\mathcal{E}_{AB}) \leq \frac{3}{8} \left(\frac{d_B^2 - 1 + d_B}{d_B^2}\right) + \frac{1}{4} \leq \frac{3}{8} \cdot \frac{5}{4} + \frac{1}{4} = \frac{15}{32} + \frac{1}{4} = \frac{23}{32}. \quad (\text{C47})$$

For the final case $d_A = d_B = 2$ we make use of the tighter lower bound of $-1 \leq \langle T_1, T_2 \rangle$ from Lemma C.4, and so the analysis proceeds as before, but replacing β_A with α_A . Doing this we find that

$$u_c(\mathcal{E}_{AB}) \leq \frac{d_B^2}{(d_A^2 - 1)(d_B^2 - 1)} \left(1 - \frac{1}{d_B^2}\right) + \frac{1}{4} = \frac{1}{3} + \frac{1}{4} = \frac{7}{12}. \quad (\text{C48})$$

This completes the proof. \square

Appendix D: Analysis of local independent twirls on A and B

1. Definition of subspace projectors

Lemma D.1. *The operator*

$$P := \int d\mu_{\text{Haar}}(U) \mathcal{U}^{\otimes 2} = \int d\mu_{\text{Haar}}(U) (U \otimes U^*)^{\otimes 2}, \quad (\text{D1})$$

on $\mathcal{H}^{\otimes 4} = V \oplus V^\perp$ is a projector into the subspace $V = \text{span}(|\mathbf{1}^{\otimes 2}\rangle, |\mathbf{F}\rangle)$, where \mathbf{F} is the Flip operator on the sub-systems, and therefore $P = 0$ on V^\perp .

Proof. (Of Lemma D.1) For any group G with an invariant measure (i.e. finite or compact) and a representation V , the averaging over all elements of the group gives a projector,

$$P = \int V(g) dg, \quad (\text{D2})$$

onto the invariant subspace $\{|\psi\rangle : V(g)|\psi\rangle = |\psi\rangle \forall g \in G\}$. To find the invariant subspace for $V(U) = (U \otimes U^*)^{\otimes 2}$ it is easier to look at $V'(U) = U \otimes U \otimes U^* \otimes U^*$. According to the definition of the invariant subspace, we must find X such that

$$V'(U) |X\rangle = |X\rangle, \quad (\text{D3})$$

or equivalently $[X, U \otimes U] = 0$.

We can decompose $U \otimes U$ into irreducible representations of $U(d)$. There are 2 of them: the symmetric subspace and the alternating subspace. This is related to the fact that symmetric group on two elements has two irreducible representations: the trivial one ($\mathbb{1}$) and the alternating one (\mathbb{F}).

Using Schur's lemma [79] the operator X must be a multiple of the identity when restricted to either of these two subspaces. Putting everything together, (up to reordering of spaces) the invariant subspace is spanned by $|\mathbf{1}^{\otimes 2}\rangle$ and $|\mathbb{F}\rangle$. \square

Lemma D.2. *A normalized basis for the invariant vector space $V = \text{span}(|\mathbf{1}^{\otimes 2}\rangle, |\mathbb{F}\rangle)$ is given by*

$$\begin{aligned} |0\rangle &= |\mathbf{X}_0\rangle \otimes |\mathbf{X}_0\rangle, \\ |1\rangle &= \frac{1}{\sqrt{d^2-1}} \sum_{k=1}^{d^2-1} |\mathbf{X}_k\rangle \otimes |\mathbf{X}_k^\dagger\rangle, \end{aligned} \quad (\text{D4})$$

where $X_\mu = (X_0 = \mathbf{1}/\sqrt{d}, X_i)$.

Proof. We defined the tensor product of two vectorized matrices as:

$$|\mathbf{A} \otimes \mathbf{B}\rangle := |\mathbf{A}\rangle \otimes |\mathbf{B}\rangle, \quad (\text{D5})$$

Applying this definition to the 1st vector that spans the space $|\mathbf{1}^{\otimes 2}\rangle = |\mathbf{1}\rangle \otimes |\mathbf{1}\rangle = d |\mathbf{X}_0\rangle \otimes |\mathbf{X}_0\rangle$. Normalizing, the first eigenvector is therefore $|0\rangle := |\mathbf{X}_0\rangle \otimes |\mathbf{X}_0\rangle$.

The Flip operator in our basis is given by considering the permutation of computational basis states:

$$\mathbb{F} := \sum_{i,j}^{d,d} |j\rangle\langle i| \otimes |i\rangle\langle j| = \sum_{i,j}^{d,d} |j\rangle\langle i| \otimes (|j\rangle\langle i|)^\dagger = \sum_{\mu}^{d^2} X_\mu \otimes X_\mu^\dagger \quad (\text{D6})$$

up to a dimensional factor. Therefore $|\mathbb{F}\rangle = \sum_{\mu=0}^{d^2-1} |\mathbf{X}_\mu\rangle \otimes |\mathbf{X}_\mu^\dagger\rangle$. From inspection the 2nd normalized eigenvector that spans this subspace is

$$|1\rangle = \frac{1}{\sqrt{d^2-1}} \sum_{k=1}^{d^2-1} |\mathbf{X}_k\rangle \otimes |\mathbf{X}_k^\dagger\rangle. \quad (\text{D7})$$

\square

We can now write the decomposition of the projector $P := |0\rangle\langle 0| + |1\rangle\langle 1|$ as

$$P = |\mathbf{X}_0\rangle\langle \mathbf{X}_0| \otimes |\mathbf{X}_0\rangle\langle \mathbf{X}_0| + \frac{1}{d^2-1} \sum_{i,j}^{d^2-1} |\mathbf{X}_i\rangle\langle \mathbf{X}_j| \otimes |\mathbf{X}_i^\dagger\rangle\langle \mathbf{X}_j^\dagger|. \quad (\text{D8})$$

Definition D.1. *The projector*

$$P_{AB} := \int d\mu_{\text{Haar}}(U_A) \int d\mu_{\text{Haar}}(U_B) (\mathbf{U}_A \otimes \mathbf{U}_B)^{\otimes 2}, \quad (\text{D9})$$

for the tensor product of two copies of a bipartite system with subsystems A & B .

Since the integrals are independent, it is readily seen that,

$$P_{AB} = P_A \otimes P_B = \sum_{i,j} |ij\rangle\langle ij| \quad (\text{D10})$$

where P_A is the projector P on subsystem A , and similarly for B . We can now calculate the action of the projector P_{AB} on two copies of the Liouville representation of a bipartite channel $P_{AB} \mathcal{E}^{\otimes 2} P_{AB}$.

2. Calculation of elements of $P_{AB}\mathcal{E}^{\otimes 2}P_{AB}$ & the matrix of sub-unitarities \mathcal{S} .

We now show that the operator $P_{AB}\mathcal{E}^{\otimes 2}P_{AB}$ can be viewed as encoding the quadratic order invariants of the quantum channel, and in particular the traceless components form a 3×3 matrix of sub-unitarities \mathcal{S} for the bipartite quantum channel. A basis of four eigenvectors of P_{AB} can be written in the basis $(|\mathbf{X}_\mu\rangle \otimes |\mathbf{Y}_\nu\rangle)^{\otimes 2}$ to match the order of the subspaces of $\mathcal{E}^{\otimes 2}$. This gives

$$\begin{aligned}
|00\rangle &= |\mathbf{X}_0\rangle \otimes |\mathbf{Y}_0\rangle \otimes |\mathbf{X}_0\rangle \otimes |\mathbf{Y}_0\rangle, \\
|10\rangle &= \sqrt{\alpha_A} \sum_{n=1}^{d_A^2-1} |\mathbf{X}_n\rangle \otimes |\mathbf{Y}_0\rangle \otimes |\mathbf{X}_n^\dagger\rangle \otimes |\mathbf{Y}_0\rangle, \\
|01\rangle &= \sqrt{\alpha_B} \sum_{m=1}^{d_B^2-1} |\mathbf{X}_0\rangle \otimes |\mathbf{Y}_m\rangle \otimes |\mathbf{X}_0\rangle \otimes |\mathbf{Y}_m^\dagger\rangle, \\
|11\rangle &= \sqrt{\alpha_A\alpha_B} \sum_{n,m=1}^{d_A^2-1, d_B^2-1} |\mathbf{X}_n\rangle \otimes |\mathbf{Y}_m\rangle \otimes |\mathbf{X}_n^\dagger\rangle \otimes |\mathbf{Y}_m^\dagger\rangle,
\end{aligned} \tag{D11}$$

where $\alpha_i = 1/(d_i^2 - 1)$. We can now calculate the matrix elements of $P_{AB}\mathcal{E}^{\otimes 2}P_{AB}$ in this basis. Firstly, for each subsystem, as the $\mu = 0$ elements are proportional to the identity we have $X_0^\dagger = X_0$ & $Y_0^\dagger = Y_0$. Secondly, as the channel \mathcal{E} is a CPTP map, we have that $\mathcal{E}((X_\mu \otimes Y_\nu)^\dagger) = (\mathcal{E}(X_\mu \otimes Y_\nu))^\dagger$ for any elements of the basis, and so

$$\begin{aligned}
\langle \mathbf{X}_\mu^\dagger \otimes \mathbf{Y}_\nu^\dagger | \mathcal{E} | \mathbf{X}_\sigma^\dagger \otimes \mathbf{Y}_\omega^\dagger \rangle &= \langle \mathbf{X}_\mu^\dagger \otimes \mathbf{Y}_\nu^\dagger | \mathcal{E}(\mathbf{X}_\sigma^\dagger \otimes \mathbf{Y}_\omega^\dagger) \rangle, \\
&= \text{tr}[(X_\mu^\dagger \otimes Y_\nu^\dagger)^\dagger \mathcal{E}(X_\sigma^\dagger \otimes Y_\omega^\dagger)], \\
&= \text{tr}[\mathcal{E}(X_\sigma^\dagger \otimes Y_\omega^\dagger) X_\mu \otimes Y_\nu], \\
&= \text{tr}[\mathcal{E}(X_\sigma \otimes Y_\omega)^\dagger X_\mu \otimes Y_\nu], \\
&= \langle \mathcal{E}(X_\sigma \otimes Y_\omega) | \mathbf{X}_\mu \otimes \mathbf{Y}_\nu \rangle, \\
&= \langle \mathbf{X}_\sigma \otimes \mathbf{Y}_\omega | \mathcal{E}^\dagger | \mathbf{X}_\mu \otimes \mathbf{Y}_\nu \rangle,
\end{aligned} \tag{D12}$$

where \mathcal{E}^\dagger corresponds to the adjoint of \mathcal{E} that is defined via $\text{tr}(A\mathcal{E}(B)) = \text{tr}(\mathcal{E}^\dagger(A)B)$. Furthermore note that if the non-unital block of \mathcal{E} is T , then the non-unital block of \mathcal{E}^\dagger is T^\dagger .

We can now calculate the 16 possible combinations $\langle a | \mathcal{E}^{\otimes 2} | b \rangle$. One element is simply equivalent to the trace preserving property of a quantum channel $\langle 00 | \mathcal{E}^{\otimes 2} | 00 \rangle = (\text{tr}[\frac{1}{\sqrt{d}} \mathcal{E}(\frac{1}{\sqrt{d}})])^2 = 1$. The remaining elements can be divided into 3 sub-blocks to be defined

$$P_{AB}\mathcal{E}^{\otimes 2}P_{AB} = \begin{matrix} & |00\rangle & |ij\rangle \\ \langle 00| & 1 & \mathbf{0} \\ \langle ij| & \mathbf{x} & \mathcal{S} \end{matrix} \text{ where } ij \in \{01, 10, 11\}. \tag{D13}$$

Consider a diagonal $\langle 10 | \mathcal{E}^{\otimes 2} | 10 \rangle$ element in the matrix \mathcal{S} , from the above properties it follows that

$$\begin{aligned}
\langle 10 | \mathcal{E}^{\otimes 2} | 10 \rangle &= \alpha_A \sum_{i,j=1}^{d_A^2-1} \langle \mathbf{X}_i | \otimes \langle \mathbf{Y}_0 | \mathcal{E} | \mathbf{X}_j \rangle \otimes |\mathbf{Y}_0\rangle \langle \mathbf{X}_i^\dagger | \otimes \langle \mathbf{Y}_0 | \mathcal{E} | \mathbf{X}_j^\dagger \rangle \otimes |\mathbf{Y}_0\rangle, \\
&= \alpha_A \sum_{i,j=1}^{d_A^2-1} \langle \mathbf{X}_i \otimes \mathbf{Y}_0 | \mathcal{E} | \mathbf{X}_j \otimes \mathbf{Y}_0 \rangle \langle \mathbf{X}_j \otimes \mathbf{Y}_0 | \mathcal{E}^\dagger | \mathbf{X}_i \otimes \mathbf{Y}_0 \rangle, \\
&= \alpha_A \text{tr}[T_{A \rightarrow A} T_{A \rightarrow A}^\dagger] = \alpha_A \text{tr}[T_{A \rightarrow A}^\dagger T_{A \rightarrow A}] = u_{A \rightarrow A}(\mathcal{E}).
\end{aligned} \tag{D14}$$

and similarly $\langle 01 | \mathcal{E}^{\otimes 2} | 01 \rangle = u_{B \rightarrow B}(\mathcal{E})$ & $\langle 11 | \mathcal{E}^{\otimes 2} | 11 \rangle = u_{AB \rightarrow AB}(\mathcal{E})$. Off diagonal elements in A can be calculated with an additional dimensional factor. For example, following the same line

$$\begin{aligned}
\langle 01 | \mathcal{E}^{\otimes 2} | 10 \rangle &= \sqrt{\alpha_A\alpha_B} \sum_{i,j=1}^{(d_B^2-1)(d_A^2-1)} \langle \mathbf{X}_0 \otimes \mathbf{Y}_i | \mathcal{E} | \mathbf{X}_j \otimes \mathbf{Y}_0 \rangle \langle \mathbf{X}_j \otimes \mathbf{Y}_0 | \mathcal{E}^\dagger | \mathbf{X}_0 \otimes \mathbf{Y}_i \rangle, \\
&= \sqrt{\alpha_A\alpha_B} \text{tr}[T_{A \rightarrow B} T_{A \rightarrow B}^\dagger] = \sqrt{\frac{\alpha_B}{\alpha_A}} u_{A \rightarrow B}(\mathcal{E}).
\end{aligned} \tag{D15}$$

Further we have elements such as

$$\begin{aligned} \langle 11 | \mathcal{E}^{\otimes 2} | 10 \rangle &= \alpha_A \sqrt{\alpha_B} \sum_{k,j,n=1}^{(d_A^2-1)(d_B^2-1)} \langle \mathbf{X}_j \otimes \mathbf{Y}_n | \mathcal{E} | \mathbf{X}_k \otimes \mathbf{Y}_0 \rangle \langle \mathbf{X}_k \otimes \mathbf{Y}_0 | \mathcal{E}^\dagger | \mathbf{X}_j \otimes \mathbf{Y}_n \rangle, \\ &= \alpha_A \sqrt{\alpha_B} \text{tr} \left[T_{A \rightarrow AB}^\dagger T_{A \rightarrow AB} \right] = \sqrt{\alpha_B} u_{A \rightarrow AB}(\mathcal{E}) \end{aligned} \quad (\text{D16})$$

and $\langle 10 | \mathcal{E}^{\otimes 2} | 11 \rangle = \alpha_A \sqrt{\alpha_B} \text{tr} \left[T_{AB \rightarrow A}^\dagger T_{AB \rightarrow A} \right] = \frac{1}{\sqrt{\alpha_B}} u_{AB \rightarrow A}(\mathcal{E})$. The remaining elements of S can be found by swapping the labeling of the subsystems. Putting this together we have the matrix of sub-unitarities given by,

$$S = \begin{array}{c} \langle 10 | \\ \langle 11 | \\ \langle 01 | \end{array} \begin{array}{ccc} |10\rangle & |11\rangle & |01\rangle \\ \left(\begin{array}{ccc} u_{A \rightarrow A}(\mathcal{E}) & \frac{1}{\sqrt{\alpha_B}} u_{AB \rightarrow A}(\mathcal{E}) & \sqrt{\frac{\alpha_A}{\alpha_B}} u_{B \rightarrow A}(\mathcal{E}) \\ \sqrt{\alpha_B} u_{A \rightarrow AB}(\mathcal{E}) & u_{AB \rightarrow AB}(\mathcal{E}) & \sqrt{\alpha_A} u_{B \rightarrow AB}(\mathcal{E}) \\ \sqrt{\frac{\alpha_B}{\alpha_A}} u_{A \rightarrow B}(\mathcal{E}) & \frac{1}{\sqrt{\alpha_A}} u_{AB \rightarrow B}(\mathcal{E}) & u_{B \rightarrow B}(\mathcal{E}) \end{array} \right) \end{array}. \quad (\text{D17})$$

The three elements $\langle ij | \mathcal{E}^{\otimes 2} | 00 \rangle$ with $ij \in \{01, 10, 11\}$ quantify the non-unitality of the channel for each subsystem to quadratic order, through the H-S inner product of the generalized Bloch vector \mathbf{x} for each subsystem. We can define $x_i := \mathbf{x}_{i \rightarrow i}^\dagger \mathbf{x}_{i \rightarrow i}$. Therefore we have

$$\begin{aligned} \langle 10 | \mathcal{E}^{\otimes 2} | 00 \rangle &= \sqrt{\alpha_A} \sum_{i=1}^{d_A^2-1} \langle \mathbf{X}_i \otimes \mathbf{Y}_0 | \mathcal{E} | \mathbf{X}_0 \otimes \mathbf{Y}_0 \rangle \langle \mathbf{X}_0 \otimes \mathbf{Y}_0 | \mathcal{E}^\dagger | \mathbf{X}_i \otimes \mathbf{Y}_0 \rangle, \\ &= \sqrt{\alpha_A} \mathbf{x}_{A \rightarrow A}^\dagger \mathbf{x}_{A \rightarrow A} = \sqrt{\alpha_A} x_A, \end{aligned} \quad (\text{D18})$$

similarly $\langle 11 | \mathcal{E}^{\otimes 2} | 00 \rangle = \sqrt{\alpha_A \alpha_B} x_{AB}$, $\langle 01 | \mathcal{E}^{\otimes 2} | 00 \rangle = \sqrt{\alpha_B} x_B$. Therefore $\mathbf{x}^T = (\sqrt{\alpha_A} x_A, \sqrt{\alpha_A \alpha_B} x_{AB}, \sqrt{\alpha_B} x_B)$.

The final three elements $\langle 00 | \mathcal{E}^{\otimes 2} | ij \rangle$ with $ij \in \{01, 10, 11\}$ are required to be zero from the trace preserving properties of a quantum channel. For example, considering $\langle 00 | \mathcal{E}^{\otimes 2} | 10 \rangle$ for \mathcal{E} to be a valid TP map we must have $\langle \mathbf{X}_0 \otimes \mathbf{Y}_0 | \mathcal{E} | \mathbf{X}_i \otimes \mathbf{Y}_0 \rangle = 0$ for all i . Therefore

$$\langle 00 | \mathcal{E}^{\otimes 2} | 10 \rangle = \sqrt{\alpha_A} \sum_{i=1}^{d_A^2-1} \langle \mathbf{X}_0 \otimes \mathbf{Y}_0 | \mathcal{E} | \mathbf{X}_i \otimes \mathbf{Y}_0 \rangle \langle \mathbf{X}_i \otimes \mathbf{Y}_0 | \mathcal{E}^\dagger | \mathbf{X}_0 \otimes \mathbf{Y}_0 \rangle = 0. \quad (\text{D19})$$

Through the same argument $\langle 00 | \mathcal{E}^{\otimes 2} | 01 \rangle = \langle 00 | \mathcal{E}^{\otimes 2} | 11 \rangle = 0$.

Finally, putting all elements together we have,

$$P_{AB} \mathcal{E}^{\otimes 2} P_{AB} = \begin{array}{c} \langle 00 | \\ \langle 10 | \\ \langle 11 | \\ \langle 01 | \end{array} \begin{array}{cccc} |00\rangle & |10\rangle & |11\rangle & |01\rangle \\ \left(\begin{array}{cccc} 1 & 0 & 0 & 0 \\ \sqrt{\alpha_A} x_A & u_{A \rightarrow A}(\mathcal{E}) & \frac{1}{\sqrt{\alpha_B}} u_{AB \rightarrow A}(\mathcal{E}) & \sqrt{\frac{\alpha_A}{\alpha_B}} u_{B \rightarrow A}(\mathcal{E}) \\ \sqrt{\alpha_A \alpha_B} x_{AB} & \sqrt{\alpha_B} u_{A \rightarrow AB}(\mathcal{E}) & u_{AB \rightarrow AB}(\mathcal{E}) & \sqrt{\alpha_A} u_{B \rightarrow AB}(\mathcal{E}) \\ \sqrt{\alpha_B} x_B & \sqrt{\frac{\alpha_B}{\alpha_A}} u_{A \rightarrow B}(\mathcal{E}) & \frac{1}{\sqrt{\alpha_A}} u_{AB \rightarrow B}(\mathcal{E}) & u_{B \rightarrow B}(\mathcal{E}) \end{array} \right) \end{array}. \quad (\text{D20})$$

Comparing this with decomposition of the Liouville representation of a bipartite channel \mathcal{E} in eqn. (16), we see that P_{AB} produces the normalized purity of every sub-block of \mathcal{E} . As sub-unitarities are the normalized purity of sub-blocks of the unital block T , these values are extracted, as well as the absolute value of the non-unital vector for both sub-systems. Using the form of the top row of $P_{AB} \mathcal{E}^{\otimes 2} P_{AB}$, it is easily seen that

$$\det(P_{AB} \mathcal{E}^{\otimes 2} P_{AB} - \lambda \mathbb{1}) = (1 - \lambda) \det(S - \lambda \mathbb{1}) \quad (\text{D21})$$

and therefore for any channel \mathcal{E} the 4 eigenvalues of $P_{AB} \mathcal{E}^{\otimes 2} P_{AB}$ will be $\lambda_0 = 1$ and the 3 eigenvalues of S .

3. The matrix components for separable channels

For a product channel $\mathcal{E} = \mathcal{E}_A \otimes \mathcal{E}_B$ the sub-unitarity matrix S takes a particularly simple form. Since the channel is separable coherent information does not flow between A and B and Theorem B.3 tells us that $u_{A \rightarrow B}(\mathcal{E}_A \otimes \mathcal{E}_B) =$

$u_{B \rightarrow A}(\mathcal{E}_A \otimes \mathcal{E}_B) = 0$ and $u_{AB \rightarrow AB}(\mathcal{E}_A \otimes \mathcal{E}_B) = u_{A \rightarrow A}(\mathcal{E}_A \otimes \mathcal{E}_B) \cdot u_{B \rightarrow B}(\mathcal{E}_A \otimes \mathcal{E}_B)$. Thus, for a product channel $\mathcal{E} = \mathcal{E}_A \otimes \mathcal{E}_B$

$$P_{AB} \mathcal{E}^{\otimes 2} P_{AB} = \begin{array}{c} \langle 00| \\ \langle 10| \\ \langle 11| \\ \langle 01| \end{array} \begin{pmatrix} |00\rangle & |10\rangle & |11\rangle & |01\rangle \\ \hline 1 & 0 & 0 & 0 \\ \sqrt{\alpha_A} x_A & u(\mathcal{E}_A) & 0 & 0 \\ \sqrt{\alpha_A \alpha_B} x_A x_B & \sqrt{\alpha_B} u(\mathcal{E}_A) x_B & u(\mathcal{E}_A) u(\mathcal{E}_B) & \sqrt{\alpha_A} u(\mathcal{E}_B) x_A \\ \sqrt{\alpha_B} x_B & 0 & 0 & u(\mathcal{E}_B) \end{pmatrix}. \quad (\text{D22})$$

From this it is readily seen that the eigenvalues for a product channel are $\{1, u(\mathcal{E}_A), u(\mathcal{E}_B), u(\mathcal{E}_A)u(\mathcal{E}_B)\}$. More generally, for the case of a *separable* channel \mathcal{E}_{AB} from Lemmas B.5 & B.6 we find instead that

$$P_{AB} \mathcal{E}^{\otimes 2} P_{AB} = \begin{array}{c} \langle 00| \\ \langle 10| \\ \langle 11| \\ \langle 01| \end{array} \begin{pmatrix} |00\rangle & |10\rangle & |11\rangle & |01\rangle \\ \hline 1 & 0 & 0 & 0 \\ \sqrt{\alpha_A} x_A & u_{A \rightarrow A}(\mathcal{E}_{AB}) & 0 & 0 \\ \sqrt{\alpha_A \alpha_B} x_{AB} & \sqrt{\alpha_B} u_{A \rightarrow AB}(\mathcal{E}_{AB}) & u_{AB \rightarrow AB}(\mathcal{E}_{AB}) & \sqrt{\alpha_A} u_{B \rightarrow AB}(\mathcal{E}_{AB}) \\ \sqrt{\alpha_B} x_B & 0 & 0 & u_{B \rightarrow B}(\mathcal{E}_{AB}) \end{pmatrix}. \quad (\text{D23})$$

and so now the eigenvalues are $\{1, u_{A \rightarrow A}(\mathcal{E}_{AB}), u_{B \rightarrow B}(\mathcal{E}_{AB}), u_{AB \rightarrow AB}(\mathcal{E}_{AB})\}$. Therefore $(P_{AB} \mathcal{E}^{\otimes 2} P_{AB})^m$, will have eigenvalues

$$\{\lambda_i\} = \{1, u_{A \rightarrow A}(\mathcal{E}_{AB})^m, u_{B \rightarrow B}(\mathcal{E}_{AB})^m, u_{AB \rightarrow AB}(\mathcal{E}_{AB})^m\}, \quad (\text{D24})$$

which implies that the sub-unitarities are the decay constants for the benchmarking protocol.

More generally we do not have such a simple link between the eigenvalues and sub-unitarities. Indeed, it may be the case that the matrix cannot be diagonalized fully, and so one must instead use a Jordan decomposition to determine the decay law for the protocol. We provide the details for the fully general case in the next section.

4. Jordan decomposition for arbitrary bipartite channels

For a general bipartite channel \mathcal{E} we can use the Jordan normal form of the matrix $P_{AB} \mathcal{E}^{\otimes 2} P_{AB}$ to study the structure scales with a power, $(P_{AB} \mathcal{E}^{\otimes 2} P_{AB})^m$.

Definition D.2. Using the Jordan matrix decomposition of any square matrix M , we can find the Jordan normal form such that

$$M = S^{-1} J S, \quad (\text{D25})$$

where S is a invertible matrix, and J is a block diagonal matrix of Jordan blocks [60].

Corollary D.1. The Jordan matrix decomposition of a square matrix M to the power n follows

$$M^n = S^{-1} J^n S. \quad (\text{D26})$$

Proof. This follows simply from $S S^{-1} = \mathbf{1}$. □

This implies that if write $P_{AB} \mathcal{E}^{\otimes 2} P_{AB}$, in a Jordan normal form, J , then the decay law of $(P_{AB} \mathcal{E}^{\otimes 2} P_{AB})^m$ will be determined entirely by J^m . There are 3 possibilities that could occur:

$$J = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \lambda_1 & 0 & 0 \\ 0 & 0 & \lambda_3 & 0 \\ 0 & 0 & 0 & \lambda_2 \end{pmatrix}, \quad J = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \lambda_1 & 1 & 0 \\ 0 & 0 & \lambda_1 & 0 \\ 0 & 0 & 0 & \lambda_2 \end{pmatrix}, \quad J = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \lambda_1 & 1 & 0 \\ 0 & 0 & \lambda_1 & 1 \\ 0 & 0 & 0 & \lambda_1 \end{pmatrix}, \quad (\text{D27})$$

where λ_i are the eigenvalues of the block S . Which form the Jordan decomposition takes depends on the degeneracy of λ_i and whether the geometric and algebraic multiplicities of each λ_i coincide [60].

For J diagonal, we have that

$$(P_{AB} \mathcal{E}^{\otimes 2} P_{AB})^m = S^{-1} J^m S = S^{-1} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \lambda_1^m & 0 & 0 \\ 0 & 0 & \lambda_3^m & 0 \\ 0 & 0 & 0 & \lambda_2^m \end{pmatrix} S, \quad (\text{D28})$$

where $\{\lambda_i\}$ are the eigenvalues of \mathcal{S} . Therefore,

$$(P_{AB}\mathcal{E}^{\otimes 2}P_{AB})^m = S^{-1}(|00\rangle\langle 00| + \lambda_1^m |10\rangle\langle 10| + \lambda_2^m |01\rangle\langle 01| + \lambda_3^m |11\rangle\langle 11|)S. \quad (\text{D29})$$

If the Jordan decomposition of $P_{AB}\mathcal{E}^{\otimes 2}P_{AB}$ is not completely diagonal, then $(P_{AB}\mathcal{E}^{\otimes 2}P_{AB})^m$ still scales with the eigenvalues of \mathcal{S} but in a slightly more complex manner. From above, the 2 remaining options are

$$(P_{AB}\mathcal{E}^{\otimes 2}P_{AB})^m = S^{-1} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \lambda_1 & 1 & 0 \\ 0 & 0 & \lambda_1 & 0 \\ 0 & 0 & 0 & \lambda_2 \end{pmatrix}^m S = S^{-1} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \lambda_1^m & m\lambda_1^{m-1} & 0 \\ 0 & 0 & \lambda_1^m & 0 \\ 0 & 0 & 0 & \lambda_2^m \end{pmatrix} S, \quad (\text{D30})$$

and

$$(P_{AB}\mathcal{E}^{\otimes 2}P_{AB})^m = S^{-1} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \lambda_1 & 1 & 0 \\ 0 & 0 & \lambda_1 & 1 \\ 0 & 0 & 0 & \lambda_1 \end{pmatrix}^m S = S^{-1} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \lambda_1^m & \lambda_1^{m-1} & \frac{m(m-1)}{2}\lambda_1^{m-2} \\ 0 & 0 & \lambda_1^m & \lambda_1^{m-1} \\ 0 & 0 & 0 & \lambda_1^m \end{pmatrix} S. \quad (\text{D31})$$

Therefore, in this more general scenario the decay law behaviour of $(P_{AB}\mathcal{E}^{\otimes 2}P_{AB})^m$ is still described by the constants $\{\lambda_i\}$.

5. Analysis of the $\mathcal{C} \times \mathcal{C}$ unitarity benchmarking protocol

We now show that the unitarity benchmarking protocol detailed in Protocol 1 generates the claimed decay law for the noise channel associated to the gate-set Γ_{AB} .

Lemma D.3. *Over all sequences s , and for a gate-independent noise channel \mathcal{E} , the expectation value of a observable M squared can be written as:*

$$\mathbb{E}_s[m(s)^2] = \langle \mathbf{M} |^{\otimes 2} (P_{AB}\mathcal{E}^{\otimes 2}P_{AB})^{k-1} | \mathcal{E}(\rho) \rangle^{\otimes 2}. \quad (\text{D32})$$

with circuit of depth k , and sequences indexed via $s = (s_A, s_B)$ with $s_A = (a_1, a_2, \dots, a_k)$ and $s_B = (b_1, b_2, \dots, b_k)$ specifying the particular target unitary in each of the local gate-sets $\Gamma_{AB} = \Gamma_A \otimes \Gamma_B$.

Proof. From eqn.(33) over all sequences we have

$$\begin{aligned} \mathbb{E}_s[m(s)^2] &:= \frac{1}{|\Gamma_{AB}|^k} \sum_s m(s)^2 = \frac{1}{|\Gamma_{AB}|^k} \sum_s (\text{tr}[M\tilde{U}_s(\rho)])^2 \\ &= \frac{1}{|\Gamma_{AB}|^k} \sum_s \langle \mathbf{M} | \tilde{\mathbf{U}}_s(\rho) \rangle^2 = \frac{1}{|\Gamma_{AB}|^k} \sum_s \langle \mathbf{M} | \tilde{\mathbf{U}}_s | \rho \rangle^2, \\ &= \frac{1}{|\Gamma_{AB}|^k} \sum_s \langle \mathbf{M} | \tilde{\mathbf{U}}_{s_k} \tilde{\mathbf{U}}_{s_{k-1}} \dots \tilde{\mathbf{U}}_{s_1} | \rho \rangle^2, \\ &= \frac{1}{|\Gamma_{AB}|^k} \sum_s \langle \mathbf{M} | (\mathbf{U}_{s_k} \mathcal{E})(\mathbf{U}_{s_{k-1}} \mathcal{E}) \dots (\mathbf{U}_{s_1} \mathcal{E}) | \rho \rangle^2. \end{aligned} \quad (\text{D33})$$

Which we can write equivalently as a bipartite system,

$$\mathbb{E}_s[m(s)^2] = \frac{1}{|\Gamma_{AB}|^k} \sum_s \langle \mathbf{M} |^{\otimes 2} (\mathbf{U}_{s_k}^{\otimes 2} \mathcal{E}^{\otimes 2})(\mathbf{U}_{s_{k-1}}^{\otimes 2} \mathcal{E}^{\otimes 2}) \dots (\mathbf{U}_{s_1}^{\otimes 2} \mathcal{E}^{\otimes 2}) | \rho \rangle^{\otimes 2}. \quad (\text{D34})$$

The summation over \mathcal{U}_s for each gate k , can be expanded

$$\mathbb{E}_s[m(s)^2] = \langle \mathbf{M} |^{\otimes 2} \left(\frac{1}{|\Gamma_{AB}|} \sum_{U_{s_k} \in \Gamma_{AB}} \mathbf{U}_{s_k}^{\otimes 2} \mathcal{E}^{\otimes 2} \right) \left(\frac{1}{|\Gamma_{AB}|} \sum_{U_{s_{k-1}} \in \Gamma_{AB}} \mathbf{U}_{s_{k-1}}^{\otimes 2} \mathcal{E}^{\otimes 2} \right) \dots \left(\frac{1}{|\Gamma_{AB}|} \sum_{U_{s_1} \in \Gamma_{AB}} \mathbf{U}_{s_1}^{\otimes 2} \mathcal{E}^{\otimes 2} \right) | \rho \rangle^{\otimes 2}, \quad (\text{D35})$$

recalling $\mathcal{U}_s = \mathcal{U}_{s_A} \otimes \mathcal{U}_{s_B}$ and the sequences expand as $\sum_s^{k^2} = \sum_{s_A, s_B}^{k, k}$. We now have the form to use the property of the unitarity 2-design gate-set on each sub-system from eqns. (30) & (35),

$$\mathbb{E}_s[m(s)^2] = \langle \mathbf{M} |^{\otimes 2} \left(\int d\mu_{\text{Haar}}(U_A) \int d\mu_{\text{Haar}}(U_B) (\mathbf{U}_A \otimes \mathbf{U}_B)^{\otimes 2} \mathcal{E}^{\otimes 2} \right) \dots \left(\int d\mu_{\text{Haar}}(U_A) \int d\mu_{\text{Haar}}(U_B) (\mathbf{U}_A \otimes \mathbf{U}_B)^{\otimes 2} \mathcal{E}^{\otimes 2} \right) | \rho \rangle^{\otimes 2}, \quad (\text{D36})$$

there are now k identical integrals over U_A and U_B . So we can write

$$\mathbb{E}_s[m(s)^2] = \langle \mathbf{M} |^{\otimes 2} \left(\int d\mu_{\text{Haar}}(U_A) \int d\mu_{\text{Haar}}(U_B) (\mathbf{U}_A \otimes \mathbf{U}_B)^{\otimes 2} \mathcal{E}^{\otimes 2} \right)^k | \rho \rangle^{\otimes 2}. \quad (\text{D37})$$

This is just the projector P_{AB} , where $P_{AB} = P_A \otimes P_B$ up to reordering of subsystems, given by

$$\begin{aligned} \mathbb{E}_s[m(s)^2] &= \langle \mathbf{M} |^{\otimes 2} (P_{AB} \mathcal{E}^{\otimes 2})^k | \rho \rangle^{\otimes 2}, \\ &= \langle \mathbf{M} |^{\otimes 2} (P_{AB} \mathcal{E}^{\otimes 2})^{k-1} (P_{AB} \mathcal{E}^{\otimes 2}) | \rho \rangle^{\otimes 2}, \\ &= \langle \mathbf{M} |^{\otimes 2} (P_{AB} \mathcal{E}^{\otimes 2})^{k-1} (P_{AB}) | \mathcal{E}(\rho) \rangle^{\otimes 2}, \end{aligned} \quad (\text{D38})$$

where we have absorbed the first noise channel to the initial state of the system ρ . As $P_{AB} = (P_{AB})^2$, we are free to write all the intermediate projectors twice

$$\begin{aligned} \mathbb{E}_s[m(s)^2] &= \langle \mathbf{M} |^{\otimes 2} (P_{AB} \mathcal{E}^{\otimes 2}) (P_{AB}^2 \mathcal{E}^{\otimes 2})^{k-2} (P_{AB}) | \mathcal{E}(\rho) \rangle^{\otimes 2}, \\ &= \langle \mathbf{M} |^{\otimes 2} (P_{AB} \mathcal{E}^{\otimes 2} P_{AB}) (P_{AB} \mathcal{E}^{\otimes 2} P_{AB})^{k-2} | \mathcal{E}(\rho) \rangle^{\otimes 2}, \\ &= \langle \mathbf{M} |^{\otimes 2} (P_{AB} \mathcal{E}^{\otimes 2} P_{AB})^{k-1} | \mathcal{E}(\rho) \rangle^{\otimes 2}. \end{aligned} \quad (\text{D39})$$

Which completes the proof. \square

From Section D 4 if the Jordan decomposition is diagonal

$$(P_{AB} \mathcal{E}^{\otimes 2} P_{AB})^{k-1} = S^{-1} (|00\rangle\langle 00| + \lambda_1^{k-1} |10\rangle\langle 10| + \lambda_2^{k-1} |01\rangle\langle 01| + \lambda_3^{k-1} |11\rangle\langle 11|) S, \quad (\text{D40})$$

where λ_i are the eigenvalues of the matrix S . Therefore from Lemma D.3 we can write

$$\begin{aligned} \mathbb{E}_s[m(s)^2] &= \langle \mathbf{M} |^{\otimes 2} (P_{AB} \mathcal{E}^{\otimes 2} P_{AB})^{k-1} | \mathcal{E}(\rho) \rangle^{\otimes 2}, \\ &= \langle \mathbf{M} |^{\otimes 2} S^{-1} J^{k-1} S | \mathcal{E}(\rho) \rangle^{\otimes 2}, \\ &= \langle \mathbf{M} |^{\otimes 2} S^{-1} (|00\rangle\langle 00| + \lambda_1^{k-1} |10\rangle\langle 10| + \lambda_2^{k-1} |01\rangle\langle 01| + \lambda_3^{k-1} |11\rangle\langle 11|) S | \mathcal{E}(\rho) \rangle^{\otimes 2}. \end{aligned} \quad (\text{D41})$$

The transformation matrix S can be absorbed into the initial state of the system and the final measurement

$$\begin{aligned} \mathbb{E}_s[m(s)^2] &= \langle \mathbf{S}^{-1\dagger} (\mathbf{M}^{\otimes 2}) | J^{k-1} | \mathbf{S}(\mathcal{E}(\rho)^{\otimes 2}) \rangle, \\ &= \langle \mathbf{S}^{-1\dagger} (\mathbf{M}^{\otimes 2}) | (|00\rangle\langle 00| + \lambda_1^{k-1} |10\rangle\langle 10| + \lambda_2^{k-1} |01\rangle\langle 01| + \lambda_3^{k-1} |11\rangle\langle 11|) | \mathbf{S}(\mathcal{E}(\rho)^{\otimes 2}) \rangle, \end{aligned} \quad (\text{D42})$$

and further expanded as

$$\begin{aligned} \mathbb{E}_s[m(s)^2] &= \langle \mathbf{S}^{-1\dagger} (\mathbf{M}^{\otimes 2}) | 00 \rangle \langle 00 | \mathbf{S}(\mathcal{E}(\rho)^{\otimes 2}) \rangle \\ &\quad + \lambda_1^{k-1} \langle \mathbf{S}^{-1\dagger} (\mathbf{M}^{\otimes 2}) | 10 \rangle \langle 10 | \mathbf{S}(\mathcal{E}(\rho)^{\otimes 2}) \rangle \\ &\quad + \lambda_2^{k-1} \langle \mathbf{S}^{-1\dagger} (\mathbf{M}^{\otimes 2}) | 01 \rangle \langle 01 | \mathbf{S}(\mathcal{E}(\rho)^{\otimes 2}) \rangle \\ &\quad + \lambda_3^{k-1} \langle \mathbf{S}^{-1\dagger} (\mathbf{M}^{\otimes 2}) | 11 \rangle \langle 11 | \mathbf{S}(\mathcal{E}(\rho)^{\otimes 2}) \rangle. \end{aligned} \quad (\text{D43})$$

Or simply,

$$\mathbb{E}_s[m(s)^2] = c_{00} + c_{10} \lambda_1^{k-1} + c_{01} \lambda_2^{k-1} + c_{11} \lambda_3^{k-1}. \quad (\text{D44})$$

So if a channel \mathcal{E} produces a diagonal Jordan decomposition J , the protocol will produce a fit of this form where λ_i are the eigenvalues of S .

If the Jordan decomposition is not diagonal, then there are 2 remaining options. Firstly,

$$J^{k-1} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \lambda_1^{k-1} & (k-1)\lambda_1^{k-2} & 0 \\ 0 & 0 & \lambda_1^{k-1} & 0 \\ 0 & 0 & 0 & \lambda_2^{k-1} \end{pmatrix}, \quad (\text{D45})$$

where the fit will take the following form: $\mathbb{E}_s[m(s)^2] = c_0 + c_1 \lambda_1^{k-1} + c_2 \lambda_2^{k-1}$, where λ_i are the degenerate eigenvalues of \mathcal{S} , and constants c_i are dependent on M, ρ, S, S^{-1} & \mathbf{x} . Secondly,

$$J^{k-1} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \lambda_1^{k-1} & \lambda_1^{k-2} & \frac{(k-1)(k-2)}{2} \lambda_1^{k-3} \\ 0 & 0 & \lambda_1^{k-1} & \lambda_1^{k-2} \\ 0 & 0 & 0 & \lambda_1^{k-1} \end{pmatrix}, \quad (\text{D46})$$

where the fit will take the following form: $\mathbb{E}_s[m(s)^2] = c_0 + c_1 \lambda_1^{k-1}$, where λ_1 is the degenerate eigenvalue of S , and for different constants c_i dependent on M, ρ, S, S^{-1} and \mathbf{x} .

Appendix E: Estimating sub-unitarities via mid-circuit re-set protocols

The local subunitarities $u_{A \rightarrow A}(\mathcal{E}_{AB})$ and $u_{B \rightarrow B}(\mathcal{E}_{AB})$ of any bipartite channel \mathcal{E}_{AB} are measures of interest in their own right. However the exact estimation of the subunitarity of gate noise through unitarity benchmarking requires the repeated preparation of the maximally mixed state on the ancillary subsystem. As shown in [23], this introduces additional noise from the imperfect depolarization.

In the main text, figures were given of simulations of the estimation of local subunitarities under the assumption that any error in the preparation of the maximally mixed state was purely local to the ancillary subsystem. What follows is a discussion of possible methods to extract estimates of local subunitarities under more physically realistic assumptions about the nature of induced re-set errors and the quantum device in question.

1. Estimating local sub-unitarities with re-set errors

The manner in which the induced error is modelled determines the accuracy of the predicted estimate of the subunitarity. If we model the noisy re-set channel $\tilde{\mathcal{R}}_B$ as

$$\tilde{\mathcal{R}}_B = \mathcal{E}_P \circ (\text{id}_A \otimes \mathcal{R}_B) \circ \mathcal{E}_M, \quad (\text{E1})$$

where \mathcal{R}_B is the exact reset, and where \mathcal{E}_M and \mathcal{E}_P are SPAM errors on whole system related to the imperfect reset of the sub-system B . Then it can be shown that Protocol 2 allows the estimation of the subunitarity of the combined channel

$$\mathbb{E}_{s_A}[m(s_A)^2] = c_1 + c_2 u_{A \rightarrow A}(\mathcal{E}_M \circ \mathcal{E} \circ \mathcal{E}_P)^{k-1} \quad (\text{E2})$$

for a sequence of length k where \mathcal{E} is the noise channel associated to the gate-set. The constants c_1 & c_2 depend on the initial and final SPAM and non-unitality of the channel \mathcal{E} .

The Protocol 2 requires the preparation of the maximally mixed state ($|\mathbf{Y}_0\rangle / \sqrt{d_B}$ in our notation) on subsystem B , albeit noisily. However, we can consider an alternative, where we randomly re-set to one of the computational basis states. For two qubits, we can consider the Liouville representation of the preparation channel

$$\text{prep}_{B, \pm Z} := \text{id}_A \otimes (|\mathbf{Y}_0\rangle / \sqrt{2} \pm |\mathbf{Y}_Z\rangle / \sqrt{2}), \quad (\text{E3})$$

which prepares the state $|0\rangle\langle 0| = \frac{1}{2}(\mathbb{1}_B \pm Z)$ on sub-system B . For a bipartite channel \mathcal{E} , the related channel \mathcal{E}_{+Z} on qubit A is defined as

$$\mathcal{E}_{+Z} := \text{tr}_B \cdot \mathcal{E} \cdot \text{prep}_{B, +Z} = (\text{id}_A \otimes \langle \mathbf{Y}_0 |) \mathcal{E} (\text{id}_A \otimes (|\mathbf{Y}_0\rangle + |\mathbf{Y}_Z\rangle)), \quad (\text{E4})$$

and similarly $\mathcal{E}_{-Z} := \text{tr}_B \cdot \mathcal{E} \cdot \text{prep}_{B, -Z}$.

We can calculate the structure of the unitarity of these channels using the Liouville representation. The definition of unitarity can be written in our basis as

$$u(\mathcal{E}_A) = \frac{1}{d^2 - 1} \sum_{ij} \langle \mathbf{X}_i | \mathcal{E}^\dagger | \mathbf{X}_j \rangle \langle \mathbf{X}_j | \mathcal{E} | \mathbf{X}_i \rangle, \quad (\text{E5})$$

for some channel \mathcal{E}_A that maps $\mathcal{B}(\mathcal{H}_A) \rightarrow \mathcal{B}(\mathcal{H}_A)$. The unitarity of the channel \mathcal{E}_{+Z} can then be related to the local sub-unitarity of the channel \mathcal{E} as

$$\begin{aligned} u(\mathcal{E}_{+Z}) = u_{A \rightarrow A}(\mathcal{E}) + \frac{1}{3} \sum_{ij} & \langle \mathbf{X}_i \otimes \mathbf{Y}_Z | \mathcal{E}^\dagger | \mathbf{X}_j \otimes \mathbf{Y}_0 \rangle \langle \mathbf{X}_j \otimes \mathbf{Y}_0 | \mathcal{E} | \mathbf{X}_i \otimes \mathbf{Y}_Z \rangle \\ & + \langle \mathbf{X}_i \otimes \mathbf{Y}_Z | \mathcal{E}^\dagger | \mathbf{X}_j \otimes \mathbf{Y}_0 \rangle \langle \mathbf{X}_j \otimes \mathbf{Y}_0 | \mathcal{E} | \mathbf{X}_i \otimes \mathbf{Y}_0 \rangle \\ & + \langle \mathbf{X}_i \otimes \mathbf{Y}_0 | \mathcal{E}^\dagger | \mathbf{X}_j \otimes \mathbf{Y}_0 \rangle \langle \mathbf{X}_j \otimes \mathbf{Y}_0 | \mathcal{E} | \mathbf{X}_i \otimes \mathbf{Y}_Z \rangle, \end{aligned} \quad (\text{E6})$$

and similarly

$$\begin{aligned} u(\mathcal{E}_{-Z}) = u_{A \rightarrow A}(\mathcal{E}) + \frac{1}{3} \sum_{ij} & \langle \mathbf{X}_i \otimes \mathbf{Y}_Z | \mathcal{E}^\dagger | \mathbf{X}_j \otimes \mathbf{Y}_0 \rangle \langle \mathbf{X}_j \otimes \mathbf{Y}_0 | \mathcal{E} | \mathbf{X}_i \otimes \mathbf{Y}_Z \rangle \\ & - \langle \mathbf{X}_i \otimes \mathbf{Y}_Z | \mathcal{E}^\dagger | \mathbf{X}_j \otimes \mathbf{Y}_0 \rangle \langle \mathbf{X}_j \otimes \mathbf{Y}_0 | \mathcal{E} | \mathbf{X}_i \otimes \mathbf{Y}_0 \rangle \\ & - \langle \mathbf{X}_i \otimes \mathbf{Y}_0 | \mathcal{E}^\dagger | \mathbf{X}_j \otimes \mathbf{Y}_0 \rangle \langle \mathbf{X}_j \otimes \mathbf{Y}_0 | \mathcal{E} | \mathbf{X}_i \otimes \mathbf{Y}_Z \rangle. \end{aligned} \quad (\text{E7})$$

This follows from expansion of the definitions of the channels and the Liouville definition of unitarity. By taking the mean of the unitarity of these two channels we find

$$\frac{1}{2}(u(\mathcal{E}_{+Z}) + u(\mathcal{E}_{-Z})) = u_{A \rightarrow A}(\mathcal{E}) + \frac{1}{3} \sum_{ij} \langle \mathbf{X}_i \otimes \mathbf{Y}_Z | \mathcal{E}^\dagger | \mathbf{X}_j \otimes \mathbf{Y}_0 \rangle \langle \mathbf{X}_j \otimes \mathbf{Y}_0 | \mathcal{E} | \mathbf{X}_i \otimes \mathbf{Y}_Z \rangle. \quad (\text{E8})$$

As the 2nd term in eqn. (E8) is strictly non-negative we can use this measure to bound the sub-unitarity of the target channel. Therefore, if we can better re-set to one of the computational basis state, then we can estimate the $A \rightarrow A$ sub-unitarity via the following.

Lemma E.1. *The local sub-unitarity of a bipartite channel $u_{A \rightarrow A}(\mathcal{E})$ can be bounded by the average unitarity of the channel with two specific initial conditions,*

$$u_{A \rightarrow A}(\mathcal{E}) \leq \frac{1}{2}(u(\mathcal{E}_{+Z}) + u(\mathcal{E}_{-Z})) \quad (\text{E9})$$

where $\mathcal{E}_{+Z}(\rho) = \text{tr}_B[\mathcal{E}(\rho \otimes |0\rangle\langle 0|)]$ and $\mathcal{E}_{-Z}(\rho) = \text{tr}_B[\mathcal{E}(\rho \otimes |1\rangle\langle 1|)]$.

Proof. This follows from Lemma E1. and the non-negativity of any element $\mathcal{E}_{ij}^* \mathcal{E}_{ij}$. \square

Corollary E.1. *If \mathcal{E} is a product channel.*

$$u_{A \rightarrow A}(\mathcal{E}) = \frac{1}{2}(u(\mathcal{E}_{+Z}) + u(\mathcal{E}_{-Z})) \quad (\text{E10})$$

Proof. If $\mathcal{E} = \mathcal{E}_A \otimes \mathcal{E}_B$, the 2nd term always contains the element $\langle \mathbf{Y}_0 | \mathcal{E}_B | \mathbf{Y}_i \rangle$, which must be zero for a valid CPTP map. \square

Additionally, it can be shown that Lemma E.1 holds for any two orthogonal initial states on qubit B .

Corollary E.2. *The local sub-unitarity of a bipartite channel $u_{A \rightarrow A}(\mathcal{E})$ can be bounded by the average unitarity of the channel with two specific initial conditions,*

$$u_{A \rightarrow A}(\mathcal{E}) \leq \min \left[\frac{1}{2}(u(\mathcal{E}_{+b}) + u(\mathcal{E}_{-b})) \right], \quad (\text{E11})$$

where $\mathcal{E}_{\pm b}(\rho) = \text{tr}_B[\mathcal{E}(\rho \otimes \frac{1}{2}(\mathbb{1}_B \pm \mathbf{b} \cdot \boldsymbol{\sigma}))]$.

Proof. This follows from Lemma E.1, replacing Z with a general Bloch vector on qubit B . \square

Under the assumption that computational basis states induce fewer errors when prepared compared to the maximally mixed state, then estimating $u(\mathcal{E}_{+Z})$ and $u(\mathcal{E}_{-Z})$ with a RB protocol allows an upper bound to be placed on the local sub-unitarity $u_{A \rightarrow A}(\mathcal{E})$, where \mathcal{E} is the noisy channel associated with the target gate-set.

In such a case, the RB protocol would simply entail two experiments: firstly performing unitarity RB on qubit A with a reset of qubit B to $|0\rangle$, and then secondly with a reset to $|1\rangle$. If we assume the reset is performed completely incoherently, but with bipartite SPAM errors we have for the 1st experiment will produce a fit of the form

$$\mathbb{E}_{s_A} [m(s_A)^2] = c_1 + c_2 u(\mathcal{E}_{+Z,M} \circ \mathcal{E}_{+Z} \circ \mathcal{E}_{+Z,P})^{k-1}, \quad (\text{E12})$$

where $\Lambda_{+Z,M}$ & $\Lambda_{+Z,P}$ are the bipartite SPAM errors associated with the noisy reset of qubit B to $|0\rangle$. Similarly the 2nd experiment will produce a fit of the form

$$\mathbb{E}_{s_A} [m(s_A)^2] = c_1 + c_2 u(\mathcal{E}_{-Z,M} \circ \mathcal{E}_{-Z} \circ \mathcal{E}_{-Z,P})^{m-1}, \quad (\text{E13})$$

where $\mathcal{E}_{\pm Z,M}$ & $\mathcal{E}_{\pm Z,P}$ are the bipartite SPAM errors associated with the noisy reset of qubit B . Such a modification could then be used when the preparation of a maximally mixed state is significantly noisier compared to computational basis state preparation and reset which would detrimentally affect estimation of $u_{A \rightarrow A}(\mathcal{E})$. In the case when $\mathcal{E}_{\pm Z,M,P} \approx id$ an upper bound could be estimated as shown above.

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- [1] M. Kliesch and I. Roth, Theory of quantum system certification, *PRX Quantum* **2**, 010201 (2021).
- [2] J. Helsen, I. Roth, E. Onorati, A. H. Werner, and J. Eisert, A general framework for randomized benchmarking, arXiv preprint arXiv:2010.07974 (2020).
- [3] T. J. Proctor, A. Carignan-Dugas, K. Rudinger, E. Nielsen, R. Blume-Kohout, and K. Young, Direct randomized benchmarking for multiqubit devices, *Physical review letters* **123**, 030503 (2019).
- [4] J. P. Gaebler, A. M. Meier, T. R. Tan, R. Bowler, Y. Lin, D. Hanneke, J. D. Jost, J. Home, E. Knill, D. Leibfried, *et al.*, Randomized benchmarking of multiqubit gates, *Physical review letters* **108**, 260503 (2012).
- [5] A. Erhard, J. J. Wallman, L. Postler, M. Meth, R. Stricker, E. A. Martinez, P. Schindler, T. Monz, J. Emerson, and R. Blatt, Characterizing large-scale quantum computers via cycle benchmarking, *Nature communications* **10**, 1 (2019).
- [6] J. Eisert, D. Hangleiter, N. Walk, I. Roth, D. Markham, R. Parekh, U. Chabaud, and E. Kashefi, Quantum certification and benchmarking, *Nature Reviews Physics* **2**, 382 (2020).
- [7] E. Derbyshire, R. Mezher, T. Kapourniotis, and E. Kashefi, Randomized benchmarking with stabilizer verification and gate synthesis, arXiv preprint arXiv:2102.13044 (2021).
- [8] G. D’Ariano and P. L. Presti, Quantum tomography for measuring experimentally the matrix elements of an arbitrary quantum operation, *Physical review letters* **86**, 4195 (2001).
- [9] D. Greenbaum, Introduction to quantum gate set tomography, arXiv preprint arXiv:1509.02921 (2015).
- [10] S. Sheldon, L. S. Bishop, E. Magesan, S. Filipp, J. M. Chow, and J. M. Gambetta, Characterizing errors on qubit operations via iterative randomized benchmarking, *Physical Review A* **93**, 012301 (2016).
- [11] D. Aharonov and M. Ben-Or, Fault-tolerant quantum computation with constant error rate, *SIAM Journal on Computing* (2008).
- [12] R. Harper and S. T. Flammia, Fault-tolerant logical gates in the ibm quantum experience, *Physical review letters* **122**, 080504 (2019).
- [13] J. Wallman, C. Granade, R. Harper, and S. T. Flammia, Estimating the coherence of noise, *New Journal of Physics* **17**, 113020 (2015).
- [14] B. Dirkse, J. Helsen, and S. Wehner, Efficient unitarity randomized benchmarking of few-qubit clifford gates, *Physical Review A* **99**, 012315 (2019).
- [15] N. Sundaresan, I. Lauer, E. Pritchett, E. Magesan, P. Jurcevic, and J. M. Gambetta, Reducing unitary and spectator errors in cross resonance with optimized rotary echoes, *PRX Quantum* **1**, 020318 (2020).
- [16] J. Preskill, Sufficient condition on noise correlations for scalable quantum computing, arXiv preprint arXiv:1207.6131 (2012).
- [17] N. H. Nickerson and B. J. Brown, Analysing correlated noise on the surface code using adaptive decoding algorithms, *Quantum* **3**, 131 (2019).
- [18] J. K. Iverson and J. Preskill, Coherence in logical quantum channels, *New Journal of Physics* **22**, 073066 (2020).
- [19] J. Preskill, Quantum computing in the nisq era and beyond, *Quantum* **2**, 79 (2018).
- [20] J. M. Gambetta, A. Córcoles, S. T. Merkel, B. R. Johnson, J. A. Smolin, J. M. Chow, C. A. Ryan, C. Rigetti, S. Poletto, T. A. Ohki, *et al.*, Characterization of addressability by simultaneous randomized benchmarking, *Physical review letters* **109**, 240504 (2012).
- [21] Y. Nakata, D. Zhao, T. Okuda, E. Bannai, Y. Suzuki, S. Tamiya, K. Heya, Z. Yan, K. Zuo, S. Tamate, Y. Tabuchi, and Y. Nakamura, Quantum circuits for exact unitary t -designs and applications to higher-order randomized benchmarking (2021), arXiv:2102.12617 [quant-ph].
- [22] J. Helsen, X. Xue, L. M. Vandersypen, and S. Wehner, A new class of efficient randomized benchmarking protocols, *npj Quantum Information* **5**, 1 (2019).
- [23] J. Combes, C. Granade, C. Ferrie, and S. T. Flammia, Logical randomized benchmarking, arXiv preprint arXiv:1702.03688 (2017).
- [24] E. Derbyshire, J. Y. Malo, A. Daley, E. Kashefi, and P. Walden, Randomized benchmarking in the analogue setting, *Quantum Science and Technology* **5**, 034001 (2020).
- [25] R. Blume-Kohout, J. K. Gamble, E. Nielsen, J. Mizrahi, J. D. Sterk, and P. Maunz, Robust, self-consistent, closed-form tomography of quantum logic gates on a trapped ion qubit, arXiv preprint arXiv:1310.4492 (2013).
- [26] J. Poyatos, J. I. Cirac, and P. Zoller, Complete characterization of a quantum process: the two-bit quantum gate, *Physical Review Letters* **78**, 390 (1997).
- [27] I. L. Chuang and M. A. Nielsen, Prescription for experimental determination of the dynamics of a quantum black box, *Journal of Modern Optics* **44**, 2455 (1997).
- [28] E. Chitambar and G. Gour, Quantum resource theories, *Reviews of Modern Physics* **91**, 025001 (2019).
- [29] G. Gour and C. M. Scandolo, Dynamical entanglement, *Physical Review Letters* **125**, 180505 (2020).
- [30] S. Bäuml, S. Das, X. Wang, and M. M. Wilde, Resource theory of entanglement for bipartite quantum channels, arXiv preprint arXiv:1907.04181 (2019).
- [31] C.-Y. Hsieh, M. Lostaglio, and A. Acín, Entanglement preserving local thermalization, *Physical Review Research* **2**, 013379 (2020).
- [32] G. Gutoski, Properties of local quantum operations with shared entanglement (2009), arXiv:0805.2209 [quant-ph].
- [33] K. Korzekwa, S. Czachórski, Z. Puchała, and K. Życzkowski, Coherifying quantum channels, *New Journal of Physics* **20**, 043028 (2018).
- [34] C.-Y. Hsieh, M. Lostaglio, and A. Acín, Quantum channel marginal problem (2021), arXiv:2102.10926 [quant-ph].

- [35] T. Heinosaari, T. Miyadera, and M. Ziman, An invitation to quantum incompatibility, *Journal of Physics A: Mathematical and Theoretical* **49**, 123001 (2016).
- [36] D. Kretschmann, D. Schlingemann, and R. F. Werner, The information-disturbance tradeoff and the continuity of stinespring's representation, *IEEE transactions on information theory* **54**, 1708 (2008).
- [37] W. K. Wootters and W. H. Zurek, A single quantum cannot be cloned, *Nature* **299**, 802 (1982).
- [38] H. P. Yuen, Amplification of quantum states and noiseless photon amplifiers, *Physics Letters A* **113**, 405 (1986).
- [39] H. Barnum, C. M. Caves, C. A. Fuchs, R. Jozsa, and B. Schumacher, Noncommuting mixed states cannot be broadcast, *Physical Review Letters* **76**, 2818 (1996).
- [40] H. Barnum, J. Barrett, M. Leifer, and A. Wilce, Generalized no-broadcasting theorem, *Physical review letters* **99**, 240501 (2007).
- [41] C. Cîrstoiu, K. Korzekwa, and D. Jennings, Robustness of noether's principle: Maximal disconnects between conservation laws and symmetries in quantum theory, *Physical Review X* **10**, 041035 (2020).
- [42] J. Watrous, *The theory of quantum information* (Cambridge University Press, 2018) p. 23.
- [43] Note that the basis $|\mathbf{X} \otimes \mathbf{Y}\rangle$ is a tensor product basis for $(\mathcal{H}_A \otimes \mathcal{H}_A) \otimes (\mathcal{H}_B \otimes \mathcal{H}_B)$ and up to re-ordering of (second and third) Hilbert spaces the same as vectorization of the matrix $X \otimes Y$. As these basis are isomorphic, the Liouville representation will be invariant under such permutations.
- [44] W. Bruzda, V. Cappellini, H.-J. Sommers, and K. Życzkowski, Random quantum operations, *Physics Letters A* **373**, 320 (2009).
- [45] J. Johansson, Nation pd& nori f. 2013 qutip 2: a python framework for the dynamics of open quantum systems, *Comp. Phys. Comm* **184**, 1234.
- [46] E. Knill, Non-binary unitary error bases and quantum codes, arXiv preprint quant-ph/9608048 (1996).
- [47] A. Y. Kitaev, Quantum computations: algorithms and error correction, *Uspekhi Matematicheskikh Nauk* **52**, 53 (1997).
- [48] J. J. Wallman and S. T. Flammia, Randomized benchmarking with confidence, *New Journal of Physics* **16**, 103032 (2014).
- [49] A. Carignan-Dugas, J. J. Wallman, and J. Emerson, Bounding the average gate fidelity of composite channels using the unitarity, *New Journal of Physics* **21**, 053016 (2019).
- [50] R. Kueng, D. M. Long, A. C. Doherty, and S. T. Flammia, Comparing experiments to the fault-tolerance threshold, *Physical review letters* **117**, 170502 (2016).
- [51] T. Proctor, K. Rudinger, K. Young, M. Sarovar, and R. Blume-Kohout, What randomized benchmarking actually measures, *Physical review letters* **119**, 130502 (2017).
- [52] J. J. Wallman, Randomized benchmarking with gate-dependent noise, *Quantum* **2**, 47 (2018).
- [53] S. T. Merkel, E. J. Pritchett, and B. H. Fong, Randomized benchmarking as convolution: Fourier analysis of gate dependent errors, arXiv preprint arXiv:1804.05951 (2018).
- [54] W. T. Gowers and O. Hatami, Inverse and stability theorems for approximate representations of finite groups, *Sbornik: Mathematics* **208**, 1784 (2017).
- [55] D. S. França and A. Hashagen, Approximate randomized benchmarking for finite groups, *Journal of Physics A: Mathematical and Theoretical* **51**, 395302 (2018).
- [56] H. Zhu, Multiqubit clifford groups are unitary 3-designs, *Physical Review A* **96**, 062336 (2017).
- [57] E. Magesan, J. M. Gambetta, B. R. Johnson, C. A. Ryan, J. M. Chow, S. T. Merkel, M. P. Da Silva, G. A. Keefe, M. B. Rothwell, T. A. Ohki, *et al.*, Efficient measurement of quantum gate error by interleaved randomized benchmarking, *Physical review letters* **109**, 080505 (2012).
- [58] S. Kimmel, M. P. da Silva, C. A. Ryan, B. R. Johnson, and T. Ohki, Robust extraction of tomographic information via randomized benchmarking, *Physical Review X* **4**, 011050 (2014).
- [59] This assumes a non-degenerate form of a Jordan matrix decomposition. Degenerate cases give rise to similar expressions. See Appendix D4 for details.
- [60] R. A. Horn and C. R. Johnson, *Matrix analysis*, 2nd ed. (Cambridge university press, 2012).
- [61] J. J. Wallman and J. Emerson, Noise tailoring for scalable quantum computation via randomized compiling, *Physical Review A* **94**, 052325 (2016).
- [62] A. Hashim, R. K. Naik, A. Morvan, J.-L. Ville, B. Mitchell, J. M. Kreikebaum, M. Davis, E. Smith, C. Iancu, K. P. O'Brien, *et al.*, Randomized compiling for scalable quantum computing on a noisy superconducting quantum processor, arXiv preprint arXiv:2010.00215 (2020).
- [63] J. M. Pino, J. M. Dreiling, C. Figgatt, J. P. Gaebler, S. A. Moses, M. Allman, C. Baldwin, M. Foss-Feig, D. Hayes, K. Mayer, *et al.*, Demonstration of the qccd trapped-ion quantum computer architecture, arXiv preprint arXiv:2003.01293 (2020).
- [64] A. D. Corcoles, M. Takita, K. Inoue, S. Lekuch, Z. K. Mineev, J. M. Chow, and J. M. Gambetta, Exploiting dynamic quantum circuits in a quantum algorithm with superconducting qubits, arXiv preprint arXiv:2102.01682 (2021).
- [65] S. Sivarajah, S. Dilkes, A. Cowtan, W. Simmons, A. Edgington, and R. Duncan, Tket: a retargetable compiler for nisq devices, *Quantum Science and Technology* **6**, 014003 (2020).
- [66] Qiskit: An open-source framework for quantum computing (2019).
- [67] M. Sarovar, T. Proctor, K. Rudinger, K. Young, E. Nielsen, and R. Blume-Kohout, Detecting crosstalk errors in quantum information processors, *Quantum* **4**, 321 (2020).
- [68] D. C. McKay, A. W. Cross, C. J. Wood, and J. M. Gambetta, Correlated randomized benchmarking, arXiv preprint arXiv:2003.02354 (2020).
- [69] A. Winick, J. J. Wallman, and J. Emerson, Simulating and mitigating crosstalk, arXiv preprint arXiv:2006.09596 (2020).
- [70] H. Ball, T. M. Stace, S. T. Flammia, and M. J. Biercuk, Effect of noise correlations on randomized benchmarking, *Physical Review A* **93**, 022303 (2016).

- [71] J. Qi and H. K. Ng, Randomized benchmarking in the presence of time-correlated dephasing noise, *Physical Review A* **103**, 022607 (2021).
- [72] R. Harper, I. Hincks, C. Ferrie, S. T. Flammia, and J. J. Wallman, Statistical analysis of randomized benchmarking, *Physical Review A* **99**, 052350 (2019).
- [73] X. Xue, T. Watson, J. Helsen, D. R. Ward, D. E. Savage, M. G. Lagally, S. N. Coppersmith, M. Eriksson, S. Wehner, and L. Vandersypen, Benchmarking gate fidelities in a si/sige two-qubit device, *Physical Review X* **9**, 021011 (2019).
- [74] J. Helsen, F. Battistel, and B. M. Terhal, Spectral quantum tomography, *npj Quantum Information* **5**, 1 (2019).
- [75] Alternatively this formula can be calculated from the definition involving Haar measure.
- [76] M. S. Byrd and N. Khaneja, Characterization of the positivity of the density matrix in terms of the coherence vector representation, *Physical Review A* **68**, 062322 (2003).
- [77] P. Rungta, V. Bužek, C. M. Caves, M. Hillery, and G. J. Milburn, Universal state inversion and concurrence in arbitrary dimensions, *Physical Review A* **64**, 042315 (2001).
- [78] R. Horodecki *et al.*, Information-theoretic aspects of inseparability of mixed states, *Physical Review A* **54**, 1838 (1996).
- [79] Schur's Lemma states that the only matrices that commute with all elements of an irreducible representation of a group are scalar multiples of $\mathbb{1}$.