

General Framework for Randomized Benchmarking

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Randomized benchmarking refers to a collection of protocols that in the past decade have become central methods for characterizing quantum gates. These protocols aim at efficiently estimating the quality of a set of quantum gates in a way that is resistant to state preparation and measurement errors. Over the years many versions have been developed, however a comprehensive theoretical treatment of randomized benchmarking has been missing. In this work, we develop a rigorous framework of randomized benchmarking general enough to encompass virtually all known protocols as well as novel, more flexible extensions. Overcoming previous limitations on error models and gate sets, this framework allows us, for the first time, to formulate realistic conditions under which we can rigorously guarantee that the output of any randomized benchmarking experiment is well described by a linear combination of matrix exponential decays. We complement this with a detailed analysis of the fitting problem associated with randomized benchmarking data. We introduce modern signal processing techniques to randomized benchmarking, prove analytical sample complexity bounds, and numerically evaluate performance and limitations. In order to reduce the resource demands of this fitting problem, we introduce novel, scalable postprocessing techniques to isolate exponential decays, significantly improving the practical feasibility of a large set of randomized benchmarking protocols. These postprocessing techniques overcome shortcomings in efficiency of several previously proposed methods such as character benchmarking and linear-cross entropy benchmarking. Finally, we discuss, in full generality, how and when randomized benchmarking decay rates can be used to infer quality measures like the average fidelity. On the technical side, our work substantially extends the recently developed Fourier-theoretic perspective on randomized benchmarking by making use of the perturbation theory of invariant subspaces, as well as ideas from signal processing.

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I. INTRODUCTION

In the last few years significant steps have been taken towards the development of large-scale quantum computers. A key part of the development of these quantum computers are tools that provide diagnostics, certification,

and benchmarking. Particularly for quantum operations, stringent conditions have to be met to achieve fault tolerance. Motivated by this observation, in recent years a significant body of work has been dedicated to the development of tools for the certification and benchmarking of quantum gates. A prominent role in this collection of tools is taken by methods that can be collectively referred to as *randomized benchmarking* (RB). These methods have risen to prominence because they conform well to the demands of realistic experimental settings. They estimate the magnitude of an average error of a set of quantum gates in a fashion that is robust to errors in *state preparation and measurement* (SPAM) and moreover is, in many settings,

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efficient, in the sense that the resources required scale polynomially with the number of qubits in the device. The various versions of RB apply sequences of randomly chosen quantum gates of varying length. Small errors are thus amplified with the sequence length, and gate quality measures can be extracted from the dependence of the output data on sequence length.

In RB protocols, group structures feature strongly, in that the gate set considered is in almost all cases a subset of a finite group. Such group structures not only make it possible to efficiently make predictions for error-free sequences and compute inverses, but they also provide the means to analyze the error contribution after averaging. Originally proposed for random unitary gates [1–3], RB is now most prominently executed with gates from the so-called *Clifford group* [4–6], a set of efficiently classically simulatable quantum gates that take a key role specifically in fault-tolerant quantum computing [7]. It has also been considered for other (subsets of) finite groups [8–15]. Moreover RB has been generalized to capture other figures of merit of gate sets, such as relative average gate fidelities to specific anticipated target gates [4], fidelities within a symmetry sector [9,10], or the unitarity [16]. Specifically recently, with challenges of realizing fault-tolerant quantum computers in mind, emphasis has been put on capturing losses, leakage, and crosstalk in a scheme [17–19]. Also, data from RB—or rather suitably combining data from multiple such experiments—can be sufficient to acquire full tomographic information about a quantum gate [20–22]. This adds up to a wealth of RB protocols [23] proposed over the previous years. Figure 2 summarizes (to our knowledge) an up to date list of theoretical proposals for RB procedures presently known.

A significant body of work moreover deals with the limitations and precise preconditions of RB. The originally rather stringent assumptions on noise being necessarily identical across different quantum gates have over time been relaxed for particular protocols in later work [24–26], and the connection between the output of RB and operationally relevant quantities (such as average fidelity) has been studied in some detail [26,27].

And yet, it seems fair to say that a comprehensive picture of RB schemes for the quantum technologies [28] has been lacking so far. In particular, a theoretical framework that is broad enough to formalize the required preconditions ensuring the proper functioning of RB protocols beyond case-by-case arguments for specific protocols. This is unsatisfactory, as the development of higher-quality quantum gates and currently relies heavily on a plethora of tailor-made variants of RB. This motivates our current effort at providing a clear rigorous underpinning for RB and exploring its underlying mathematical structure, putting all variants of RB on a common footing.

With this effort we aim to not only *better understand* these protocols, but also to *increase trust* in them, making

it possible to *reliably use them* without a detailed understanding of their inner workings. This is a timely effort, as procedures that fit within the RB framework, such as linear-cross-entropy benchmarking [29] and the behavior of noisy random circuits more generally, have been the topic of significant attention recently [30–32], including for the purpose of benchmarking [33]. Given how we identify linear-cross-entropy benchmarking as a randomized benchmarking procedure, we relate our general framework to this timely discussion.

At the same time our framework allows us to *go significantly beyond current protocols* and establish a series of novel theoretical results and benchmarking schemes, addressing several shortcomings of the current state of the art. Among others, these novel results include a rigorous error bound for generator-style randomized benchmarking, a formal equivalence between linear-cross-entropy benchmarking and randomized benchmarking and a novel, scalable method for isolating signals in RB experiments, an absolute requirement if one wants to apply RB to nonstandard gate sets. This latter method, which we call *filtered RB*, is a significant conceptual improvement over standard RB schemes, promising greater flexibility and applicability. Notably, it also obviates the need for physically implemented inversion gates in randomized benchmarking experiments and the preparation of specific input states, making its implementation significantly more straightforward. As such, this framework therefore also constitutes a solid basis for *developing new schemes* of randomized benchmarking. Altogether these results substantially advance the understanding of the possibilities and requirements of randomized benchmarking as a practical tool for estimation and certification.

II. OVERVIEW OF RESULTS

In this work, we aim at developing a *mathematically comprehensive framework of randomized benchmarking protocols*, synthesizing, generalizing, and substantially strengthening previous work. This paper covers a variety of different aspects of randomized benchmarking, from general theorems on the validity of RB data, to a detailed study of the classical postprocessing of data generated by RB and an in-depth discussion of the connection between the outputs of RB and average fidelity. As our work is often quite technical, we formulate a series of “take-home” messages at the end of this section, summarizing the key takeaways of our work for experimental practice.

A. A general framework for randomized benchmarking

We begin by providing a general framework that generalizes and covers (to the best of our knowledge) all RB procedures currently present in the literature. This can also be thought of as an attempt at a *formal definition of RB*

protocols, and is largely an effort to organize and formalize knowledge already present in the RB literature. RB protocols can be divided into two separate phases: a data-collection phase, and a data-processing phase (see Fig. 1).

- (a) The *data-collection phase* corresponds to the part of the protocol involving the actual quantum computer and can be described as (1) the preparation of a quantum state, (2) the application of a sequence of random quantum operations, capped by (3) an inversion operator mapping the state (ideally) to a specified final state (usually the initial state), upon which (4) a measurement is then performed.
- (b) This process yields estimates of a success probability $p(m)$ for different sequence lengths m , which constitutes the input to the *data-processing phase*. In this phase—which is completely classical—the data $p(m)$ is fitted to a functional model, generally a linear combination of exponential decays. One can consider the decay rates of these exponential decays as direct measures of quality of the implementation, or further relate it to operational quantities like the average fidelity.

Starting with the data-collection phase, we write down a general RB protocol (Algorithm 1). This protocol depends on a number of input parameters, and by making particular choices for these parameters we can obtain all RB protocols currently in the literature. The key parameters are as follows:

1. A **group** \mathbb{G} , encoding the gates that are applied during the RB protocol. A common choice for this group is the multiqubit Clifford group \mathbb{C}_q but many other choices are possible.
2. A **reference implementation** ϕ , assigning to each element of the group \mathbb{G} an ideal quantum operation to be implemented. In the standard scenario this map is a *representation* of the group \mathbb{G} (denoted ω). In general this map need not be a representation, but it is in all known cases obtained from a representation by some fixed mapping. The paradigmatic example of such an implementation map is the standard conjugation action $g \mapsto U_g \rho U_g^\dagger$, which associates a unitary action to every element g of the group.
3. A **probability distribution** ν encoding the probability with which gates are selected from \mathbb{G} . In the standard case this probability distribution is simply the uniform distribution over the group. We also consider the situation where this probability distribution can vary throughout different steps of the protocol.
4. An **ending gate** g_{end} governing the total operation performed in each RB sequence. Typically this is

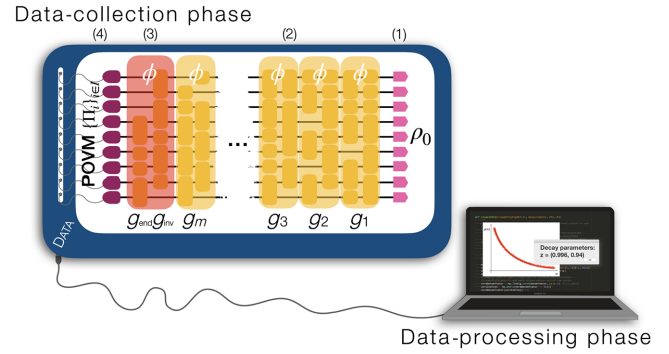


FIG. 1. The basic structure of RB. The RB data-collection phase iterates the following steps: after (1) the preparation of an initial state ρ_0 , (2) a sequence of m random gates g_i is applied, (3) followed by the gate inverting the sequence g_{inv} up to an end gate g_{end} and (4) a final POVM measurement. In the data-processing phase the measurement data, for many random sequences and different sequence lengths is postprocessed in a classical computer to extract decay parameters quantifying the imperfections in the implemented gates.

the identity, but other choices are relevant, and it can even be chosen at random.

Different choices for these key parameters can be collected into classes, yielding a *typology of randomized benchmarking procedures*, an overview of which can be seen in Fig. 2. This typology consists of three classes:

- (a) **Uniform RB**, which is characterized by uniform random sampling of operations and reference implementations that are representations.
- (b) **Interleaved RB**, where the reference implementations involve the application of “interleaved” gates.
- (c) **Nonuniform RB**, which is characterized by nonuniform random sampling of operations. This last class comes with two subtypes: **approximate RB**, where the sampling distribution is close to uniform, and **subset RB**, where the sampling distribution is very far from being uniform (for instance, taking only nonzero values on a small set of generators).

These classes of RB procedures are motivated by the qualitatively different behavior of the associated output data $p(m)$, which we discuss in more detail later. They also partially but not completely align with notions already present in the literature. In particular, we see that the behavior of this data is dictated by the group \mathbb{G} and the reference representation ω . We can always decompose this representation ω into a direct sum of *irreducible* subrepresentations, i.e., $\omega = \bigoplus_{\lambda \in \Lambda} \sigma_\lambda^{\oplus n_\lambda}$ where the σ_λ are irreducible (and occur with multiplicity n_λ).

A key tenet of RB is that this decomposition decides the functional form of the output data $p(m)$ as a function of sequence length m . More precisely, we expect behavior of

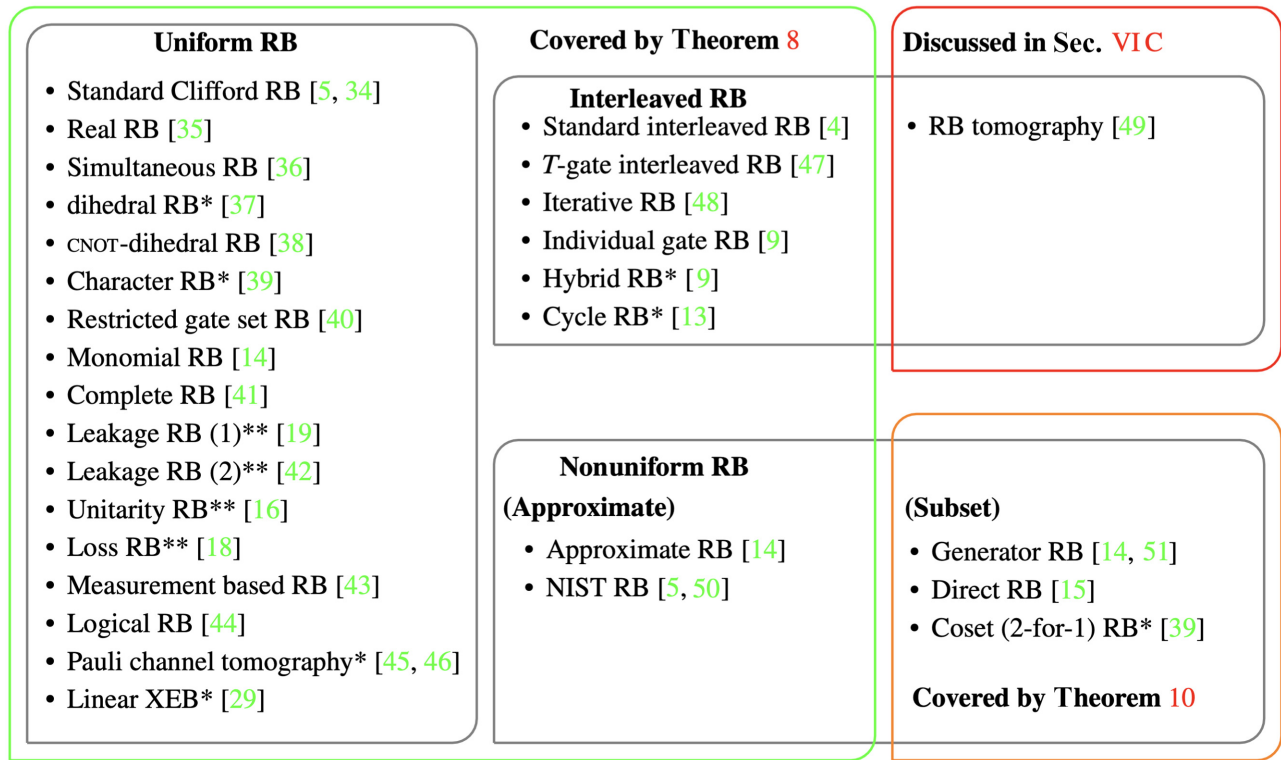


FIG. 2. An overview of RB schemes, indicating how they fit within our typology (see Sec. VD) of RB schemes and what theorem covers the behavior of their output data (see Sec. VI). An * indicates that the protocol has a nontrivial postprocessing scheme, while ** indicates that the protocol in its original specification has no inversion gate. We discuss how this is equal to uniform RB (with inversion) together with a postprocessing step in Sec. VIII.

the form

$$p(m) \approx \sum_{\lambda \in \Lambda} \text{Tr}(A_\lambda M_\lambda^m), \quad (1)$$

where A_λ, M_λ are $n_\lambda \times n_\lambda$ matrices encoding *state preparation and measurement errors*, and the quality of gate implementation, respectively. This formalizes in a precise way the general idea that RB data is well described by a linear combination of exponential decays and allows for the classical processing of RB output data, thus providing the connection between the data-collection and the data-processing phases. Note, however, that if irreducible subrepresentations appear with nontrivial multiplicities the functional form of Eq. (1) includes *matrix* exponential decays. These can have qualitatively different features than scalar exponential decays, requiring a more sophisticated data-processing approach. It is, for instance, possible for these matrices to have *complex* eigenvalue pairs, which will lead to damped-oscillation behavior in randomized benchmarking data.

B. The functional form of randomized benchmarking data

At the core of the RB literature is the promise that RB output data has a very specific form, namely that of a linear

combination of (matrix) exponential decays [as expressed in Eq. (1)], decaying with the length of the sequences of random gates. Moreover, this linear combination is of a specific structure, determined by the implemented gate set. However, this functional form of the RB output data is not guaranteed by the protocol itself, but is instead derived from assumptions on the noisy implementation of the random quantum operations. In early work this assumption took the form of the *gate-independent noise assumption*. Later, it was realized that this assumption is not satisfactory [26] and it was subsequently generalized for standard Clifford RB to the more general assumption that the noisy implementations of gates are Markovian and time independent, and moreover either that the gate-dependent variation of the noise is upper bounded in the diamond norm (in the work of Ref. [24]), or lower bounded in average fidelity (in the work of Ref. [25]). Here, we provide a series of theorems generalizing these works to (almost) all existing RB protocols, justifying Eq. (1) in broad circumstances. The theorems we prove make claims of different strength for different classes of RB protocols, as per the typology outlined in Fig. 2.

- (a) We prove that the output data of *uniform RB* protocols (as per the typology in Fig. 2) can be described as a linear combination of exponentials, up to an

exponentially small error, provided that the gate implementations are Markovian, time independent, and are on average close *in diamond norm* to an ideal implementation that is a representation. This closeness is independent of the particular RB protocol and independent of the underlying Hilbert-space dimension. The complete statement is given as Theorem 8 that can be summarized as follows.

Theorem 1: (Informal version of Theorem 8.) *Consider a RB experiment with sequence length m , with gates uniformly drawn from a group \mathbb{G} and implemented through a reference representation $\omega(g) = \bigoplus_{\lambda \in \Lambda} \sigma_{\lambda}^{\oplus n_{\lambda}}(g)$. Denote the corresponding noisy implementation on the quantum computer as $\phi(g)$ (note that this assumes time independent and Markovian noise). If we have*

$$\frac{1}{|\mathbb{G}|} \sum_{g \in \mathbb{G}} \|\omega(g) - \phi(g)\|_{\diamond} \leq \delta \leq \frac{1}{9}, \quad (2)$$

then the output data $p(m)$ of the RB experiment obeys the relation

$$\left| p(m) - \sum_{\lambda \in \Lambda} \text{Tr}(A_{\lambda} M_{\lambda}^m) \right| \leq O(\delta^m), \quad (3)$$

with the error exponentially suppressed in m . Here A_{λ} and M_{λ} are $n_{\lambda} \times n_{\lambda}$ matrices, with M_{λ} depending only on the actual implementation ϕ .

The proof of this theorem relies on a combination of techniques from earlier works: taking the matrix Fourier-transform perspective introduced to RB in Ref. [25] and combining it with the realization in Ref. [24] that the diamond distance (averaged over random gates) is the correct distance measure for the formulation of assumptions on noisy gate implementations. We also make heavy use of the perturbation theory of invariant subspaces of non-normal matrices [52,53]. We note that the specific parameter $1/9$ is an artifact of the proof techniques and probably suboptimal.

- (b) Building on Theorem 8, we prove multiple theorems for *nonuniform RB* protocols. The first subtype, approximate RB, is covered by Theorem 9, a direct generalization of Theorem 8, and also features an exponentially suppressed error. For the second subtype, subset RB, on the other hand, we can give only a weaker statement, guaranteeing that the RB output data is described by a linear combination of exponentials up to *constant error* (in sequence length) as long as the sequence length m is taken to be larger than a mixing length m_{mix} . This mixing length indicates the moment where the m -fold convolution ν^{*m} of the probability distribution ν , which governs the

sampling of random gates, becomes close to the uniform distribution and is a function of both the initial distribution ν and the underlying group \mathbb{G} . We can summarize our result on subset RB as follows.

Theorem 2: (Informal version of Theorem 10). *Consider a RB experiment with sequence length m , with gates drawn from a group \mathbb{G} according to a probability distribution ν and implemented through a reference representation $\omega(g) = \bigoplus_{\lambda \in \Lambda} \sigma_{\lambda}^{\oplus n_{\lambda}}(g)$. Denote the corresponding (noisy) actual implementation on the quantum computer as $\phi(g)$. If we have, for some sequence length m_{mix} that*

$$\sum_{g \in \mathbb{G}} \nu(g) \|\omega(g) - \phi(g)\|_{\diamond} \leq \frac{\delta}{m_{\text{mix}}}, \quad (4)$$

$$\sum_{g \in \mathbb{G}} \left| \nu^{*m_{\text{mix}}}(g) - \frac{1}{|\mathbb{G}|} \right| \leq \delta', \quad (5)$$

and $\delta + \delta' \leq 1/9$, then the output data $p(m)$ of the RB experiment obeys the relation

$$\left| p(m) - \sum_{\lambda \in \Lambda} \text{Tr}(A_{\lambda} M_{\lambda}^{m-m_{\text{mix}}}) \right| \leq O(\delta + \delta'), \quad (6)$$

with the error bound independent of m . Here A_{λ} and M_{λ} are $n_{\lambda} \times n_{\lambda}$ matrices, with M_{λ} depending only on the actual implementation ϕ .

This theorem cannot guarantee an exponential error bound, but still improves on the state of the art [14,15], both in the generality of the assumptions made and the size of the possible error. Note also the appearance of the m_{mix}^{-1} term in the average diamond-norm deviation. This can be read as the requirement that the generating gates are of sufficiently high quality that any (composite) uniformly randomly chosen gate will be close in diamond norm to its ideal version. In this sense this requirement is of the same stringency as Eq. (2).

- (c) We discuss the behavior of *interleaved RB* protocols, illustrating how standard interleaved RB, as well as all but one nonstandard interleaved RB protocol, are covered by Theorem 8. We consider two nonstandard interleaved RB protocols, namely cycle benchmarking [13], which is covered by our theorems in a nontrivial way and robust RB tomography [50], which is not covered by our theorems. We argue that this is not a weakness of our argument but rather that the RB output data of this protocol behaves in a nonstandard manner, requiring tailor-made analysis.
- (d) In Sec. X, we provide a discussion of the central assumption $|\mathbb{G}|^{-1} \sum_{g \in \mathbb{G}} \|\omega(g) - \phi(g)\|_{\diamond} \leq \delta$, made on the behavior of noisy gates in the above

theorems. We argue that this assumption is a natural one to make (Theorem 18) and moreover that it cannot be replaced by a similar assumption involving the average fidelity without requiring the gate to be exponentially close to perfect in the number of qubits. This also answers an open question posed in Ref. [25] in the negative.

The unifying conceptual theme of all of our theorems is the fact that RB can be seen as a “power iteration in frequency space.” The behavior of the output data is dictated by the dominant eigenvalues of a fixed matrix that is obtained from the Fourier transform [25] (in a specific sense defined later) of the noisy implementation map ϕ . Taking powers of this matrix results in the exponential suppression of all but the largest eigenvalues.

Together, these results provide a rigorous justification for the folkloric knowledge that RB protocols function under broad experimental circumstances.

C. A framework for randomized benchmarking data processing

The second phase of the RB protocol, the data-processing phase, takes in RB output data, which is well described by a linear combination of exponentials and outputs the decay rates associated with those exponentials. If the data is well described by a single exponential decay this can be done by off-the-shelf curve-fitting procedures, but if the RB output data is of a more complex form (such as a linear combination of several exponentials) a more flexible approach is required. Here we provide a self-contained discussion of modern signal-processing methods for extracting decay parameters from data with a functional form given by Eq. (1). We review signal-processing algorithms, in particular the multiple signal classification (MUSIC) and estimation of signal parameters via rational invariance techniques (ESPRIT) algorithms, that are at least, in principle, applicable to the most general form of RB output data, even including matrix exponentials. Beyond that, we discuss theoretical guarantees that were derived for these algorithms and discuss their implications for RB data processing. Building upon these guarantees, we derive a sampling complexity statement that ensures the recovery of decay rates with these algorithms under measurements with finite statistics. We complement our analytical discussion with numerical evaluations and simulations that demonstrate the practical performance of these algorithms. Importantly, our discussions detail the fundamental limitations of postprocessing RB output data featuring many exponential decays.

D. A general postprocessing scheme for isolating exponential decays

Even with modern methods, fitting multiple exponential decays is a difficult affair, and in many scenarios one is

only interested in a subset of the decay parameters that describe the output data of a particular RB experiment. Because of this, several methods have been developed to isolate particular exponential decays. Examples of this include the class of uniform RB protocols without inversion gates (indicated with a double asterisk “**” in Fig. 2) and a variety of other protocols that take linear combinations of RB output data with different ending gates g_{end} to isolate particular exponential decays (indicated with a single asterisk “*”). In Sec. VIII, we give a novel class of protocols called filtered RB that subsumes all these earlier approaches. For simplicity, we consider only uniform RB, but our results generalize to other types of RB.

This class of protocols is based on the realization that RB output data (indexed by an ending gate g_{end}) can be seen as a vector in the group algebra of the group being benchmarked. This allows for the design of *filter functions* $\alpha_\lambda : \mathbb{G} \rightarrow \mathbb{C}$, based on the matrix elements of irreducible representations, that isolate exponential decays associated with subrepresentations of the ideal implementation of the gates in the group \mathbb{G} . Using these filter functions we can write down a general postprocessing scheme for the isolation of exponential decays and prove that it works when the assumptions of Theorem 8 are satisfied. We prove a theorem of the following form.

Theorem 3: [Theorem 16 (informal)]. *Let $\alpha_\lambda : \mathbb{G} \rightarrow \mathbb{C}$ be the filter function associated with the irreducible representation σ_λ and let $p(m, g_{\text{end}})$ be the output data associated with a uniform RB experiment with ending gate g_{end} , satisfying the condition Eq. (2) with parameter δ . We have that*

$$k_\lambda(m) := \frac{1}{|\mathbb{G}|} \sum_{g_{\text{end}} \in \mathbb{G}} \alpha_\lambda(g_{\text{end}}) p(m, g_{\text{end}}) \quad (7)$$

satisfies

$$|k_\lambda(m) - \text{Tr}(B_\lambda M_\lambda^m)| \leq O(\delta^m), \quad (8)$$

with M_λ associated with the irreducible subrepresentation σ_λ [as per Eq. (1)].

Beyond this theoretical result we note that this novel class of protocols allows one (by a simple reparametrization) to eliminate the need for an explicitly implemented inversion gate in RB, making the protocol significantly simpler to implement in practice.

We also give a statistical analysis of this postprocessing scheme. In particular, we prove that if the measurement positive operator-valued measure (POVM) performed in the RB experiment is (proportional to) a state 3-design, the sample complexity of the complete benchmarking procedure (data collection plus postprocessing) is asymptotically independent of the dimension of the underlying

Hilbert space for arbitrary benchmarking groups. This is a strong improvement on previous attempts at such a general postprocessing procedure. Note that the 3-design condition appearing here plays a similar role in controlling the variance in scalable estimation procedures such as shadow estimation [54,55].

We stress, however, that the 3-design condition is a sufficient condition and there are examples in the literature covered by this postprocessing scheme where this condition is not met but the overall procedure is still scalable. In particular, we discuss the recently proposed *linear-cross-entropy benchmarking procedure* (XEB) [29] in Sec. VIII C. We argue that the variant of XEB that performs multiple random gate sequences is an *example of uniform RB* (as per the typology) combined with an instance of our general postprocessing scheme. Furthermore, we argue that the sample complexity of linear XEB is asymptotically independent of the underlying Hilbert-space dimension even though the POVM being measured is not itself a 3-design.

E. Randomized benchmarking and average fidelity

RB has originally been designed to estimate the *average gate fidelity* of a group of gates. Under the assumption of gate-independent noise, it can be proven (as has already been done in Ref. [1]) that the decay rates estimated in a RB experiment correspond exactly to the average fidelity of the noise associated to the gates. However, if this condition is relaxed, the connection between these decay rates and the average fidelity is less clear. Even more strongly, it has been argued in Ref. [26] that due to a so-called gauge freedom in the representation of the gate set, the entire premise of a connection between RB decay rates and average fidelity may be suspect. This is because the choice of the gauge does not influence the RB decay rates, but it does affect the average gate fidelity. Indeed, it has been shown that under some transformations the two quantities may differ by orders of magnitude, even in the gate-dependent noise case (where the previously proven connection can be seen as a “natural” gauge choice).

Subsequently proposals have been made to reconnect the average gate fidelity and RB decay rates in the context of standard Clifford RB: a natural gauge called the depolarizing gauge [25] and the noise-in-between-gates framework. Both of these proposals provide an exact connection between the decay rates of RB and the average fidelity. However, several crucial questions of interpretation have still been left open, and in this work we aim to address some of them, and sharpen others.

In Sec. IX B 2, we substantially generalize both proposed connections between decay rates and average fidelity to RB with *arbitrary* finite groups. What is more, we argue that these two proposals are in fact *equivalent*. Moreover, we present an explicit example of a completely

positive implementation map, which is not completely positive in the depolarizing gauge (or equivalently has non-completely positive noise in-between gates). This implies that both these interpretations of RB decay rates are not fully satisfactory, because they cannot be guaranteed to correspond to the average fidelity of a *physical* process. That said, this does not mean that RB decay rates are not useful figures of merit, as they can always be interpreted as meaningful benchmarks in their own right.

Complementing this, following the approximate approach of Ref. [27], we show that the problem of connecting RB decay rates with the average gate fidelity can be (approximately) reduced to the deviation between the dominant (ideal) unperturbed eigenvectors and their (implemented) perturbed version in Fourier space. We show that, as long as this overlap is sufficiently close to 1, any gauge choice that corresponds to a completely positive and trace-preserving (CPT) channel will connect RB parameters to the average gate fidelity. Hence we obtain, under precise conditions, an approximate version of the connection between average fidelity and RB decay rates.

More formally, we leverage the Fourier-transform framework introduced in Ref. [25] to derive the following expression for the *entanglement fidelity*, which is linearly related to the average fidelity, averaged over all elements of the group as

$$F_e(\phi, \omega) = \frac{1}{d^2} \sum_{\lambda \in \Lambda} d_{\sigma_\lambda} f_{\max}(\sigma_\lambda) \alpha_{\text{overlap}} + \alpha_{\text{res}}, \quad (9)$$

where $f_{\max}(\sigma_\lambda)$ is the RB decay parameter associated with the irreducible subrepresentation σ_λ . In the Fourier framework $f_{\lambda, \max}$ corresponds to the largest eigenvalue of the Fourier transform of the implementation map ϕ evaluated at σ_λ . Furthermore, the parameter α_{overlap} encodes the overlap between the (left and right) eigenvectors associated with this largest eigenvalue, and the eigenvector of the Fourier transform of the reference representation ω evaluated at σ_λ . Finally, the term α_{res} , the residuum, encodes information about the subdominant eigenspaces of the Fourier transform. The factors $\alpha_{\text{overlap}}, \alpha_{\text{res}}$ are gauge dependent. We give bounds on the overlap and residuum in terms of the deviation of ϕ from the reference ω and discuss relevant scenarios where these terms contribute only negligibly to the entanglement fidelity (and thus when RB decay data corresponds approximately to an average fidelity).

F. Nontechnical discussion

In this work, we develop a comprehensive theory of randomized benchmarking. Our main motivation has been our desire to give a mathematical framework for RB and to classify known schemes. It should be clear, however, that our work goes significantly beyond a mere classification of what is present in the literature. Since our

work is in parts rather technical, in the following we formulate a series of “take-home messages”: actionable advice for experimentalists interested in using RB in the laboratory and developing new protocols to suit their needs.

1. **RB gives exponential decays under broad (Markovian) circumstances.** Confirming experimental intuition, and extending earlier results for specific groups, our main result (Theorem 8) proves that RB protocols behave (up to an exponentially small correction factor) as expected whenever the noise afflicting the gate set is Markovian and time independent. Because the correction factor is so small, any deviation from the prescribed functional form can in fact be taken as evidence of non-Markovian or time-dependent noise processes (as suggested earlier by Ref. [24]). We do wish to emphasize that the error term in Theorem 8 can be quite significant for small sequence lengths. Hence we recommend as a rule of thumb that RB experiments should not include very short ($m \leq 5$) sequence lengths, especially when strong gate-dependent (but Markovian) noise is suspected, as this might bias the estimator for the decay rate.
2. **RB is broadly resistant to deviations from uniform sampling.** Similar to robustness against gate-dependent Markovian noise, we prove (Theorem 9) that RB gives correct results even when the group is not being sampled exactly uniformly. This broadly justifies the use of (generically applicable) Markov chain techniques for sampling group elements [14], overcoming a key technical hurdle in running RB protocols with new groups.
3. **The decay rates given by RB can be interpreted as an average fidelity (but caveats apply).** We find that the decay rates of general RB experiments can always be exactly associated to the average fidelity of a fixed process, however, this process need not be physical (i.e., it does not always correspond to a completely positive and trace-preserving map). Alternatively, we show that RB decay rates can always be connected approximately to the average fidelity of a physical process, but the degree of approximation is dependent upon external beliefs about the underlying noise process. Hence, we believe the interpretation of RB decay rates as an average fidelity to be broadly valid, but subject to technical caveats.

These three messages can be considered folklore knowledge in the RB community, for which we provide a rigorous underpinning. However, our work also contains new conceptual developments, notably the following.

1. **Filtering scalably extends RB to a large class of groups.** As formalized in Sec. VII, a major practical hurdle to applying RB with *arbitrary* finite groups, is that this generically requires the fitting of output data to multiexponential decays. This is a difficult problem both in theory and in practice and it has so far contributed to the limited experimental use of RB beyond a few groups (such as the Clifford group). Our new procedure, which we call *filtering* (or filtered RB), takes a major step towards solving this problem by giving a generic procedure for isolating exponential decays in a fully scalable manner. This approach is discussed in great detail in Sec. VIII, with the protocol given explicitly in Algorithm Box 2. This procedure is guaranteed to be scalable for all groups as long as the measurement POVM forms a 3-design, but we believe that it applies beyond that (see, in particular, the example of linear cross-entropy benchmarking discussed in Sec. VIII C).
2. **Inversion gates are not required for RB.** Another key practical difficulty in performing randomized benchmarking has been the necessity to compute and implement a global inversion gate. However, filtered RB has the bonus property that it does not require the application of inverses. Instead a random noisy gate sequence can be directly compared to a perfect classical simulated version to extract the same RB decay rates, making the quantum part of the protocol significantly easier to implement. However, this simplicity is gained at a (constant) extra sampling overhead, as the inversion gate in standard RB also suppresses the sampling complexity [56].

With these new contributions, our framework serves as a convenient basis to design new schemes that *come with rigorous performance bounds built in*. We expect this to facilitate and accelerate the development of more sophisticated and tailor-made benchmarking schemes as required by experimental practitioners. Steps in this direction have already been made [57–59]. In particular, Ref. [58] explores the framework put forth here for continuous groups of quantum gates.

G. Structure of this work

In Sec. III, we discuss mathematical preliminaries: we set the notation for the rest of the work and recall standard notions from representation theory. This section can be skipped by experienced readers.

In Sec. IV, we discuss implementation maps: linear maps from finite groups to superoperators, a central concept in our treatment of RB. We also give an introduction into matrix-valued Fourier theory and explicitly state

several results from the perturbation theory of non-normal matrices, which we use throughout the rest of the work.

In Sec. V, we give a general framework for RB, with its two phases: the *data-collection* and *data-processing phases*, and give a general protocol for the data-collection phase. This protocol, which depends on a range of input parameters, covers (the data-collection phase of) all known versions of RB. We also discuss a typology of RB schemes, dividing up the known protocols into a few generic classes.

In Sec. VI, we present a series of general theorems that govern the behavior of the output data of a RB protocol. We confirm the folklore knowledge that RB data is well described by a linear combination of (matrix) exponentials, under some general assumptions.

In Sec. VII, we discuss general procedures for extracting decay parameters from RB output data. We discuss implementation and general limitations and prove a sampling complexity statement for RB.

In Sec. VIII, we propose a general postprocessing method for isolating exponential decays associated with particular subrepresentations. We argue that this postprocessing method covers many previously proposed procedures. We also prove a sufficient condition under which this postprocessing scheme is scalable for any RB protocol and analyze linear cross-entropy benchmarking as an example.

In Sec. IX, we discuss the relation between the decay rates generated by RB and the average fidelity, focusing in particular on the gauge freedom in the presentation of the underlying noise channels.

Finally, in Sec. X, we finally argue that the assumptions made in Sec. VI are natural and in some sense necessary for the correct behavior of RB.

III. PRELIMINARIES: QUANTUM CHANNELS AND GROUP REPRESENTATIONS

In this section, we go over some of the basic mathematical machinery needed to talk about randomized benchmarking and prove our central theorems. We discuss quantum channels and their matrix representations (Sec. III A), and groups and group representations (Sec. III B). This is fairly standard material, and beyond the setting of notation it can be skipped by an experienced reader.

We begin by setting the stage and introducing some basic notation used throughout our work. We denote complex vector spaces by V or more explicitly by \mathbb{C}^d . We denote by \mathcal{M}_d the vector space of complex linear transformation of \mathbb{C}^d and by \mathcal{S}_d the space of linear transformations of \mathcal{M}_d , often called superoperators. Here d is an integer that in many cases can be thought of as being a power of 2 ($d = 2^q$), however, all theorems are valid for general d unless explicitly stated. We denote by Tr_V the partial trace over a tensor factor V (of an implied tensor product space

$V \otimes W$ for some W). Finally we denote the complex conjugate by a bar (i.e., \bar{A} is the entrywise complex conjugate of A).

A. Quantum channels and the operator-matrix representation

Unitary operations as they are generated by quantum gates—in the focus of attention in this work—are quantum channels. Formally, quantum channels are superoperators, that is elements of \mathcal{S}_d , that are trace preserving and completely positive. In order to represent quantum channels (and elements of \mathcal{S}_d more generally), we make use of the *operator matrix representation*. Given a quantum channel $\mathcal{E} \in \mathcal{S}_d$, we can represent it as an element of \mathcal{M}_{d^2} by choosing an orthonormal basis (with respect to the trace or Hilbert-Schmidt inner product) $\{b_j\}_{j=1}^{d^2}$ for \mathcal{M}_d . Thus \mathcal{E} (abusing notation) is a $d^2 \times d^2$ matrix with components

$$\mathcal{E}_{j,k} := \text{Tr} \left[b_j^\dagger \mathcal{E}(b_k) \right]. \quad (10)$$

Analogously, (density) matrices $\rho \in \mathcal{M}_d$ can be represented as vectors,

$$|\rho\rangle\rangle = \begin{pmatrix} \rho_1 \\ \rho_2 \\ \dots \\ \rho_{d^2} \end{pmatrix} \quad \text{with} \quad \rho_k := \text{Tr} \left[b_k^\dagger \rho \right]. \quad (11)$$

Note that the action $\mathcal{E}(\rho)$ now corresponds to a matrix-vector multiplication $\mathcal{E}|\rho\rangle\rangle$ and the concatenation of two channels \mathcal{E} and \mathcal{E}' into a matrix multiplication $\mathcal{E}\mathcal{E}'$. We can analogously write a (POVM element) matrix $\Pi \in \mathcal{M}_d$ as a covector

$$\langle\langle \Pi | = (\Pi_1 \ \Pi_2 \ \dots \ \Pi_{d^2}) \quad \text{with} \\ \Pi_k := \langle\langle \Pi, b_k \rangle\rangle = \text{Tr} [\Pi b_k]. \quad (12)$$

With this, the probability to obtain an outcome described by the POVM element Π when measuring ρ is $p(\Pi|\rho) = \langle\langle \Pi, \rho \rangle\rangle = \text{Tr}[\Pi\rho]$.

B. Representations of groups

At the heart of our discussion are notions of representations of groups. In this section, we hence recall some basic facts about the representations of finite (and compact) groups over complex vector spaces, with a focus on their use in quantum computation. For a more in-depth treatment of this topic we refer to Refs. [60,61]. In this work we restrict our attention to finite groups keeping the notation more concise. Most results can be analogously stated for continuous, compact groups and derived following the same strategy. Reference [58] carefully discusses the required modifications and gives explicit reformulations for continuous compact groups.

1. Representations

Let \mathbb{G} be a finite group and consider the space \mathcal{M}_d of linear transformations of \mathbb{C}^d . A representation ω is a map $\omega : \mathbb{G} \rightarrow \mathcal{M}_d$ that preserves the group multiplication, i.e.,

$$\omega(g)\omega(h) = \omega(gh), \quad \forall g, h \in \mathbb{G}. \quad (13)$$

We require the operators $\omega(g)$ to be unitary as well (for finite groups this can always be done).

2. Reducible and irreducible representations

If there is a nontrivial subspace W of \mathbb{C}^d such that for all vectors $w \in W$ we have

$$\omega(g)w \in W, \quad \forall g \in \mathbb{G}, \quad (14)$$

then the representation ω is called *reducible*. The restriction of ω to the subspace W is also a representation, which we call a *subrepresentation* of ω . If there are no nontrivial subspaces W such that Eq. (14) holds the representation ω is called *irreducible*. We generally reserve the letter σ to denote irreducible representations.

Two representations ω, ω' of a group \mathbb{G} are called *equivalent* if there exists an invertible linear map T such that

$$T\omega(g) = \omega'(g)T, \quad \forall g \in \mathbb{G}. \quad (15)$$

We denote this by $\omega \simeq \omega'$. For finite groups \mathbb{G} the set of irreducible representations (up to the above equivalence) is finite. We denote it by $\text{Irr}(\mathbb{G})$.

3. Sums, products, and Maschke's lemma

We make use of sums and products of representations. Given representations ω, ω' , the maps

$$\omega \oplus \omega' : \mathbb{G} \rightarrow \mathcal{M}_d \oplus \mathcal{M}_{d'} : g \mapsto \omega(g) \oplus \omega'(g), \quad (16)$$

$$\omega \otimes \omega' : \mathbb{G} \rightarrow \mathcal{M}_d \otimes \mathcal{M}_{d'} : g \mapsto \omega(g) \otimes \omega'(g), \quad (17)$$

are again representations. They are, however, generally not irreducible (even if ω and ω' are). However, Maschke's lemma ensures that every representation ω of a group can be uniquely written as a direct sum of irreducible representations, that is

$$\omega(g) \simeq \bigoplus_{\lambda \in \Lambda} \sigma_\lambda(g)^{\oplus n_\lambda}, \quad \forall g \in \mathbb{G}, \quad (18)$$

where the index set Λ is a subset of the set $\text{Irr}(\mathbb{G})$ and n_λ is an integer denoting the number of copies (or multiplicity) of σ_λ present in ω .

4. Characters

Characters are a central object in representation theory, given by the trace of a representation.

Definition 4: (Character of a representation). The character χ_ω of a representation ω of a group \mathbb{G} is defined as

$$\chi_\omega(g) = \text{Tr}[\omega(g)]. \quad (19)$$

One of the most important properties for characters of irreducible representations is the following orthogonality relation.

Proposition 5: (Orthogonality formula). *Let $\chi_\lambda, \chi_{\lambda'}$ be the characters of two irreducible representations $\sigma_\lambda, \sigma_{\lambda'}$ of a group \mathbb{G} . Then*

$$\frac{1}{|\mathbb{G}|} \sum_{g \in \mathbb{G}} \bar{\chi}_\lambda(g) \chi_{\lambda'}(g) = \begin{cases} 1 & \text{if } \sigma_\lambda \simeq \sigma_{\lambda'} \\ 0 & \text{if } \sigma_\lambda \not\simeq \sigma_{\lambda'}. \end{cases} \quad (20)$$

5. Projections onto irreducible representation

Given a representation $\omega = \bigoplus_{\lambda \in \Lambda} \sigma_\lambda^{\oplus n_\lambda}$ on a vector space $V_\omega = \bigoplus V_\lambda^{\oplus n_\lambda}$ we can choose a basis $\{v_j^\lambda \mid j \in 1, \dots, d_\lambda\}$ for each V_λ . Each vector v in V_ω can thus be written as a linear combination $v = \sum_{\lambda \in \Lambda} \sum_{j=1}^{d_\lambda} c_j^\lambda v_j^\lambda$. We can conversely identify the basis vector components of any vector v by application of an appropriate projection P_j^λ , such that $P_j^\lambda v = c_j^\lambda v_j^\lambda$, where

$$P_j^\lambda = \frac{d_\lambda}{|\mathbb{G}|} \sum_{g \in \mathbb{G}} [\bar{\sigma}_\lambda(g)]_{j,j} \omega(g). \quad (21)$$

Note that, in order to construct these projections, the knowledge of the diagonal elements of the corresponding irreducible representation σ_λ is required. However, it is also possible to project any vector onto distinct irreducible subspaces (up to multiplicity) by using only knowledge of the character of a representation:

$$P_\lambda = \frac{d_\lambda}{|\mathbb{G}|} \sum_{g \in \mathbb{G}} \bar{\chi}_\lambda(g) \omega(g). \quad (22)$$

This last formula follows simply from the definition of the character as $\chi_\lambda(g) = \text{Tr}[\sigma_\lambda(g)]$.

IV. FOURIER TRANSFORMS AND PERTURBATION THEORY OF IMPLEMENTATION MAPS

In this section, we review the concept of *group implementation maps* and their *Fourier theory* (Sec. IV B).

Mathematically this corresponds to noncommutative harmonic analysis of matrix-valued functions. We also discuss perturbation theory for non-normal matrices. This material is somewhat less well known, so we spend more time discussing these concepts.

A. Implementation maps

Given a group \mathbb{G} , we can assign quantum circuits [elements of $U(d)$] to each group element, which gives rise to a representation of the group. However, in practice, quantum circuits will not be executed perfectly, but rather include noise. This noise can be modeled by a quantum channel, and we can thus envision assigning to each group element a quantum channel modeling the real implementation of that circuit. These quantum channels can be composed, but this composition will not necessarily maintain group structure and will thus in general not form a representation. However, we can define the more general concept of an “implementation map” ϕ , which is a function from a finite group \mathbb{G} to the space of superoperators \mathcal{S}_d ,

$$\phi : \mathbb{G} \rightarrow \mathcal{S}_d, \quad (23)$$

where we usually assume that $\phi(g)$ is a trace nonincreasing quantum channel for all g . If we want to draw explicit attention to this fact we call ϕ completely positive if and only if $\phi(g)$ is completely positive for all $g \in \mathbb{G}$. Finally, note that if $\phi(g)\phi(h) = \phi(gh)$ for all $g, h \in \mathbb{G}$ then ϕ would be a representation. We can think of the implementation map as being an abstract presentation of the noisy implementation of the group elements, which depends on the noise processes in the quantum computer but also on other choices such as the compilation of circuits into elementary gates.

B. Fourier transforms of implementation maps

When considering an implementation map one can ask precisely when it is a representation, and failing that, if it is close to a representation (in some reasonable way). To answer this question we need to introduce some mathematical machinery. This machinery was first introduced into the theory of randomized benchmarking by Ref. [25], based on work by Gowers and Hatami [62], which is itself a partial review of older mathematical work. In this section, we consider general maps ϕ from a group \mathbb{G} to a space of $d \times d$ matrices \mathcal{M}_d . Thinking of \mathcal{S}_d as a matrix space, our notion of implementation map can be seen to be a special case of these maps. Given a map ϕ we define its *Fourier transform* $\mathcal{F}(\phi)$ as

$$\mathcal{F}(\phi)[\sigma_\lambda] = \frac{1}{|\mathbb{G}|} \sum_{g \in \mathbb{G}} \overline{\sigma_\lambda}(g) \otimes \phi(g) \quad (24)$$

for all $\lambda \in \text{Irr}(\mathbb{G})$. So the Fourier transform $\mathcal{F}(\phi)$ is a function from the set $\text{Irr}(\mathbb{G})$ of irreducible representations of \mathbb{G}

to a set of matrices. This definition has all the properties of a Fourier transform. Firstly, it has an inverse transform, which maps $\mathcal{F}(\phi)$ back to ϕ , given by

$$\mathcal{F}^{-1}[\mathcal{F}(\phi)](g) = \sum_{\lambda \in \text{Irr}(\mathbb{G})} d_\lambda \text{Tr}_{V_\lambda} \{ \mathcal{F}(\phi)[\sigma_\lambda] \overline{\sigma_\lambda}(g^{-1}) \otimes \mathbb{1} \} \quad (25)$$

for all $g \in \mathbb{G}$ and where d_λ is the dimension of V_λ , the space on which the representation σ_λ acts.

Secondly, it has the correct behavior with respect to convolutions of implementation maps: the Fourier transform of a convolution corresponds to a product of Fourier transforms. Recalling the definition of a convolution of two implementation maps ϕ, ϕ'

$$\phi * \phi'(g) = \frac{1}{|\mathbb{G}|} \sum_{g' \in \mathbb{G}} \phi(gg'^{-1})\phi'(g') \quad (26)$$

we can easily see the following:

$$\begin{aligned} \mathcal{F}(\phi * \phi')[\sigma_\lambda] &= \frac{1}{|\mathbb{G}|} \sum_{g, g' \in \mathbb{G}} \overline{\sigma_\lambda}(g) \otimes \phi(gg'^{-1})\phi'(g') \\ &= \frac{1}{|\mathbb{G}|} \sum_{g, g' \in \mathbb{G}} \overline{\sigma_\lambda}(gg') \otimes \phi(g)\phi'(g') \\ &= \mathcal{F}(\phi)[\sigma_\lambda] \mathcal{F}(\phi')[\sigma_\lambda] \end{aligned} \quad (27)$$

for all $\lambda \in \text{Irr}(\mathbb{G})$. Another useful property is the Parseval identity

$$\begin{aligned} &\frac{1}{|\mathbb{G}|} \sum_{g \in \mathbb{G}} \text{Tr}[\phi(g)^\dagger \phi'(g)] \\ &= \sum_{\lambda \in \text{Irr}(\mathbb{G})} d_\lambda \text{Tr}\{\mathcal{F}(\phi)[\sigma_\lambda]^\dagger \mathcal{F}(\phi')[\sigma_\lambda]\}. \end{aligned} \quad (28)$$

Finally, we note that the Fourier transform (evaluated at an irreducible representation) of a representation is an orthogonal projector with its rank given by the multiplicity of that irreducible representation. To see this, consider a representation $\omega = \bigoplus_{\lambda \in \Lambda} \sigma_\lambda^{\oplus n_\lambda}$. We have that

$$\begin{aligned} \{\mathcal{F}(\omega)[\sigma_{\lambda'}]\}^2 &= \frac{1}{|\mathbb{G}|^2} \sum_{g, g' \in \mathbb{G}} \overline{\sigma_{\lambda'}}(gg') \otimes \omega(gg') \\ &= \frac{|\mathbb{G}|}{|\mathbb{G}|^2} \sum_{g \in \mathbb{G}} \overline{\sigma_{\lambda'}}(g) \otimes \omega(g) = \mathcal{F}(\omega)[\sigma_{\lambda'}] \end{aligned} \quad (29)$$

for all $\lambda' \in \text{Irr}(\mathbb{G})$. Moreover for $\lambda' \in \Lambda$ we have

$$\text{Tr}\{\mathcal{F}(\omega)[\sigma_{\lambda'}]\} = \frac{1}{|\mathbb{G}|} \sum_{g \in \mathbb{G}} \overline{\chi_{\sigma_{\lambda'}}}(g) \chi_\omega(g) = n_{\lambda'} \quad (30)$$

by the character orthogonality formula.

1. Fourier operators

We also give another, useful way to think about the matrix Fourier transform, namely in terms of what we call *Fourier operators*.

Note that the set of maps $\phi \rightarrow \mathcal{S}_d$ can be seen as a vector space under pointwise addition (of the superoperators). We can further lift this vector space to an algebra by considering the convolution operator $*$ [as defined in Eq. (26)] on the functions in the vector space. We can construct a faithful (i.e., injective) matrix representation of this algebra as

$$\begin{aligned} F(\phi) &= \frac{1}{|\mathbb{G}|} \sum_{g \in \mathbb{G}} \bigoplus_{\lambda \in \text{Irr}(\mathbb{G})} \bar{\sigma}_\lambda(g) \otimes \phi(g) \\ &= \frac{1}{|\mathbb{G}|} \sum_{g \in \mathbb{G}} \overline{\omega_{\mathbb{G}}}(g) \otimes \phi(g), \end{aligned} \quad (31)$$

with $\omega_{\mathbb{G}} = \bigoplus_{\lambda \in \text{Irr}(\mathbb{G})} \sigma_\lambda$. This is just the Fourier transform of ϕ gathered in a direct sum [note that $\text{Irr}(\mathbb{G})$, and hence the sum, is finite for any finite group]. By the Peter-Weyl theorem for finite groups one can equally well think of $\omega_{\mathbb{G}}(g)$ as an element of the group algebra $\mathbb{C}[\mathbb{G}]$ associated with \mathbb{G} , we do not use this point of view explicitly. We call $F(\phi)$ the *Fourier operator* of ϕ . From the properties of the Fourier transform we immediately see that $F(\phi)F(\phi') = F(\phi * \phi')$. It is useful to equip the algebra of Fourier operators with several norms, based on the diamond norm $\|\cdot\|_\diamond$ for \mathcal{S}_d (in principle, this construction will work for any norm on \mathcal{S}_d). We define

$$\begin{aligned} \|F(\phi)\|_{\max} &= \max_{g \in \mathbb{G}} \left\| \text{Tr}_{V_{\omega_{\mathbb{G}}}} [D_{\omega_{\mathbb{G}}} \overline{\omega_{\mathbb{G}}}(g^{-1}) \otimes \mathbb{1}F(\phi)] \right\|_\diamond \\ &= \max_{g \in \mathbb{G}} \|\phi(g)\|_\diamond, \end{aligned} \quad (32)$$

$$\begin{aligned} \|F(\phi)\|_m &= \frac{1}{|\mathbb{G}|} \sum_{g \in \mathbb{G}} \left\| \text{Tr}_{V_{\omega_{\mathbb{G}}}} [D_{\omega_{\mathbb{G}}} \overline{\omega_{\mathbb{G}}}(g^{-1}) \otimes \mathbb{1}F(\phi)] \right\|_\diamond \\ &= \frac{1}{|\mathbb{G}|} \sum_{g \in \mathbb{G}} \|\phi(g)\|_\diamond, \end{aligned} \quad (33)$$

where $D_{\omega'} = \bigoplus_{\lambda \in \text{Irr}(\mathbb{G})} d_\lambda \mathbb{1}_\lambda$ collects the relevant dimensional factors and where the second equality follows from the properties of the Fourier transform. These norms are bona fide matrix norms on the algebra of Fourier operators, notably they are submultiplicative, viz.,

$$\begin{aligned} \|F(\phi)F(\phi')\|_{\max} &= \|F(\phi * \phi')\|_{\max} = \max_{g \in \mathbb{G}} \|\phi * \phi'(g)\|_\diamond \\ &\leq \max_{g \in \mathbb{G}} \frac{1}{|\mathbb{G}|} \sum_{\hat{g} \in \mathbb{G}} \|\phi(g\hat{g}^{-1})\|_\diamond \|\phi'(\hat{g})\|_\diamond \end{aligned}$$

$$\begin{aligned} &\leq \max_{g, \hat{g} \in \mathbb{G}} \|\phi(g)\|_\diamond \|\phi'(\hat{g})\|_\diamond \\ &= \|F(\phi)\|_{\max} \|F(\phi')\|_{\max} \end{aligned} \quad (34)$$

and similarly for $\|\cdot\|_m$. We also have an identity involving both norms

$$\|F(\phi)F(\phi')\|_{\max} = \|F(\phi * \phi')\|_{\max} = \max_{g \in \mathbb{G}} \|\phi * \phi'(g)\|_\diamond \quad (35)$$

$$\begin{aligned} &\leq \max_{g \in \mathbb{G}} \frac{1}{|\mathbb{G}|} \sum_{\hat{g} \in \mathbb{G}} \|\phi(g\hat{g}^{-1})\|_\diamond \|\phi'(\hat{g})\|_\diamond \\ &= \|F(\phi)\|_{\max} \|F(\phi')\|_m, \end{aligned} \quad (36)$$

which will be helpful later.

C. Perturbation theory

In this section, we gather some technical tools from matrix perturbation theory that are essential to many of the proofs in this paper. Our sources for this section are the standard books of Stewart and Sun [53] and Kato [52]. For the rest of this section, we assume that $\|\cdot\|$ denotes a submultiplicative matrix norm on \mathcal{M}_d , i.e., $\|AB\| \leq \|A\| \|B\|$ for all $A, B \in \mathcal{M}_d$.

Let $A \in \mathcal{M}_d$ be a complex Hermitian matrix. Assume that there exists a unitary matrix $X = [X_1, X_2]$ such that the columns of X_1 and X_2 span invariant subspaces of A , that is

$$[X_1, X_2]^\dagger A [X_1, X_2] = \begin{pmatrix} A_1 & 0 \\ 0 & A_2 \end{pmatrix}, \quad (37)$$

with $A_1 = X_1^\dagger A X_1$ and $A_2 = X_2^\dagger A X_2$. We call this a *spectral resolution* of A . We can think of A_1, A_2 as the matrix A restricted to subspaces of \mathbb{C}^d spanned by the columns of X_1, X_2 , respectively, and furthermore we assume that the eigenvalues of A_1 are all distinct from the ones of A_2 : the subspaces are then said to be *simple*. These subspaces are invariant under the action of A in the sense that $A X_1 = X_1 A_1$ and are hence called invariant subspaces. It turns out that spectral resolutions, and invariant subspaces more generally, are stable against (small) perturbations. That is, given a perturbation matrix E (not necessarily Hermitian) we can find matrices $R = [R_1, R_2]$ and $L = [L_1, L_2]$ such that $L^\dagger = R^{-1}$ and

$$[L_1, L_2]^\dagger (A + E) [R_1, R_2] = \begin{pmatrix} A'_1 & 0 \\ 0 & A'_2 \end{pmatrix} \quad (38)$$

for some A'_1, A'_2 and the matrices R, L are close to X in a well-specified sense. This is what one would expect from a perturbation theorem. It, however, holds only if the perturbation E is small with respect to the difference between

A_1 and A_2 . This difference is made quantitative by the so-called separation function:

$$\text{sep}(A_1, A_2) = \min_{Z \neq 0} \frac{\|A_1 Z - Z A_2\|}{\|X_1 Z X_2^\dagger\|}. \quad (39)$$

This separation function has some rather nice properties. Firstly, it is symmetric in its arguments:

$$\text{sep}(A_1, A_2) = \text{sep}(A_2, A_1). \quad (40)$$

Secondly, it is stable against perturbations, i.e., given a perturbation $A + E$ of A we have

$$|\text{sep}(A_1 + E_1, A_2 + E_2) - \text{sep}(A_1, A_2)| \leq \|E_1\| + \|E_2\|. \quad (41)$$

With this function we can state the following theorem, which can be derived from Theorem 2.8 in Ref. [53, p. 238].

Theorem 6: (Reference [53]). *Let A be a complex Hermitian matrix with spectral resolution $\text{diag}(A_1, A_2)$ induced by a unitary $X = [X_1, X_2]$. Also, let $\|\cdot\|$ be a matrix norm. Now let E be a complex matrix. If E has the properties*

$$\frac{\|X_1^\dagger E X_2\| \|X_2^\dagger E X_1\|}{[\text{sep}(A_1, A_2) - \|X_1^\dagger E X_1\| - \|X_2^\dagger E X_2\|]^2} < \frac{1}{4}, \quad (42)$$

$$\frac{\|X_1^\dagger E X_2\| \|X_2^\dagger E X_1\| + \|X_1^\dagger E X_2\| \|X_1^\dagger E X_2\|}{[\text{sep}(A_1, A_2) - \|X_1^\dagger E X_1\| - \|X_2^\dagger E X_2\|]^2} < \frac{1}{2} \quad (43)$$

then there exist matrices P_1, P_2 such that

$$\|P_1\| \leq \frac{\|X_2^\dagger E X_1\|}{\text{sep}(A_1, A_2) - \|X_1^\dagger E X_1\| - \|X_2^\dagger E X_2\|}, \quad (44)$$

$$\|P_2\| \leq \frac{\|X_2^\dagger E X_1\|}{\text{sep}(A_1, A_2) - \|X_1^\dagger E X_1 + X_1^\dagger E X_2 P_1\| - \|X_2^\dagger E X_2 - P_1 X_1^\dagger E X_2\|} \quad (45)$$

and

$$[L_1, L_2]^\dagger (A + E) [R_1, R_2] = \begin{pmatrix} A'_1 & 0 \\ 0 & A'_2 \end{pmatrix}, \quad (46)$$

with

$$[R_1, R_2] = [X_1, X_2] \begin{pmatrix} \mathbb{1} & 0 \\ P_1 & I \end{pmatrix} \begin{pmatrix} \mathbb{1} & P_2 \\ 0 & I \end{pmatrix}, \quad (47)$$

$$[L_1, L_2]^\dagger = \begin{pmatrix} \mathbb{1} & -P_2 \\ 0 & I \end{pmatrix} \begin{pmatrix} \mathbb{1} & 0 \\ -P_1 & I \end{pmatrix} [X_1, X_2]^\dagger, \quad (48)$$

and $A'_1 = A_1 + X_1^\dagger E X_1 - X_2^\dagger E X_1 P_1$ and $A'_2 = A_2 + X_2^\dagger E X_2 - P_1 X_1^\dagger E X_2$. Equivalently, we have

$$A + E = R_1 A'_1 L_1^\dagger + R_2 A'_2 L_2^\dagger. \quad (49)$$

Proof. From the first property in Eq. (42), and Theorem 2.8 in Ref. [53] we conclude the existence of a matrix P_1 such that

$$\|P_1\| \leq \frac{\|X_2^\dagger E X_1\|}{\text{sep}(A_1, A_2) - \|X_2^\dagger E X_2\| - \|X_1^\dagger E X_1\|}, \quad (50)$$

and

$$\begin{aligned} & \begin{pmatrix} \mathbb{1} & 0 \\ -P_1 & I \end{pmatrix} [X_1, X_2]^\dagger (A + E) [X_1, X_2] \begin{pmatrix} \mathbb{1} & 0 \\ P_1 & I \end{pmatrix} \\ &= \begin{pmatrix} A'_1 & E_{12} \\ 0 & A'_2 \end{pmatrix}, \end{aligned} \quad (51)$$

with $E_{12} = X_1^\dagger E X_2$ and $A'_1 = A_1 + X_1^\dagger E X_1 - X_2^\dagger E X_1 P_1$ and $A'_2 = A_2 + X_2^\dagger E X_2 - P_1 X_1^\dagger E X_2$. Now considering the above as a perturbation of $A' = \begin{pmatrix} A'_1 & 0 \\ 0 & A'_2 \end{pmatrix}$ we can apply Theorem 2.8 from Ref. [53] again so long as

$$\text{sep}(A'_2, A'_1) > 0. \quad (52)$$

Using the stability and symmetry of the sep function a necessary condition for the above is

$$\begin{aligned} & \text{sep}(A_1, A_2) - \|X_1^\dagger E X_1 + X_1^\dagger E X_2 P\| \\ & - \|X_1^\dagger E X_1 - P X_1^\dagger E X_2\| > 0, \end{aligned} \quad (53)$$

which by submultiplicativity and the norm bound on P_1 is true if the second property in Eq. (42) holds. Hence Theorem 2.8 in Ref. [53] provides for the existence of a P_2 with norm bound

$$\|P_2\| \leq \frac{\|X_2^\dagger EX_1\|}{\text{sep}(A_1, A_2) - \|X_2^\dagger EX_2 + X_1^\dagger EX_2 P_1\| - \|X_2^\dagger EX_2 - P_1 X_1^\dagger EX_2\|} \quad (54)$$

and the property that

$$[L_1, L_2]^\dagger (A + E)[R_1, R_2] = \begin{pmatrix} A'_1 & 0 \\ 0 & A'_2 \end{pmatrix}, \quad (55)$$

with

$$[R_1, R_2] = [X_1, X_2] \begin{pmatrix} \mathbb{1} & 0 \\ P_1 & I \end{pmatrix} \begin{pmatrix} \mathbb{1} & P_2 \\ 0 & I \end{pmatrix}, \quad (56)$$

$$[L_1, L_2]^\dagger = \begin{pmatrix} \mathbb{1} & -P_2 \\ 0 & I \end{pmatrix} \begin{pmatrix} \mathbb{1} & 0 \\ -P_1 & I \end{pmatrix} [X_1, X_2]^\dagger. \quad (57)$$

■

We note that in Eq. (42) the first property implies the second if $\|X_1^\dagger EX_2\| \leq \|X_2^\dagger EX_1\|$.

While eigenvalues and invariant subspaces are stable under small perturbations (as discussed above), that is, they are holomorphic functions with respect to analytic perturbations, the same is not true for eigenvectors. This is due to the fact that a vector basis spanning a multidimensional eigenspace is not uniquely determined, and thus the eigenvectors of the perturbed eigenspace may be completely different from the unperturbed basis. However, if an unperturbed eigenvalue a_1 is simple, the related eigenvector x_1 is unique (up to a scalar factor), and it is thus stable. We can make this more explicit by specializing Theorem 6 to simple invariant subspaces of dimension one. Let us again consider a Hermitian matrix A and adopt a unitary basis transformation $X = [x_1, X_2]$ so that

$$[x_1, X_2]^\dagger A [x_1, X_2] = \begin{pmatrix} a_1 & 0 \\ 0 & A_2 \end{pmatrix}, \quad (58)$$

where $A_2 \in \mathcal{M}_{d-1}$. In this specific setting, the separation function becomes [63]

$$\text{sep}(a_1, A_2) = \|(a_1 \mathbb{1} - A_2)^{-1}\|^{-1}. \quad (59)$$

From Theorem 6, we then have the following.

Corollary 7: (Perturbation of a 1-dim simple subspace). *The left and right perturbed eigenvectors originated from x_1 are*

$$\begin{aligned} r_1 &\approx x_1 + X_2 (a_1 \mathbb{1} - A_2)^{-1} X_2^\dagger E x_1 \quad \text{and} \\ \ell_1^\dagger &\approx x_1^\dagger + x_1^\dagger E X_2 (a_1 \mathbb{1} - A_2)^{-1} X_2^\dagger, \end{aligned} \quad (60)$$

where we neglect terms $O(\|E\|^2)$.

Finally, to analyze perturbations of eigenvalues, we make use of the Bauer-Fike Theorem [53, Theorem 1.6]: let A be diagonalizable such that $S^{-1}AS = \text{diag}[(a_j)_j]$ and let E be an arbitrary operator of the same dimension. Then, for any eigenvalue \tilde{a} of $A + E$, the bound

$$|\tilde{a} - a_j| \leq \|S\| \|S^{-1}\| \|E\| \quad (61)$$

is satisfied for some eigenvalue a_j in any vector-induced norm. This implies that, if A is Hermitian, then

$$|\tilde{a} - a_j| \leq \|E\|. \quad (62)$$

V. THE RANDOMIZED BENCHMARKING PROTOCOL

The name randomized benchmarking is conventionally given to a class of methods that assess the quality of a set of quantum gates. These methods are probabilistic, and can be seen as constructing an estimator for a quantity that captures some notion of gate quality. In this section, we make an attempt at *defining* randomized benchmarking. By this we mean that we attempt to organize and make explicit various ideas that have been present in the literature. We begin (in Sec. V A) by dividing RB into two parts: a data-collection phase and a data-processing phase. These correspond roughly to the parts of RB performed on a quantum computer and on a classical computer, respectively. Within this division we focus first on the data-collection phase. In Secs. V B and V C, we give a general protocol for the data-collection phase of RB. This general protocol depends on a number of input parameters, and we can obtain every known RB protocol from a choice of these input parameters. We complement this protocol with a classification of RB protocols into a few types in Sec. V D. This classification, which pertains only to the data-collection phase of RB is largely a formalization of knowledge implicit in the literature but we see that it is a useful organizing tool when proving theorems about the data generated by RB. This data we discuss in Sec. V E.

We note that the output of RB data is assumed to be of a very particular form, namely that of a linear combination of (matrix) exponential decays. However, this form is incumbent upon assumptions on the quantum computer on which (the data-collection phase of) RB is implemented. We discuss what assumptions have been made before in the literature and propose our own set of assumptions, which we justify later in the text.

A. The data-collection and data-processing phases

RB is composed of two major parts, a *data-collection phase* and a *data-processing phase*. The data-collection phase consists of what one typically thinks of as RB: one randomly selects a sequence of quantum gates and applies them to a quantum state together with a global inverse, and measures the resulting state. Averaging over many random choices of these gates one obtains RB output data that depends on the length of the random sequence in a controlled way. This vague description can be made more precise in many different ways and we provide a general framework for this procedure in the next few subsections.

The data-processing phase, on the other hand, consists of what one then does with the data given by a RB experiment. This can be as simple as fitting the data to an exponential decay, but in many cases also involves more sophisticated processing techniques. The key feature of the RB protocol that allows for a structured approach to data processing is the fact that the RB output data has a very controlled form. We discuss this form in Sec. VE after more formally discussing the data-collection phase of RB.

B. Input parameters

The data-collection phase of a RB procedure is characterized by a set of input parameters. These input parameters fully define a protocol (which we write down in Sec. VC) that can be executed on a quantum computer, yielding probabilistic data that can then be interpreted. Below is a list of all input parameters to RB, together with an explanation and examples of choices for these parameters that correspond to versions of RB present in the literature.

1. **A gate-set/group:** A finite set of unitaries (quantum gates) on \mathbb{C}^d . In (almost) all RB protocols this gate set is also a finite subgroup $\mathbb{G} \subset U(d)$ of the unitary group. In a large section of the RB literature the group considered is the q -qubit Clifford group \mathbb{C}_q , but a range of other choices (such as the Pauli group \mathbb{P}_q [13], the real Clifford group [35] or the CNOT-dihedral group [37,38]) are possible. Choosing a group fixes what gates RB assesses the quality of and partially determines the structure of the output data. In generator-style RB [14,15] this group is defined implicitly by the set of generators.
2. **A reference implementation and representation:** A map ϕ_r from the gate-set/group \mathbb{G} to the d -dimensional superoperators that specifies how the gates in \mathbb{G} should be implemented in the quantum computer. This map takes into account aspects of the specific RB protocol but also how gates are composed of elementary gates and other implementation details. In uniform RB the map ϕ_r is a representation of the group \mathbb{G} on \mathcal{S}_d . The prototypical example is

the action on the space of Hermitian matrices ρ by conjugation, i.e., $\phi_r(g)(\rho) = \omega(g)(\rho) = U_g \rho U_g^\dagger$. In general, however, the reference implementation ϕ_r is not a representation, though we see that for any known RB procedure the reference implementation can be written as $\phi_r(g) = \mathcal{A}\omega(g)\mathcal{B}$, where \mathcal{A}, \mathcal{B} are (unitary) quantum channels. We refer to ω as *the reference representation*.

3. **An ending gate:** A group element g_{end} that dictates the global action of a RB sequence. For most proposals this gate is simply the identity, but in other proposals nontrivial choices for g_{end} (such as choosing it uniformly at random [13,37,39,45]) play an essential role in data-processing schemes. This ending gate also allows us to include RB schemes that do not involve an inversion gate [16,19,42,64]. We emphasize that it is not necessary to implement this gate physically, but rather it arises from compilation.
4. **A set of sequence lengths:** A set of integers \mathbb{M} denoting the length of the random sequences of gates implemented in a RB experiment. We denote elements of this set by m and the largest element of this set by M .
5. **An input state:** A state ρ_0 that is prepared at the beginning of a RB experiment. This state will typically be a pure state (such as the $|0, \dots, 0\rangle$ state vector), but is chosen mixed in some versions of RB [56].
6. **An output POVM:** A POVM that is measured at the end of a RB experiment. We denote this POVM as $\{\Pi_i\}_{i \in I}$ with some index set I . In many cases this is a two-component POVM, but some RB procedures explicitly call for more complex measurements (such as a computational basis measurement [29]).
7. **A set of sampling distributions:** A set of probability distributions ν_i for $i \in \{1, \dots, M\}$ over the group \mathbb{G} that govern the random sampling of group elements in RB. We often consider the scenario where all these probability distributions are the same, in which case we drop the subscript i and just write ν for *the* probability distribution. Moreover, in almost all instances in the literature this distribution is uniform, i.e., $\nu(g) = 1/|\mathbb{G}|$, and unless stated explicitly we always assume this to be the case.

C. The data-collection protocol

Given the input parameters discussed above we can write down a formal procedure for the data-collection phase of RB. It has as output an estimator $\hat{p}(i, m)$ of a probability $p(i, m)$ for each POVM element Π_i for $i \in I$ and each sequence length $m \in \mathbb{M}$.

Note that the probabilities $p(i, m)$ depend in a nontrivial manner on the initial state ρ_0 , the POVM $\{\Pi_i\}_{i \in I}$ and the

ending gate g_{end} . We, however, suppress this dependence unless it is explicitly necessary to refer to it.

D. A typology of randomized benchmarking protocols

Given protocol Algorithm 1, different choices of the parameters discussed in Sec. VB give rise to different RB procedures. More strongly, (the data-collection phases of) all variants of RB currently in the literature can be expressed by choosing these input parameters correctly. Surveying the literature we can distinguish three major types that are differentiated by their reference implementations and sampling distributions. The output data associated with these classes of protocols has varying behavior and we treat each class separately in Sec. VI. All protocols included in these classes can be found in Fig. 2 (here we give only illustrative examples).

1. **Uniform randomized benchmarking:** This is the basic type of RB. It is characterized by the fact that the probability distributions ν_i are the uniform distribution for all $i \in \{1, \dots, m_{\text{max}}\}$, and that the reference implementation map ϕ_r is exactly a representation ω , usually the standard action by conjugation given by $\omega(g) = \phi_r(g)(\rho) = U_g \rho U_g^\dagger$ for unitaries U_g (other choices have been made in Refs. [42,65]). Randomized benchmarking proposals of this type are mainly distinguished by what group \mathbb{G} they consider as a gate set (at least when it comes to the data-collection phase, different proposals in this class might have radically different data-processing procedures). Protocols of this type

include the original RB proposals [1,66] and many others.

2. **Nonuniform randomized benchmarking:** The defining feature of this class is that the sampling distributions ν_i are not the uniform distribution. It comes in two flavors, which we discuss separately:

- (a) **Subset RB:** Here, the distributions ν_i are far from uniform (and typically only have support on a small subset of the group \mathbb{G}). Examples from the literature are Refs. [14,15,39,67].
- (b) **Approximate RB:** Here the ν_i are close to uniform. This latter class will turn out to be essentially the same as uniform RB. This class has been discussed in Ref. [14] and also arises in the original ‘‘NIST’’ RB proposal [5] (as per the analysis of Ref. [51]).

In all works of this type so far the reference implementations are representations (akin to uniform RB).

3. **Interleaved randomized benchmarking:** This class of RB protocol is characterized by the addition of an extra ‘‘interleaving gate’’ in the RB procedure. This is a class that is somewhat idiosyncratic, having one standard subtype and a collection of ‘‘nonstandard’’ protocols:

- (a) **Standard interleaved randomized benchmarking:** In this class the interleaving gate is an element of the benchmarked group \mathbb{G} . In this

```

1 for  $m \in \mathbb{M}$  do
2   Prepare the initial state  $\rho_0$ 
3   for  $i \in \{1, \dots, m\}$  do
4     Choose  $g_i$  at random from  $\mathbb{G}$  according to the measure  $\nu_i$ 
5     Apply  $\phi_r(g_i)$  to the state
6   end
7   Compute the global inverse  $g_{\text{inv}} = (g_m \dots g_1)^{-1}$ 
8   Apply  $\phi_r(g_{\text{end}} g_{\text{inv}})$  to the state
9   Measure the state in the POVM  $\{\Pi_i\}_{i \in I}$ 
10  Repeat the above many times to obtain estimators  $\hat{p}(i; g_1, \dots, g_m)$  for the probabilities
      
$$p(i; g_1, \dots, g_m) = \text{Tr}(\Pi_i \phi_r(g_{\text{end}} g_{\text{inv}}) \phi_r(g_m) \dots \phi_r(g_1)(\rho_0))$$

11  Repeat for many random  $g_1, \dots, g_m$  and average to obtain estimators  $\hat{p}(i, m)$  for the probabilities
      
$$p(i, m) = \sum_{g_1, \dots, g_m \in \mathbb{G}} \nu_1(g_1) \dots \nu_m(g_m) p(i; g_1, \dots, g_m)$$

12 end
13 Output the estimators  $\hat{p}(i, m)$  for all  $i \in I, m \in \mathbb{M}$ 

```

Algorithm 1. RB (data-collection phase)

case we find that it is most useful to interpret interleaved RB as uniform RB, with the reference implementation a representation ω , but with the probability distributions ν_i uniform for even i and peaked on a single group element (the interleaving gate) for odd i . We consider this in more detail in Sec. VIC. The paradigmatic example is Ref. [4], but nearly all uniform RB protocols have an interleaved version.

- (b) **Nonstandard interleaved randomized benchmarking:** These protocols are characterized by the addition of interleaving gates that are not part of the group \mathbb{G} as well as nonuniform sampling distributions. We discuss these protocols on a more case-by-case basis in Sec. VIC.

1. Protocols without inversion gates

A number of RB protocols have been developed that do not feature an inversion gate g_{inv} . These protocols are indicated with ** in Fig. 2. While not immediately obvious, these protocols are actually covered by the general procedure written down in Algorithm 1. We can think of these protocols as choosing the ending gate g_{end} at random for each experimental run and averaging over the results. Because of the invariance of uniform group averages this is equivalent to not including an inversion gate and ending the protocol on a random group element. In Sec. VIII we see that protocols without inversion gate can be seen as a special case of a general postprocessing scheme for RB data.

E. Output data

There is a folkloric notion that the output data of RB has an exponential dependence on the sequence length, with the rate of decay dependent only on the implementation ϕ of the gates in \mathbb{G} . This was first established to be true for uniform RB (in our typology) with the unitary and Clifford groups, where, under certain assumptions (see Sec. VF) on the quantum computer implementing operations, one can prove that $p(i, m) = Af^m + B$, where f depends only on the implementation map ϕ and A, B are constants depending on SPAM. However, if the group \mathbb{G} was not the Clifford group it was found that the RB output data did not follow a single exponential decay but rather was of the form $p(i, m) = \sum_{\lambda} A_{\lambda} f_{\lambda}^m$ with the decay constants f_{λ} depending only on the implementation of the quantum operations and associated with the irreducible subrepresentations of the reference representation ω .

However, this functional form is only valid if the reference representation ω has no multiplicities (no irreducible subrepresentation occurs more than once), and hence does not describe all possible RB experiments. In this paper we argue that for a general reference representation of the form $\omega = \bigoplus_{\lambda \in \Lambda} \sigma_{\lambda}^{\oplus n_{\lambda}}$ for $\Lambda \subset \text{Irr}(\mathbb{G})$ RB data takes the

form

$$p(i, m) \approx \sum_{\lambda \in \Lambda} \text{Tr}(A_{\lambda} M_{\lambda}^m), \quad (63)$$

where M_{λ} is an $n_{\lambda} \times n_{\lambda}$ real matrix that depends only on the implementation ϕ and A_{λ} is an $n_{\lambda} \times n_{\lambda}$ matrix encoding SPAM behavior. Note that the matrices M_{λ} are not required to be normal, or even diagonalizable. This means that $p(i, m)$ can appear to be strikingly nonexponential (at least if m is fairly small) unless ω is known to be multiplicity-free. We discuss this in greater detail in Sec. VII when we discuss general fitting procedures.

F. Assumptions

The functional form of RB output data given in Eq. (63) does not immediately follow from the specification of the protocol in Algorithm 1. Rather it must be derived based on assumptions on the behavior of the operations being performed inside the quantum computer. Here we give a run down of assumptions that are made throughout the literature, and which we make in order to derive Eq. (63). The assumptions we make are not the most general possible that still lead to Eq. (63), but we attempt to strike a balance between generality and operational motivation. In the list we point out where assumptions can be generalized and refer to work where this is done (for some versions of RB).

- (a) **State preparation and measurement consistency:** We assume that the initial state ρ_0 and the measurement POVM $\{\Pi_i\}_{i \in I}$ are always prepared in the same manner, independently of the gates being implemented. Slightly stronger, we assume the existence of quantum channels \mathcal{E}_{SP} and \mathcal{E}_M such that the implemented initial state is given by $\mathcal{E}_{\text{SP}}(\rho_0)$ and the elements of the implemented measurement POVM are given by $\mathcal{E}_M(\Pi_i)$. This assumption is made throughout the RB literature.
- (b) **Markovianity and time independence:** We assume that the implementation of a gate $g \in \mathbb{G}$ is always the same, independently of when it is performed in the RB protocol and independently of its context (the gates being performed before and after). This assumption leads to the concept of an implementation map $\phi : \mathbb{G} \rightarrow \mathcal{S}_d$ which assigns to each group element g a completely positive superoperator $\phi(g)$ modeling the actual implementation of the gate.
- (i) This assumption is not always justified, as the implementation of a gate can in principle depend on, e.g., the gates being implemented before it or the amount of time elapsed in the protocol. It can also depend on external uncontrolled variables (either deterministic or

random). In Ref. [68], a model of time dependence has been considered and in Refs. [69–71] the effect of gate correlations and certain uncontrolled variables such as quasistatic noise were investigated. In all of these scenarios, however, the exponential behavior of Eq. (63) breaks down. It might be possible to derive assumptions beyond the setting of Markovian time independence that lead to output data of the correct form, but we do not pursue this here.

- (c) **Closeness to reference implementation:** In order to derive Eq. (63) we must make additional assumptions on the implementation map ϕ . We assume that

$$\frac{1}{|\mathbb{G}|} \sum_{g \in \mathbb{G}} \|\phi_r(g) - \phi(g)\|_{\diamond} \leq \delta, \quad (64)$$

for sufficiently small $\delta > 0$. The appearance of the diamond distance might strike one as overly pessimistic, however, we show that it is in fact required in Sec. IX. It is also not the most general possible assumption that still guarantees Eq. (63) (see below), but it has the advantage of making reference only to physical quantities and being operationally interpretable.

- (i) In early works on RB the standard assumption was that of gate-independent noise. This means the implementation map ϕ is of the form $\phi(g) = \mathcal{A}\phi_r(g)$ for all g with some fixed quantum channel \mathcal{A} . This is not a very realistic assumption and several attempts were made to replace it with a weaker assumption. In Ref. [66] it has been proposed to consider a perturbation $\phi(g) = \mathcal{A}\phi_r(g) + \mathcal{A}_g\phi_r(g)$. In Ref. [26], however, this analysis was shown to not be strong enough to actually justify behavior of the form Eq. (63). Here, an analysis of uniform Clifford randomized benchmarking as a power iteration of a matrix was proposed (see also early work in this direction by Ref. [41]), justifying the exponential decay model (but with nonoptimal correction). Subsequently, in Ref. [24] Eq. (63) was derived (with an exponentially small correction) for uniform RB with the multiqubit Clifford group under the assumption that there exist superoperators \mathcal{R}, \mathcal{L} such that

$$\frac{1}{|\mathbb{G}|} \sum_{g \in \mathbb{G}} \|\phi(g) - \mathcal{R}\omega(g)\mathcal{L}\|_{\diamond} \leq \delta \quad (65)$$

for small enough δ . This assumption is quite general, but has as its main drawback that the

operators \mathcal{R}, \mathcal{L} are not guaranteed to be completely positive, complicating the interpretation of this assumption as being a belief on physical quantities. Finally, Ref. [25] derives (introducing the Fourier analysis also used here) Eq. (63) (up to an exponentially small correction) for uniform RB with the multiqubit Clifford group under an assumption on the fidelity of the implementation map ϕ with respect to its reference implementation,

$$\frac{1}{|\mathbb{G}|} \sum_{g \in \mathbb{G}} F[\omega(g), \phi(g)] \geq 1 - \delta. \quad (66)$$

This assumption has the advantage of making reference to physical objects only, but suffers from the drawback that δ must grow inversely proportional to the underlying Hilbert-space dimension for the argument in Ref. [25] to hold. We discuss this further in Sec. X.

VI. THE RANDOMIZED BENCHMARKING FITTING MODEL

In this section, we prove a general theorem about the behavior of RB output data, i.e., the probabilities $p(i, m)$ associated with a RB experiment with its input parameters specified as in Sec. VB and described in protocol Algorithm 1. We argue that for a broad variety of choices for reference implementations and probability distributions this data is well described by a linear combination of exponential (matrix) decays [as in Eq. (63)], as long as the physical implementation ϕ is close to its ideal version: the reference implementation ϕ_r . By close we mean that the diamond distance between reference and ideal implementations, averaged over the group, has to be bounded as

$$\frac{1}{|\mathbb{G}|} \sum_{g \in \mathbb{G}} \|\phi_r(g) - \phi(g)\|_{\diamond} \leq \delta. \quad (67)$$

One can think of the above equation as a relatively weak initial belief one must hold about one’s quantum computer (instantiated in ϕ) before one can trust the outcome of RB.

For the rest of the work we adopt the transfer-matrix framework (discussed in Sec. III) for describing the action of superoperators. We also explicitly write implementation noise on the initial state ρ_0 and output POVM $\{\Pi_i\}_{i \in I}$ through quantum channels \mathcal{E}_{SP} (state preparation) and \mathcal{E}_M (measurement). This is notationally somewhat clumsy, but it makes explicit one of the assumptions underlying RB, namely that SPAM noise is independent of sequence length.

The theorems we present in this section are generalizations of the theorems given in Ref. [24], encompassing

almost all known RB procedures, but the techniques used are based on the cleaner conceptual framework of matrix-valued Fourier transforms provided by Ref. [25], which we reviewed in Sec. IV B. The central observation of Ref. [25] is that the data-collection phase of uniform RB can be seen as evaluating m -fold convolutions of the implementation map ϕ . This observation generalizes beyond uniform RB to arbitrary implementation maps, and, in particular, we see that

$$p(i, m) = \sum_{g_1, \dots, g_m \in \mathbb{G}} \langle \langle \mathcal{E}_M(\Pi_i) | v(g_1) \dots v_m(g_m) \rangle \rangle \times \phi(g_{\text{end}} g_1^{-1} \dots g_m^{-1}) \phi(g_m) \dots \phi(g_1) | \mathcal{E}_{\text{SP}}(\rho_0) \rangle \rangle \quad (68)$$

can be rewritten, using the invariance of the uniform sum over \mathbb{G} under changes of variables, as

$$\begin{aligned} p(i, m) &= \sum_{g_1, \dots, g_m \in \mathbb{G}} \langle \langle \mathcal{E}_M(\Pi_i) | \phi(g_{\text{end}} g_m^{-1}) v_m(g_m g_m^{-1}) \rangle \rangle \\ &\quad \times \phi(g_m g_{m-1}^{-1}) \dots v_1(g_1) \phi(g_1) | \mathcal{E}_{\text{SP}}(\rho_0) \rangle \rangle \quad (69) \\ &= \langle \langle \mathcal{E}_M(\Pi_i) | (\phi * (v_m \phi) * \dots * (v_1 \phi)) (g_{\text{end}}) | \rangle \rangle \\ &\quad \times \mathcal{E}_{\text{SP}}(\rho_0) \rangle \rangle \quad (70) \end{aligned}$$

where we use the definition of convolution of implementation maps given in Eq. (26) and where $(v_i \phi)(g) = v_i(g) \phi(g)$. We see that often the convolution product map $\phi * (v_m \phi) * \dots * (v_1 \phi)$ can be written exactly as an m -fold convolution ϕ'^{*m} (for some ϕ' that is not necessarily the same as ϕ).

We begin in Sec. VI A with discussing the case of uniform RB (as per the RB typology in Sec. VD). This is the easiest case, but the results derived there will go a long way in analyzing the other two types (nonuniform and interleaved RB).

A. Uniform randomized benchmarking

Here we discuss the behavior of RB output data given by a uniform RB scheme (as defined in Sec. VD). We prove that this data behaves as expected (i.e., a controlled linear combination of exponential decays), as long as the implementation map ϕ is close enough to its reference implementation ϕ_r . As we saw in Sec. VB, for uniform RB protocols this reference implementation is exactly a representation, which we denote by ω . We can always decompose ω into a direct sum of irreducible representations. We write this as $\omega = \bigoplus_{\lambda \in \Lambda} \sigma_\lambda^{\oplus n_\lambda}$ with Λ some index set and σ_λ irreducible subrepresentations appearing with multiplicity n_λ . As discussed in Sec. V, we expect the RB output data to be approximately well described by a linear

combination of the form

$$p(i, m) \approx \sum_{\lambda \in \Lambda} \text{Tr}(A_\lambda M_\lambda^m), \quad (71)$$

where M_λ is an $n_\lambda \times n_\lambda$ matrix depending only on the actual implementation ϕ . In particular, M_λ is given by the projection of the Fourier mode $\mathcal{F}(\phi)[\sigma_\lambda]$ onto the subspace associated with its n_λ largest (in absolute value) eigenvalues. This is the content of Theorem 8. The essential idea in Theorem 8 is the fact that convolutions correspond to matrix multiplication in Fourier space, together with a careful use of the subspace perturbation techniques discussed in Sec. III.

Theorem 8: (Output data of uniform randomized benchmarking). *Let $p(i, m)$ be the outcome probability associated with a uniform RB experiment with group \mathbb{G} , initial state ρ_0 , reference representation $\omega = \bigoplus_{\lambda \in \Lambda} \sigma_\lambda^{\oplus n_\lambda}$, and ending gate g_{end} , for a specific sequence length $m \in \mathbb{N}$ and POVM element Π_i in the POVM $\{\Pi_i\}_i$ (as described in protocol Algorithm 1). Let ϕ be the implementation map describing the actually implemented operations. Moreover, assume that there exists a $\delta > 0$ such that*

$$\frac{1}{|\mathbb{G}|} \sum_{g \in \mathbb{G}} \|\omega(g) - \phi(g)\|_\diamond \leq \delta \leq 1/9. \quad (72)$$

The RB output probability $p(i, m)$ is well approximated as

$$|p(i, m) - \sum_{\lambda \in \Lambda} \text{Tr}(A_\lambda M_\lambda^m)| \leq 8 \left(\delta \left[1 + \frac{2\delta}{1-5\delta} \right] \right)^m, \quad (73)$$

where M_λ, A_λ are $n_\lambda \times n_\lambda$ real matrices and M_λ depends only on the implementation ϕ .

Proof. Note from Eq. (69) with v_i the uniform probability distribution for all $i \in \{1, \dots, m\}$ that

$$p(i, m) = \langle \langle \mathcal{E}_M(\Pi_i) | (\phi * \phi^{*m})(g_{\text{end}}) | \mathcal{E}_{\text{SP}}(\rho_0) \rangle \rangle. \quad (74)$$

Inserting the Fourier transform of ϕ , we get

$$\begin{aligned} p(i, m) &= \sum_{\lambda \in \text{Ir}(\mathbb{G})} d_\lambda \langle \langle \mathcal{E}_M(\Pi_i) \rangle \rangle \\ &\quad \times |\text{Tr}_{V_\lambda} \{ \mathcal{F}(\phi)^{m+1} [\sigma_\lambda] \overline{\sigma_\lambda}(g_{\text{end}}^{-1}) \otimes \mathbb{1} \} | \mathcal{E}_{\text{SP}}(\rho_0) \rangle \rangle \quad (75) \\ &= \langle \langle \mathcal{E}_M(\Pi_i) | \text{Tr}_{V_{\omega_{\mathbb{G}}}} \left[\left[\frac{1}{|\mathbb{G}|} \sum_{g \in \mathbb{G}} \overline{\omega_{\mathbb{G}}}(g) \otimes \phi(g) \right]^{m+1} \right. \right. \\ &\quad \left. \left. \times [\mathcal{D}_{\mathbb{G}} \overline{\omega_{\mathbb{G}}}(g_{\text{end}}^{-1})] \otimes \mathbb{1} \right] | \mathcal{E}_{\text{SP}}(\rho_0) \rangle \rangle, \quad (76) \end{aligned}$$

where $\omega_{\mathbb{G}}(g) = \bigoplus_{\lambda \in \text{Irr}(\mathbb{G})} \sigma_{\lambda}(g)$ is the direct sum of all irreducible representations of \mathbb{G} and $\mathcal{D}_{\mathbb{G}} = \bigoplus_{\lambda \in \text{Irr}(\mathbb{G})} d_{\lambda} \mathbb{1}_{\lambda}$ accounts for the dimensional factor in the inverse Fourier transform. Now we can consider the Fourier operator $F(\phi)$ [as defined in Eq. (31)] associated with ϕ as a perturbation of its ideal version $F(\omega)$. From our discussion of Fourier transforms and Fourier operators we know that $F(\omega) = 1/|\mathbb{G}| \sum_{g \in \mathbb{G}} \bigoplus_{\lambda \in \Lambda} \bar{\sigma}_{\lambda}(g) \otimes \omega(g)$ is an orthogonal projection, with rank given by the number of irreducible subrepresentations of ω ($\text{Rk}[F(\omega)] = \sum_{\lambda \in \Lambda} n_{\lambda}$). Recall also that there is a natural matrix norm $\|\cdot\|_m$ on the space of Fourier operators and that

$$\begin{aligned} & \|F(\phi - \omega)\|_m \\ &= \frac{1}{|\mathbb{G}|} \sum_{g \in \mathbb{G}} \left\| \text{Tr}_{V_{\omega_{\mathbb{G}}}} [F(\phi - \omega) \mathcal{D}_{\mathbb{G}} \bar{\omega}_{\mathbb{G}}(g^{-1}) \otimes \mathbb{1}] \right\|_{\diamond} \\ &= \frac{1}{|\mathbb{G}|} \sum_{g \in \mathbb{G}} \|\phi(g) - \omega(g)\|_{\diamond}. \end{aligned} \quad (77)$$

The plan is now to use the perturbation theorem (Theorem 6) to split the above into dominant and subdominant invariant subspaces. To do this note that $F(\omega)$ is a projector so we trivially get a spectral resolution with $X_1 = F(\omega)$, $X_2 = \mathbb{1} - F(\omega)$ with $F(\omega)$ acting as the identity on the column and row space of X_1 and as the zero operator on the column and row space of X_2 . Thinking of $F(\phi - \omega)$

as a perturbation to $F(\omega)$ we need to ensure the conditions in Eq. (42) are satisfied with respect to the norm $\|\cdot\|_m$. Using the submultiplicativity of this norm and the fact that $\|X_1\|_m = 1$ by construction together with the triangle inequality, we get the following sufficient condition for the applicability of Theorem 6:

$$\begin{aligned} & \frac{\|X_1^{\dagger} F(\phi - \omega) X_2\|_m \|X_2^{\dagger} F(\phi - \omega) X_1\|_m}{[\text{sep}(\mathbb{1}, 0) - \|X_1^{\dagger} F(\phi - \omega) X_1\|_m - \|X_2^{\dagger} F(\phi - \omega) X_2\|_m]^2} \\ & \leq \frac{[2 \|F(\phi - \omega)\|_m]^2}{[1 - 5 \|F(\phi - \omega)\|_m]^2} < \frac{1}{4} \end{aligned} \quad (78)$$

where we also use that $\text{sep}(\mathbb{1}, 0) = 1$, which is easy to see from the definition of sep (see Sec. IV C). Working out, we see that the above is satisfied if Eq. (72) is true, which it is by assumption. Hence we can use Theorem 6 to conclude the existence of operators $R = [R_1, R_2], L = [L_1, L_2]$ with $L^{\dagger} = R^{-1}$ and P_1 such that

$$\begin{aligned} F(\phi) &= R_1 [X_1^{\dagger} F(\omega) X_1 + X_1^{\dagger} F(\phi - \omega) (X_1 + X_2 P_1)] L_1^{\dagger} \\ & \quad + R_2 [X_2^{\dagger} F(\omega) X_2 + (X_2^{\dagger} - P_1 X_1^{\dagger}) F(\phi - \omega) X_2] L_2^{\dagger}. \end{aligned} \quad (79)$$

Using the fact that $L^{\dagger} = R^{-1}$ (and thus that $L_2^{\dagger} R_1 = L_1^{\dagger} R_2 = 0$) we can now write $p(m, g_{\text{end}}, \Pi)$ as a sum of two terms corresponding to the above spectral resolution:

$$\begin{aligned} p(i, m) &= \langle \mathcal{E}_M(\Pi_i) | \text{Tr}_{V_{\omega_{\mathbb{G}}}} [\mathcal{D}_{\mathbb{G}} \bar{\omega}_{\mathbb{G}}(g_{\text{end}}^{-1}) \otimes \mathbb{1}] F(\phi) \{ R_1 [X_1^{\dagger} F(\omega) X_1 + X_1^{\dagger} F(\phi - \omega) (X_1 + X_2 P_1)] L_1^{\dagger} \}^m | \mathcal{E}_{\text{SP}}(\rho_0) \rangle \rangle \\ & \quad + \langle \mathcal{E}_M(\Pi_i) | \text{Tr}_{V_{\omega_{\mathbb{G}}}} [\mathcal{D}_{\mathbb{G}} \bar{\omega}_{\mathbb{G}}(g_{\text{end}}^{-1}) \otimes \mathbb{1}] \{ R_2 [X_2^{\dagger} F(\omega) X_2 + (X_2^{\dagger} - P_1 X_1^{\dagger}) F(\phi - \omega) X_2]^{m+1} L_2^{\dagger} \} | \mathcal{E}_{\text{SP}}(\rho_0) \rangle \rangle. \end{aligned} \quad (80)$$

We consider both of these terms separately. We deal first with the second term. Note that, using the definitions of R, L from Theorem 6, we have

$$(2) \leq \left\| \text{Tr}_{V_{\omega_{\mathbb{G}}}} \left\{ [\mathcal{D}_{\mathbb{G}} \bar{\omega}_{\mathbb{G}}(g_{\text{end}}^{-1}) \otimes \mathbb{1}] R_2 [X_2^{\dagger} F(\omega) X_2 + (X_2^{\dagger} - P_1 X_1^{\dagger}) F(\phi - \omega) X_2]^{m+1} L_2^{\dagger} \right\} \right\|_{\diamond} \quad (81)$$

$$\leq \left\| (X_2 + X_1 P_2 + X_2 P_1 P_2) [X_2^{\dagger} F(\omega) X_2 + (X_2^{\dagger} - P_1 X_1^{\dagger}) F(\phi - \omega) X_2]^m (X_2 - P_1 X_1)^{\dagger} \right\|_{\max}, \quad (82)$$

which is just a statement about the max norm of a Fourier operator. Note that $X_2^{\dagger} F(\omega) X_2 = 0$ by construction so the above depends only on $F(\phi - \omega)$. Now using the max-mean norm inequality in Eq. (35) several times and the fact that $X_2 = \mathbb{1} - X_1$, we can upper bound this as

$$(2) \leq \left\| (X_2 + X_1 P_2 + X_2 P_1 P_2) (X_2 - P_1 X_1)^{\dagger} F(\phi - \omega) X_2 (X_2 - P_1 X_1) \right\|_{\max} \left\| [F(\phi - \omega) X_2 (X_2 - P_1 X_1)^{\dagger}]^m \right\|_m \quad (83)$$

$$\leq 2 \left[\|F(\phi - \omega)\|_{\max} (1 + \|P_2\|_m) (1 + \|P_1\|_m) + \|P_1\|_m^2 \|P_2\|_m (3 + \|P_1\|_m) \right] \left[\|F(\phi - \omega)\|_m (1 + \|P_1\|_m) \right]^m. \quad (84)$$

Now we use from Theorem 6, the upper bounds on

$$\|P_1\|_m \leq \frac{\|X_2^{\dagger} F(\phi - \omega) X_1\|_m}{1 - \|X_1^{\dagger} F(\phi - \omega) X_1\|_m - \|X_1^{\dagger} F(\phi - \omega) X_1\|_m} \leq \frac{2 \|F(\phi - \omega)\|_m}{1 - 5 \|F(\phi - \omega)\|_m} \leq \frac{2\delta}{1 - 5\delta} \quad (85)$$

and

$$\|P_2\|_m \leq \frac{2\|F(\phi - \omega)\|_m}{1 - 5\|F(\phi - \omega)\|_m - 2\|P_1\|_m \|X_1^\dagger F(\phi - \omega) X_2\|} \quad (86)$$

$$\leq \frac{2\|F(\phi - \omega)\|_m}{1 - 5\|F(\phi - \omega)\|_m - \frac{8\|F(\phi - \omega)\|_m^2}{1 - 5\|F(\phi - \omega)\|_m}} \quad (87)$$

$$\leq \frac{2\delta(1 - 5\delta)}{1 - 8\delta^2} \quad (88)$$

$$\leq \frac{\delta}{1 - \delta}, \quad (89)$$

where we exploit the assumption $\delta \leq 1/9$ in the last line. Inserting these bounds into the main expression we get

$$(2) \leq 4 \left(\left[1 + \frac{2\delta}{1 - 5\delta} \right] \left[1 + \frac{\delta}{1 - \delta} \right] + \left[\frac{2\delta}{1 - 5\delta} \right]^2 \left[\frac{\delta}{1 - \delta^2} \right] \left[3 + \frac{2\delta}{1 - 5\delta} \right] \right) \times \left(\delta \left[1 + \frac{2\delta}{1 - 5\delta} \right] \right)^m \quad (90)$$

$$\leq \frac{115}{16} \left(\delta \left[1 + \frac{2\delta}{1 - 5\delta} \right] \right)^m \quad (91)$$

$$\leq 8 \left(\delta \left[1 + \frac{2\delta}{1 - 5\delta} \right] \right)^m, \quad (92)$$

where we use that $\|F(\phi - \omega)\|_{\max} \leq 2$ and $\delta \leq 1/9$. Next we consider the first term in Eq. (80). For this term we desire an exact expression. We begin by noting that both $F(\omega)$ and $F(\phi)$ are block diagonal with respect to the decomposition of $\omega_{\mathbb{C}}$ into irreducible representations. This implies that the matrices R, L are block diagonal with respect to this decomposition as well, and that, moreover, we can take the matrices P_1, P_2 to be block diagonal with the blocks labeled by the irreducible subrepresentations present in $\omega = \bigoplus_{\lambda \in \Lambda} \sigma_{\lambda}^{\oplus n_{\lambda}}$. Writing $P = \bigoplus_{\lambda \in \Lambda} P^{\lambda}$, and similarly for other operators we can write the first term

of Eq. (80) as

$$(1) = \sum_{\lambda \in \Lambda} d_{\sigma_{\lambda}} \langle \langle \mathcal{E}_M(\Pi_i) | \text{Tr}_{V_{\sigma_{\lambda}}} \{ [\bar{\sigma}_{\lambda}(\mathbf{g}_{\text{end}}^{-1}) \otimes \mathbb{1}] \times \mathcal{F}(\phi) [\sigma_{\lambda}] R_1^{\lambda} [(X_1^{\lambda})^{\dagger} \mathcal{F}(\phi) [\sigma_{\lambda}] (X_1^{\lambda} + X_2^{\lambda} P_1^{\lambda})]^m L_1^{\lambda \dagger} \} | \mathcal{E}_{\text{SP}}(\rho_0) \rangle \rangle, \quad (93)$$

where we also use that $F(\omega)X_2 = 0$ by construction. To continue further we need to pick a convenient basis to express $X_1^{\lambda}, R_1^{\lambda}$.

For this note that we can specify rank-1 Fourier operators in $L(V_{\omega_{\mathbb{C}}}) \otimes \mathcal{S}_d$ by specifying pairs of superoperators \mathcal{A}, \mathcal{B} and looking at Fourier operators of the form $F(\mathcal{A}\omega\mathcal{B})$. It is useful to think of the Fourier operator $F(\omega)$ as a vectorization operation on \mathcal{A}, \mathcal{B} . We can express $X_1 = F(\omega)$ in this way by considering the operators $F(\mathcal{P}_{\lambda}^j \omega \mathcal{P}_{\lambda}^j)$ where \mathcal{P}_{λ}^j is the (superoperator) projector onto the j th copy of the representation σ_{λ} in $\omega = \bigoplus_{\lambda \in \Lambda} \sigma_{\lambda}^{\oplus n_{\lambda}}$. Note that these operators are rank-one orthogonal projectors and moreover that

$$\sum_{j_{\lambda}=1}^{n_{\lambda}} F(\mathcal{P}_{\lambda}^{j_{\lambda}} \omega \mathcal{P}_{\lambda}^{j_{\lambda}}) = \sum_{j_{\lambda}=1}^{n_{\lambda}} F(\sigma_{\lambda}^{\oplus n_{\lambda}}) = X_1^{\lambda} \quad (94)$$

holds true. Now noting that $(X_1^{\lambda} + X_2^{\lambda} P_1^{\lambda}) = R_1^{\lambda}$ is a rank n_{λ} matrix with $X_1^{\lambda} R_1^{\lambda} = X_1^{\lambda}$, we can similarly find n_{λ} superoperators $\mathcal{R}_{\lambda}^{j_{\lambda}}$ ($j_{\lambda} \in 1, \dots, n_{\lambda}$) such that

$$R_1^{\lambda} = \sum_{j_{\lambda}=1}^{n_{\lambda}} F(\mathcal{R}_{\lambda}^{j_{\lambda}} \omega \mathcal{P}_{\lambda}^{j_{\lambda}}), \quad (95)$$

where $F(\mathcal{P}_{\lambda}^{j_{\lambda}} \omega \mathcal{R}_{\lambda}^{j_{\lambda}})$ is again of rank one (but no longer orthogonal). Note that $X_1^{\lambda} R_1^{\lambda} = X_1^{\lambda}$ gives rise to the orthogonality property

$$F(\mathcal{P}_{\lambda}^{j_{\lambda}} \omega \mathcal{P}_{\lambda}^{j_{\lambda}}) F(\mathcal{R}_{\lambda}^{j'_{\lambda}} \omega \mathcal{P}_{\lambda}^{j'_{\lambda}}) = \delta_{j_{\lambda} j'_{\lambda}} F(\mathcal{P}_{\lambda}^{j_{\lambda}} \omega \mathcal{P}_{\lambda}^{j_{\lambda}}). \quad (96)$$

Using these resolutions of $X_1^{\lambda}, R_1^{\lambda}$ and the orthogonality property we can express the first term in Eq. (80) further as

$$(1) = \sum_{\lambda \in \Lambda} \sum_{j_{\lambda}^1, \dots, j_{\lambda}^{2m}=1}^{n_{\lambda}} d_{\sigma_{\lambda}} \langle \langle \mathcal{E}_M(\Pi_i) | \text{Tr}_{V_{\sigma_{\lambda}}} \left[[\bar{\sigma}_{\lambda}(\mathbf{g}_{\text{end}}^{-1}) \otimes \mathbb{1}] \mathcal{F}(\phi) [\sigma_{\lambda}] R_1^{\lambda} \right. \quad (97)$$

$$\left. \times \{ F(\mathcal{P}_{\lambda}^{j_{\lambda}^1} \omega \mathcal{P}_{\lambda}^{j_{\lambda}^1}) \mathcal{F}(\phi) [\sigma_{\lambda}] F(\mathcal{R}_{\lambda}^{j_{\lambda}^2} \omega \mathcal{P}_{\lambda}^{j_{\lambda}^2}) \cdots \mathcal{F}(\phi) [\sigma_{\lambda}] F(\mathcal{R}_{\lambda}^{j_{\lambda}^{2m}} \omega \mathcal{P}_{\lambda}^{j_{\lambda}^{2m}}) \} L_1^{\lambda \dagger} \right] | \mathcal{E}_{\text{SP}}(\rho_0) \rangle \rangle \quad (98)$$

$$= \sum_{\lambda \in \Lambda} \sum_{j_{\lambda}^1, j_{\lambda}^{2m}=1}^{n_{\lambda}} d_{\sigma_{\lambda}} \langle \langle \mathcal{E}_M(\Pi_i) | \text{Tr}_{V_{\sigma_{\lambda}}} \left[[\bar{\sigma}_{\lambda}(\mathbf{g}_{\text{end}}^{-1}) \otimes \mathbb{1}] \mathcal{F}(\phi) [\sigma_{\lambda}] R_1^{\lambda} F(\mathcal{P}_{\lambda}^{j_{\lambda}^1} \omega \mathcal{P}_{\lambda}^{j_{\lambda}^1}) L_1^{\lambda \dagger} \right] | \mathcal{E}_{\text{SP}}(\rho_0) \rangle \rangle [M_{\lambda}^m]_{j_{\lambda}^1, j_{\lambda}^{2m}} \quad (99)$$

with

$$\begin{aligned} [M_\lambda]_{j_\lambda, j'_\lambda} &= \text{Tr} \left(F(\mathcal{P}_\lambda^{j_\lambda} \omega \mathcal{P}_\lambda^{j'_\lambda}) F(\phi) F(\mathcal{R}_\lambda^{j_\lambda} \omega \mathcal{P}_\lambda^{j'_\lambda}) \right) \\ &= \text{Tr} \left(F(\phi) F(\mathcal{R}_\lambda^{j_\lambda} \omega \mathcal{P}_\lambda^{j'_\lambda}) \right), \end{aligned} \quad (100)$$

by the fact that $F(\mathcal{P}_\lambda^{j_\lambda} \omega \mathcal{P}_\lambda^{j'_\lambda}), F(\mathcal{R}_\lambda^{j_\lambda} \omega \mathcal{P}_\lambda^{j'_\lambda})$ are of rank one. Now writing

$$\begin{aligned} [A_\lambda]_{j_\lambda, j'_\lambda} &= d_{\sigma_\lambda} \langle \langle \mathcal{E}_M(\Pi_i) | \text{Tr}_{V_{\sigma_\lambda}} \left[[\bar{\sigma}_\lambda (\mathfrak{g}_{\text{end}}^{-1}) \otimes \mathbb{1}] \mathcal{F}(\phi) \right. \\ &\quad \left. \times [\sigma_\lambda] R_1^\lambda F(\mathcal{P}_\lambda^{j_\lambda} \omega \mathcal{P}_\lambda^{j'_\lambda}) L_1^{\lambda\dagger} \right] | \mathcal{E}_{\text{SP}}(\rho_0) \rangle \rangle \end{aligned} \quad (101)$$

we can combine the two terms in Eq. (80) to get

$$\left| p(i, m) - \sum_{\lambda \in \Lambda} \text{Tr}(A_\lambda M_\lambda^m) \right| \leq 8 \left(\delta \left[1 + \frac{2\delta}{1-5\delta} \right] \right)^m. \quad (102)$$

■

B. Randomized benchmarking with nonuniform sampling

Several works [5,14,15,39,51] discuss adaptations of RB where the elements of the group are no longer sampled exactly at random, but are instead sampled according to (1) a distribution close to uniform [5,14,51] (which we call “approximate RB” in Sec. VB, following Ref. [14]), or (2) a distribution that only has support on a small subset of the group; group generators in the case of Ref. [14] (see also early work on the Clifford group by Ref. [67]), subgroup cosets in the case of Ref. [39], and constant depth circuits (layers) in the case of Ref. [15]. In Sec. VB, we call these approaches “subset RB.”

We begin by treating the case of approximate RB. This corresponds to performing RB as described in protocol Algorithm 1 but instead of sampling group elements from the group \mathbb{G} uniformly at random one samples group elements according to some prescribed probability distributions $\nu_i : \mathbb{G} \rightarrow [0, 1]$ (with i indicating the time at which the gate is applied). In Ref. [14] it has been argued that as long as the distributions ν_i are all close to the uniform distribution in the l_1 norm, then the output data of approximate RB is close to the output data of exact RB.

As a corollary of Theorem 8 we obtain a similar result. Our result is somewhat less general than the one given in Theorem 17 of Ref. [14]. In particular, we assume that all distributions ν_i are equal to a fixed distribution ν . In return for this restriction we are able to make a much stronger statement on the behavior of the RB output data. Moreover, our approach does not require the gate-independent noise

assumption [replacing it with the more general diamond-norm assumption of Eq. (72)]. We have the following statement.

Theorem 9: (Randomized benchmarking data with nonuniform sampling). *Let ν be a probability distribution on \mathbb{G} and $p_\nu(i, m)$ be the outcome probability associated with a nonuniform RB experiment with implementation map ϕ and reference representation $\omega(\mathfrak{g}) = \bigoplus_{\lambda \in \Lambda} \sigma_\lambda^{\oplus m_\lambda}$. Moreover, assume that there exists $\delta, \delta' > 0$ such that*

$$\frac{1}{|\mathbb{G}|} \sum_{\mathfrak{g} \in \mathbb{G}} \|\omega(\mathfrak{g}) - \phi(\mathfrak{g})\|_\diamond \leq \delta, \quad (103)$$

$$\sum_{\mathfrak{g} \in \mathbb{G}} |\nu(\mathfrak{g}) - \frac{1}{|\mathbb{G}|}| \leq \delta', \quad (104)$$

with $\delta + \delta' \leq 1/9$. Now $p_\nu(i, m)$ is well approximated as

$$\begin{aligned} |p_\nu(i, m) - \sum_{\lambda \in \Lambda} \text{Tr}[A_\lambda (M_\lambda^\nu)^m]| \\ \leq 8 \left((\delta + \delta') \left[1 + \frac{2(\delta + \delta')}{1 - 5(\delta + \delta')} \right] \right)^m, \end{aligned} \quad (105)$$

where M_λ^ν, A_λ are $n_\lambda \times n_\lambda$ real matrices, M_λ^ν depends on the implementation ϕ and the measure ν .

Proof. Consider the map $\phi_\nu : \mathbb{G} \rightarrow \mathcal{S}_d : \mathfrak{g} \rightarrow |\mathbb{G}| \nu(\mathfrak{g}) \phi(\mathfrak{g})$. Note that we can think of nonuniform RB as being uniform RB with this (not trace preserving but still completely positive) implementation map. In particular, we have

$$p_\nu(i, \mathfrak{g}_{\text{end}}, m) = \langle \langle \mathcal{E}_M(\Pi_i) | (\phi * \phi_\nu^{*m})(\mathfrak{g}_{\text{end}}) | \mathcal{E}_{\text{SP}}(\rho_0) \rangle \rangle, \quad (106)$$

which is just Eq. (74) but with the “effective implementation” ϕ_ν . From the assumptions of the theorem we have

$$\begin{aligned} \frac{1}{|\mathbb{G}|} \sum_{\mathfrak{g} \in \mathbb{G}} \|\omega(\mathfrak{g}) - \phi_\nu(\mathfrak{g})\|_\diamond \\ \leq \frac{1}{|\mathbb{G}|} \sum_{\mathfrak{g} \in \mathbb{G}} \|\omega(\mathfrak{g}) - \phi(\mathfrak{g})\|_\diamond + \sum_{\mathfrak{g} \in \mathbb{G}} |\nu(\mathfrak{g}) - \frac{1}{|\mathbb{G}|}| \leq \frac{1}{9}. \end{aligned} \quad (107)$$

Hence, the proof of Theorem 8 immediately applies to $p_\nu(i, \mathfrak{g}_{\text{end}}, m)$, yielding Eq. (105). ■

We note that in the case of NIST RB [51] the probability distribution over (a subgroup of) the single-qubit Clifford group is not strictly speaking close enough to uniform to apply the above theorem. This can be easily solved

by blocking a few gate applications together, defining a new effective implementation map $\phi' = (\nu\phi) * (\nu\phi) \cdots * (\nu\phi)$, which is close enough to uniformly distributed to apply Theorem 9.

The above approach fails utterly when applied to subset RB. In this scenario the distribution ν only has support on a small subset A of \mathbb{G} and consequently $\sum_{g \in \mathbb{G}} |\nu(g) - 1/|\mathbb{G}|| \approx 1$ in many cases. This is not necessarily a weakness of Theorem 8 but rather a statement of the fact that strong deviations from exponential behavior can be observed if one does not give the distribution ν time to converge to the uniform distribution through repeated convolution. This was already noted more or less explicitly in previous papers on subset RB. There are two approaches to solving this problem. The first, followed in Refs. [14,15,39,67] is to restrict the set of sequence lengths \mathbb{M} at which RB data is gathered to $m \geq m_{\text{mix}}$ where m_{mix} is related to the mixing time of the distribution ν . Note that in the direct RB proposal [15], this convergence time is instead enforced directly by applying a uniformly random gate before applying nonuniformly sampled gates. The second approach is to take this deviation from uniform RB behavior at face value [13] and draw conclusions from the RB output directly. We believe this latter approach is more accurately classified as an interleaved benchmarking scheme and we discuss it there.

With regards to the first approach we can make a statement akin to Theorem 8 about subset RB procedures by making the (natural) assumption that upon equilibration of the distribution ν the quality of the total gates has not degraded too much. Intuitively, this means that the gates that have high weight in the initial distribution are of high enough quality to generate (by composition) good-quality implementations of all gates in the group. Concretely, we have the following theorem.

Theorem 10: (Subset randomized benchmarking). *Let ν be a probability distribution on \mathbb{G} and $p_\nu(i, m)$ be the outcome probability associated with a nonuniform RB experiment with implementation map ϕ and reference representation $\omega(g) = \bigoplus_{\lambda \in \Lambda} \sigma_\lambda^{\oplus n_\lambda}$. Moreover, assume that there exists an integer m_{mix} and real numbers $\delta, \delta' > 0$ such that*

$$\sum_{g \in \mathbb{G}} |\nu^{*m_{\text{mix}}}(g) - \frac{1}{|\mathbb{G}|}| \leq \delta', \quad (108)$$

$$\sum_{g \in \mathbb{G}} \nu(g) \|\omega(g) - \phi(g)\|_\diamond \leq \frac{\delta}{m_{\text{mix}}} \quad (109)$$

with $\delta + \delta' \leq 1/9$. Now $p_\nu(i, m)$ is well approximated as

$$|p_\nu(i, m) - \sum_{\lambda \in \Lambda} \text{Tr}(A_\lambda M_\lambda^{m-m_{\text{mix}}})| \leq \varepsilon \quad (110)$$

with M_λ the projection onto the n_λ -dimensional dominant invariant subspace of $\mathcal{F}(\nu\phi)[\sigma_\lambda]$ and where

$$\begin{aligned} \varepsilon \leq 2\delta'' & \left(\left[1 + \frac{2\delta''}{1-5\delta''} \right] \left[1 + \frac{\delta''}{1-\delta''} \right] \right. \\ & \left. + \left[\frac{2\delta''}{1-5\delta''} \right]^2 \left[\frac{\delta''}{1-\delta''} \right] \left[3 + \frac{2\delta''}{1-5\delta''} \right] \right) \leq 4\delta'' \end{aligned} \quad (111)$$

with $\delta'' = \delta + \delta'$.

Note that this theorem is qualitatively less strong than Theorem 8. In particular, we cannot guarantee that the distance between the output data of subset RB and the exponential decays associated with the irreducible subrepresentations of the reference representation closes exponentially fast with increasing sequence length. However, our bound on this distance is stronger than previous rigorous statements (Theorem 20 in Ref. [14]) and works under weaker assumptions. The distance bound given in Ref. [39] (Theorem 3) does close exponentially but the proof relies critically on the fact that ν is uniformly nonzero on a (large) subgroup coset in \mathbb{G} , and thus applies only to a far more restricted situation. Note also that it does not directly apply to the approach taken in Ref. [15]. However, we believe that with very minor alterations the reasoning below can be made to fit.

Proof. Consider again the map $\phi_\nu : \mathbb{G} \rightarrow \mathcal{S}_d : g \rightarrow |\mathbb{G}| \nu(g)\phi(g)$. We have

$$p_\nu(i, m) = \langle \langle \mathcal{E}_M(\Pi_i) | (\phi * \phi_\nu^{*m})(g_{\text{end}}) | \mathcal{E}_{\text{SP}}(\rho_0) \rangle \rangle. \quad (112)$$

We now establish a bound on the quality of $\phi_\nu^{*m_{\text{mix}}}$, namely we show that

$$\frac{1}{|\mathbb{G}|} \sum_{g \in \mathbb{G}} \|\phi_\nu^{*m_{\text{mix}}}(g) - \omega(g)\|_\diamond \leq \delta + \delta' \leq \frac{1}{9}. \quad (113)$$

This can be seen as follows:

$$\begin{aligned} & \frac{1}{|\mathbb{G}|} \sum_{g \in \mathbb{G}} \|\phi_\nu^{*m_{\text{mix}}}(g) - \omega(g)\|_\diamond \\ & \leq \frac{1}{|\mathbb{G}|} \sum_{g \in \mathbb{G}} \|\omega_\nu^{*m_{\text{mix}}}(g) - \omega(g)\|_\diamond \\ & \quad + \frac{1}{|\mathbb{G}|} \sum_{g \in \mathbb{G}} \|\phi_\nu^{*m_{\text{mix}}} - \omega_\nu^{*m_{\text{mix}}}\|_\diamond \end{aligned} \quad (114)$$

with $\omega_\nu(g) = |\mathbb{G}| \nu(g) \omega(g)$. Writing out the convolution in the first term and changing variables, we get

$$\frac{1}{|\mathbb{G}|} \sum_{g \in \mathbb{G}} \left\| \omega_v^{*m_{\text{mix}}}(g) - \omega(g) \right\|_{\diamond} = \frac{1}{|\mathbb{G}|} \sum_{g \in \mathbb{G}} \left\| \sum_{g_1, \dots, g_{m_{\text{mix}}-1} \in \mathbb{G}} |\mathbb{G}| \nu(g g_{m_{\text{mix}}-1}^{-1}) \dots \nu(g_1) \omega(g g_{m_{\text{mix}}-1}^{-1}) \dots \omega(g_1) - \omega(g) \right\|_{\diamond} \quad (115)$$

$$\leq \frac{1}{|\mathbb{G}|} \sum_{g \in \mathbb{G}} \left| \sum_{g_1, \dots, g_{m_{\text{mix}}-1} \in \mathbb{G}} |\mathbb{G}| \nu(g g_{m_{\text{mix}}-1}^{-1}) \dots \nu(g_1) - 1 \right| \|\omega(g)\|_{\diamond} \quad (116)$$

$$= \sum_{g \in \mathbb{G}} \left| \frac{1}{|\mathbb{G}|} - \nu^{*m_{\text{mix}}}(g) \right| \quad (117)$$

for the first term and

$$\frac{1}{|\mathbb{G}|} \sum_{g \in \mathbb{G}} \left\| \phi_v^{*m_{\text{mix}}} - \omega_v^{*m_{\text{mix}}} \right\|_{\diamond} = \frac{1}{|\mathbb{G}|} \sum_{g \in \mathbb{G}} \left\| \sum_{j=1}^{m_{\text{mix}}} \phi_v^{*(m_{\text{mix}}-j)} * (\phi_v - \omega_v) * \omega_v^{*(j-1)}(g) \right\|_{\diamond} \quad (118)$$

$$\leq m_{\text{mix}} \sum_{g \in \mathbb{G}} \nu(g) \|\phi(g) - \omega(g)\|_{\diamond}, \quad (119)$$

where we use the telescoping series identity $A^m - B^m = \sum_{j=1}^m A^{m-j} (A - B) B^{j-1}$, which holds for any elements A, B of an associative algebra (such as the implementation maps with convolution), the submultiplicativity of the diamond norm, and the fact that $\|\phi(g)\|_{\diamond} = \|\omega(g)\|_{\diamond} = 1$ for all $g \in \mathbb{G}$. Together with the theorem assumptions, this yields Eq. (113). Now as in Theorem 8, we can write the RB output data as

$$p_v(i, m) = \langle \langle \mathcal{E}_M(\Pi_i) | \text{Tr}_{V_{\omega_{\mathbb{G}}}} \left(\mathcal{D}_{\mathbb{G}}[\bar{\omega}_{\mathbb{G}}(g_{\text{end}}^{-1}) \otimes \mathbb{1}] F(\phi) F(\phi_v)^{m'} F(\phi_v^{*m_{\text{mix}}}) \right) | \mathcal{E}_{\text{SP}}(\rho_0) \rangle \rangle, \quad (120)$$

where $m' = m - m_{\text{mix}}$. We can again consider $F(\phi_v^{*m_{\text{mix}}})$ as a perturbation of $F(\omega)$. Since $F(\omega)$ is a projector, the operator $F(\phi_v^{*m_{\text{mix}}})$ will resolve into a dominant and subdominant invariant subspace (as in Theorem 8). We have

$$\begin{aligned} p(i, m) &= \langle \langle \mathcal{E}_M(\Pi_i) | \text{Tr}_{V_{\omega_{\mathbb{G}}}} \left(\mathcal{D}_{\mathbb{G}}[\bar{\omega}_{\mathbb{G}}(g_{\text{end}}^{-1}) \otimes \mathbb{1}] \left\{ F(\phi) F(\phi_v)^{m-m_{\text{mix}}} R_1 [X_1^{\dagger} F(\omega) X_1 \right. \right. \\ &\quad \left. \left. + (X_1^{\dagger} - P_1 X_2^{\dagger}) F(\phi_v^{*m_{\text{mix}}} - \omega) X_1 \right] L_1^{\dagger} \right\} \right) | \mathcal{E}_{\text{SP}}(\rho_0) \rangle \rangle \\ &\quad + \langle \langle \mathcal{E}_M(\Pi_i) | \text{Tr}_{V_{\omega_{\mathbb{G}}}} \left(\mathcal{D}_{\mathbb{G}}[\bar{\omega}_{\mathbb{G}}(g_{\text{end}}^{-1}) \otimes \mathbb{1}] \left\{ F(\phi) F(\phi_v)^{m-m_{\text{mix}}} R_2 [X_2^{\dagger} F(\omega) X_2 \right. \right. \\ &\quad \left. \left. + (X_2^{\dagger} - P_1 X_1^{\dagger}) F(\phi_v^{*m_{\text{mix}}} - \omega) X_2 \right] L_2^{\dagger} \right\} \right) | \mathcal{E}_{\text{SP}}(\rho_0) \rangle \rangle. \end{aligned} \quad (121)$$

Now note that $F(\phi_v^{*m_{\text{mix}}})$ and $F(\phi_v)$ commute, and hence share invariant subspaces. This means we can write the first term in Eq. (121) as

$$(1) = \sum_{\lambda \in \Lambda} \text{Tr} (A_{\lambda} M_{\lambda}^{m-m_{\text{mix}}}). \quad (122)$$

Finally, we can bound the second term in Eq. (121) as

$$| (2) | \leq \left\| F(\phi) F(\phi_v)^{m-m_{\text{mix}}} R_2 [X_2^{\dagger} F(\omega) X_2 + (X_2^{\dagger} - P_1 X_1^{\dagger}) F(\phi_v^{*m_{\text{mix}}} - \omega) X_2] L_2^{\dagger} \right\|_{\max} \quad (123)$$

$$\leq \left\| R_2 [X_2^{\dagger} F(\omega) X_2 + (X_2^{\dagger} - P_1 X_1^{\dagger}) F(\phi_v^{*m_{\text{mix}}} - \omega) X_2] L_2^{\dagger} \right\|_m \left\| F(\phi_v)^{m-m_{\text{mix}}-1} \right\|_m \left\| F(\phi) \right\|_{\max} \quad (124)$$

using the max-mean inequality of the norms on Fourier operators. Note now that

$$\|F(\phi_\nu)^{m-m_{\text{mix}}-1}\|_m \leq \left[\sum_{g \in \mathbb{G}} \nu(g) \|\phi(g)\|_\diamond \right]^{m-m_{\text{mix}}-1} \leq 1, \quad (125)$$

where we use that ν is a probability distribution and that $\|\phi\|_\diamond \leq 1$. Moreover, we have that $\|F(\phi)\|_{\text{max}} \leq 1$. Using this and the reasoning from Theorem 8 we can thus bound the second term as

$$| (2) | \leq 2 \|F(\phi_\nu^{*m_{\text{mix}}} - \omega)\|_m \left(\left[1 + \frac{2\delta''}{1-5\delta''} \right] \left[1 + \frac{\delta''}{1-\delta''} \right] + \left[\frac{2\delta''}{1-5\delta''} \right]^2 \left[\frac{\delta''}{1-\delta''} \right] \left[3 + \frac{2\delta''}{1-5\delta''} \right] \right) \quad (126)$$

with $\delta'' = \delta + \delta'$. Inserting the assumption that $\|F(\phi^{*m_{\text{mix}}} - \omega)\|_m \leq \delta''$ we obtain the statement of the theorem. ■

C. Interleaved randomized benchmarking

As discussed in Sec. VD, a common variant of RB is interleaved randomized benchmarking (IRB). IRB is performed like uniform RB, as formulated in Algorithm 1, but the reference implementation is not a representation. Instead a fixed operation C is being interleaved between the application of randomly selected group elements. The outcome of this experiment is then compared to the same RB experiment without the interleaving gate to infer the quality of the interleaved gate C . The literature splits into two sections, standard interleaved RB [4,48] and nonstandard interleaved RB [9,47]. We emphasize here that we discuss the so-called ‘‘interleaved step’’ of the interleaved RB protocol, and do not interpret the resulting decay rate (for a thorough discussion of the relationship of interleaved RB decay rates and their interpretation see Ref. [72]).

1. Standard interleaved randomized benchmarking

In the standard protocol the interleaved operation C is applied after every randomly selected gate and is also a part of the group \mathbb{G} . Hence at the end of a random sequence, the inversion step can be performed inside the group. An IRB output data is thus of the form

$$\begin{aligned} p_{\text{IRB}}(i, g_{\text{end}}, m) &= \frac{1}{|\mathbb{G}|^m} \sum_{g_1, \dots, g_m \in \mathbb{G}} \langle \mathcal{E}_M(\Pi_i) | \phi[g_{\text{end}}(g_1 C \dots g_m C)^{-1}] \\ &\quad \times \phi(C)\phi(g_m) \dots \phi(C)\phi(g_1) | \mathcal{E}_{\text{SP}}(\rho_0) \rangle \rangle \end{aligned} \quad (127)$$

for a POVM element Π_i , an ending gate g_{end} , a sequence length m , an implementation map ϕ , and an initial state ρ_0 . It is interesting to interpret this procedure in the light of the protocol given in Sec. VC. Namely we can think of defining a probability distribution ν_C over \mathbb{G} , that takes the value 1 for $g = C$ and 0 for all other group elements. With

this probability distribution, we can reconsider the above as a RB experiment according to the protocol written in Algorithm 1, we have

$$\begin{aligned} p_{\text{IRB}}(i, g_{\text{end}}, m) &= p(i, g_{\text{end}}, 2m) = \sum_{g_1, \dots, g_{2m} \in \mathbb{G}} \langle \mathcal{E}_M(\Pi_i) | \\ &\quad \times \phi[g_{\text{end}}(g_1 g_2 \dots g_m)^{-1}] \nu_C(g_{2m}) \phi(g_{2m}) \\ &\quad \times \mu(g_{2m-1}) \phi(g_{2m-1}) \dots \nu_C(g_2) \phi(g_2) \mu(g_1) \phi(g_1) \\ &\quad \times | \mathcal{E}_{\text{SP}}(\rho_0) \rangle \rangle, \end{aligned} \quad (128)$$

where μ is the uniform distribution on \mathbb{G} . Hence, we can think of standard IRB as being a RB experiment with a particular choice of sampling distributions. In this picture, it becomes trivial to extend Theorem 8 to standard interleaved RB by considering the map $\phi_C = (\nu_C \phi) * \phi$. By the standard change of variables we can see

$$p_{\text{IRB}}(i, g_{\text{end}}, m) = \langle \mathcal{E}_M(\Pi_i) | \phi * \phi_C^{*m}(g_{\text{end}}) | \mathcal{E}_{\text{SP}}(\rho_0) \rangle \rangle \quad (129)$$

and hence interleaved RB is just uniform RB with the implementation map ϕ_C . If $\phi(C)$ is close enough to its reference representation element $\omega(C)$ the assumption Eq. (72) is reasonable for ϕ_C as well. Hence, Theorem 8 holds equally well for interleaved RB.

Nonstandard interleaved RB protocols [9,13,47,50] depart from the above framework by including interleaved gates that are not part of the group \mathbb{G} , (the Pauli group in the case of Ref. [13] and the Clifford group in the case of Ref. [47]) and sampling from the group in a nonuniform manner. These are somewhat idiosyncratic so we treat them separately. We see that the protocols of Refs. [9,47] are covered by Theorem 8, while the protocols of Ref. [13] and Ref. [50] are not covered. We expect that it is possible to make guarantees on the output data of these protocols with suitable adaptations to Theorem 8 but we do not pursue this here.

2. Interleaved T -gate randomized benchmarking

In Ref. [47] the quality of a T gate (with ideal implementation \mathcal{T}), with an associated noisy implementation $\tilde{\mathcal{T}}$ is assessed by estimating the following quantity

$$p_T(m) = \frac{1}{|\mathbb{P}_q|^m |\mathbb{C}_q|^m} \sum_{\substack{p_1, \dots, p_m \in \mathbb{P}_q \\ g_1, \dots, g_m \in \mathbb{C}_q}} \langle \mathcal{E}_M(\Pi_i) | \phi\{[g_m t(p_m) \dots g_1 t(p_1)]^{-1}\} \phi(g_m) \tilde{\mathcal{T}} \phi(p_m) \tilde{\mathcal{T}} \times \dots \times \phi(g_1) \tilde{\mathcal{T}} \phi(p_1) \tilde{\mathcal{T}} | \mathcal{E}_{\text{SP}}(\rho_0) \rangle \quad (130)$$

with \mathbb{C}_q the q -qubit Clifford group, $\mathbb{P}_q \subset \mathbb{C}_q$ the Pauli group, and $\phi : \mathbb{C} \rightarrow \mathcal{S}_d$ an implementation of the Clifford group (and the Pauli group) and $t(p) : \mathbb{P}_q \rightarrow \mathbb{C}_q$ is an injective map mapping Pauli elements p to TpT^\dagger . Because T is in the third level of the Clifford hierarchy we have $TpT^\dagger \in \mathbb{C}_q$ for all $p \in \mathbb{P}_q$ making the above well defined. By defining the map $\phi_T(g) : \mathbb{C}_q \rightarrow \mathcal{S}_d : g \mapsto v_T(g) \mathcal{T}^\dagger \phi[t^{-1}(g)] \mathcal{T}$ with

$$v_T(g) = \frac{|\mathbb{C}_q|}{|\mathbb{P}_q|} I[g \in \text{Im}(t)] \quad (131)$$

a probability distribution on \mathbb{C}_q taking nonzero value only on the image of the map t [strictly speaking $t^{-1}(g)$ is not defined for $g \notin \text{Im}(t)$, but v_T is zero there anyway]. With these definitions we can rewrite the output probability as

$$p_T(m) = \langle \mathcal{E}_M(\Pi_i) | [\phi * (\phi * \phi_T)^{*m}](e) | \mathcal{E}_{\text{SP}}(\rho_0) \rangle. \quad (132)$$

Hence, Theorem 8 generalizes to $p_T(m)$ as long as Eq. (72) is satisfied for the convoluted map $\phi * \phi_T$. In the ideal case of $\phi = \omega$ (the reference representation) and $\mathcal{T} = T$ we see that $\phi * \phi_T(g) = \omega(g)$. Hence this is a reasonable assumption to make, and Theorem 8 thus covers the protocol presented in Ref. [47].

3. Individual gate benchmarking

Individual RB, as proposed in Ref. [9], is an interleaved RB protocol characterized by uniform probability distributions and, interestingly, a reference implementation ϕ_r that is not a representation. Rather, the reference implementation is of the form $\phi_r(g) = \mathcal{U}\omega(g)$ where $\omega(g)$ is the standard action by conjugation, i.e., $\omega(g)(\rho) = U_g \rho U_g^\dagger$, and $\mathcal{U}(\rho) = U\rho U^\dagger$ is a fixed unitary gate (that is not a part of the group \mathbb{G}). Moreover, \mathcal{U} is assumed to commute with the representation $\omega(g)$. The output RB data $p(i, m)$ associated with this procedure is of the form, Eq. (74), however, the central assumption [Eq. (72)] of Theorem 8 is generally far from satisfied (unless \mathcal{U} is the identity). However,

we can make the alternative assumption that

$$\frac{1}{|\mathbb{G}|} \sum_{g \in \mathbb{G}} \|\mathcal{U}\omega(g) - \tilde{\mathcal{U}}\phi(g)\|_\diamond \leq \delta, \quad (133)$$

where $\tilde{\mathcal{U}}$ is the noisy implementation of the unitary \mathcal{U} and ϕ is the implementation of the reference representation $\omega(g)$. This is a reasonable assumption to make since

$$\begin{aligned} & \frac{1}{|\mathbb{G}|} \sum_{g \in \mathbb{G}} \|\mathcal{U}\omega(g) - \tilde{\mathcal{U}}\phi(g)\|_\diamond \\ & \leq \frac{1}{|\mathbb{G}|} \sum_{g \in \mathbb{G}} \|\mathcal{U}\omega(g) - \mathcal{U}\phi(g)\|_\diamond + \|\mathcal{U}\phi(g) - \tilde{\mathcal{U}}\phi(g)\|_\diamond \end{aligned} \quad (134)$$

$$\leq \|\mathcal{U} - \tilde{\mathcal{U}}\|_\diamond + \frac{1}{|\mathbb{G}|} \sum_{g \in \mathbb{G}} \|\omega(g) - \phi(g)\|_\diamond \quad (135)$$

so as long as the implementation of the interleaving unitary \mathcal{U} is of sufficient quality Eq. (133) is reasonable. Furthermore we note that due to the commutation assumption $[\omega(g), \mathcal{U}] = 0$ the Fourier operator $F(\mathcal{U}\omega)$ has the same dominant invariant subspace as $F(\omega)$ [since $F(\mathcal{U}\omega) = \mathbb{1}_\mathbb{G} \otimes \mathcal{U}F(\omega) = F(\omega)\mathbb{1}_\mathbb{G} \otimes \mathcal{U}$]. Hence the proof of Theorem 8 goes through for individual gate benchmarking as well, replacing the assumption Eq. (72) with Eq. (133).

4. Cycle benchmarking

Cycle benchmarking [13] is a recently developed RB protocol that can also be subsumed under the framework of Theorem 8, albeit after some nontrivial considerations we discuss in this section.

The data-collection phase of cycle benchmarking can be seen as interleaved RB over the Pauli group with the interleaving gate C being a (non-Pauli) Clifford gate. In particular, cycle benchmarking implements sequences C, g_m, \dots, C, g_1 where g is drawn uniformly at random from the Pauli group \mathbb{P}_q and C is a Clifford gate.

A key aspect of cycle benchmarking is the cycle length, i.e., an integer c such that $C^c = e$ (note that for any Clifford gate such a cycle length exists). In cycle benchmarking the number of random Pauli elements implemented is always a multiple of the cycle length. Writing $\phi(g)$ for the noisy implementation of the standard conjugation representation of the Pauli group, and \tilde{C} for the noisy implementation of the Clifford gate C we can define the cycle implementation map (on the Pauli group):

$$\phi_c(g) = \frac{1}{|\mathbb{P}_q|^{c-1}} \sum_{\substack{g_1, \dots, g_{c-1} \in \mathbb{P}_q \\ Cg_{c-1} \dots Cg_1 = g}} \tilde{C}\phi(g_{c-1}) \dots \tilde{C}\phi(g_1). \quad (136)$$

Note that because the Clifford group contains the Pauli group the equation $Cg_c \cdots Cg_1 = g$ makes sense. Now because of the cycle property

$$Cg_c \cdots Cg_1 = (C^{-(c-1)}g_c C^{(c-1)}) \cdots C^{-1}g_2 Cg_1 = g'_c \cdots g'_1 \quad (137)$$

since $C^{-1}gC$ is always a Pauli element. Hence the equation has exactly $|\mathbb{P}_1^{(c-1)}|$ solutions. Furthermore, we have that

$$\begin{aligned} \frac{1}{|\mathbb{P}_q|} \sum_{g \in \mathbb{P}_q} \phi_c(g) &= \frac{1}{|\mathbb{P}_q|^c} \sum_{g \in \mathbb{P}_q} \sum_{\substack{g_1, \dots, g_c \in \mathbb{P}_q \\ Cg_c \cdots Cg_1 = g}} \tilde{\mathcal{C}}\phi(g_c) \cdots \tilde{\mathcal{C}}\phi(g_1) \\ &= \frac{1}{|\mathbb{P}_q|^c} \sum_{g'_1, \dots, g'_c \in \mathbb{P}_q} \tilde{\mathcal{C}}\phi(g'_c) \cdots \tilde{\mathcal{C}}\phi(g'_1) \end{aligned} \quad (138)$$

and thus that

$$\frac{1}{|\mathbb{P}_q|^{mc}} \sum_{g_1, 1, \dots, g_m, c \in \mathbb{P}_q} \tilde{\mathcal{C}}\phi(g_{mc}) \cdots \tilde{\mathcal{C}}\phi(g_1) = \phi_c^{*m}(e), \quad (139)$$

which means cycle benchmarking can be framed as RB with the implementation map ϕ_c . Moreover, since in the limit of perfect gates we have, if $Cg_c \cdots Cg_1 = g$, that

$$\mathcal{C}\omega(g_c) \cdots \mathcal{C}\omega(g_1) = \omega(g) \quad (140)$$

we can reasonably make the assumption that ϕ_c is close to its reference implementation [i.e., Eq. (72)]. Hence the behavior of cycle benchmarking data is covered by Theorem 8. What is less clear is how to interpret the resulting exponential decays (especially in terms of the implementations ϕ and $\tilde{\mathcal{C}}$). This requires a more sophisticated analysis, which is done in Ref. [13].

5. Robust benchmarking tomography

In *robust benchmarking tomography* [50] one uses a RB protocol as a subroutine to extract tomographic information from a superoperator (not necessarily a unitary) \mathcal{E} . This is done by estimating the probability

$$\begin{aligned} p(i, m) &= \frac{1}{|\mathbb{G}|^m} \sum_{g_1, \dots, g_m \in \mathbb{G}} \langle\langle \mathcal{E}_M(\Pi_i) | \phi[g'(g_1 \dots g_m)^{-1}] \\ &\quad \times \mathcal{E}\phi(g'_m) \cdots \mathcal{E}\phi(g'_1) | \mathcal{E}_{\text{SP}}(\rho_0) \rangle\rangle, \end{aligned} \quad (141)$$

where g' is a fixed element of the group \mathbb{G} and ϕ is the implementation of a reference representation ω [the goal is to estimate correlations between $\omega(g')$ and \mathcal{E}]. We can consider this as an interleaved RB scheme with reference implementation $\phi_{\text{tom}}(g) = \omega(g'g)$ (thinking of \mathcal{E} as a noisy implementation of the identity gate). However,

this reference implementation is not close to a representation (unless $g' = e$), which means that Theorem 8 does not apply. This is not an artifact of the proof technique but rather a reflection of the fact that robust benchmarking tomography features extremely rapid exponential decays. In the gate-independent noise case the decay rate is set by the average fidelity $F[\omega(g'), \mathcal{E}]$, which can be very small. In the language of matrix Fourier theory this means that the dominant eigenvalues of the Fourier operator $F(\phi_{\text{tom}})$ will be small even in the ideal case. Hence, we do not expect an assumption of the form, Eq. (72), to be strong enough to guarantee exponential behavior of the RB output data in this scenario.

VII. DATA PROCESSING AND SAMPLE COMPLEXITY

As discussed before the randomized benchmarking protocol can be divided into data collection and postprocessing phases. The data-collection protocol is summarized in Algorithm 1. The outputs of the data-collection phase are mean estimators $\hat{p}(i, m, g_{\text{end}})$ that estimate the average over all sequences of length m according to the measures ν_i and the quantum-measurement statistics, simultaneously. The main theorems of the data-collection phase (Theorems 8–10) state that the expectation value, again both over the measurement statistics and the random sequences, is well-approximated by a linear combination of (matrix) exponentials in m .

The figures of merit that RB experiments report are the decay parameters associated with the linear combination of (matrix) exponentials. Extracting these decay parameters is the objective of the data-processing phase that is the focus of the current section. For gate-independent noise and reference representations without multiplicities the decay parameters can be directly connected to the average gate fidelity of the noise. In the more general case, the interpretation of the decay parameters in terms of other operational measures of quality can be more complicated. We consider the connection between the decay parameters and the average gate-set fidelity in Sec. IX. Here we want to take a more pragmatic approach for the postprocessing phase. The deviation of the decay parameters from unity can directly be regarded as a measure of quality that captures the deviation of the actually implemented gates from an ideal implementation. In principle, the set of decay parameters itself provides a refined image of the quality of the implementation, as compared to the average gate fidelity. This motivates us to limit the postprocessing phase to the extraction of the decay parameters. The estimation of other measures of quality from the decay parameters is then left to an optional subsequent processing phase.

In the simplest RB setting (e.g., uniform RB with the Clifford group), featuring a single noise-affected

representation, the data-processing phase involves only fitting a single exponential decay curve. The analysis of RB data arising in more general settings, however, requires a considerably more flexible approach for the data processing.

Extracting multiple decay coefficients, or poles, from a discrete series of data points is a well-studied problem in signal processing that arises in many different disciplines. For this reason, this section includes a review of modern approaches to this fitting problem that not only have been generalized to the fitting of matrix exponentials but also come with theoretical performance guarantees and bounds. The pole-finding algorithms we review (MUSIC and ESPRIT) come with multiple merits: (1) they are easily and efficiently implementable, (2) they are flexible enough to in principle analyze any RB signal of the general form, Eq. (63), (3) they come with in-built denoising and super-resolution capabilities, (4) they feature theoretical bounds that can (4a) inform the design of experimental parameters, and (4b)—very importantly—can be used to identify parameter regimes where distinguishing the different decay parameters becomes infeasible in practice.

Following this review we combine analytical guarantees and numerical simulations to evaluate the performance of these algorithmic approaches for the processing of RB data. In particular, we discuss the effect of the configuration of the decay parameters, such as their number and spacings, on the overall number of required measurements and the maximal sequence length in the experiment. We thereby provide theoretical guiding principles for designing RB experiments and explicitly work out limitations where the experimental precision required in order to separate multiple decays become impractical.

These fundamental limitations in analyzing RB data have previously motivated a variety of more resource-intensive data-gathering protocols that take further data from which one can isolate different decay curves in the classical postprocessing phase. We turn our attention to devising a novel general method for isolating matrix exponentials in Sec. VIII. We begin by a detailed description of the data-processing problem.

A. The randomized benchmarking data-processing phase

The theorems on the data-collection phase, morally summarized by Eq. (63), state that in expectation RB output data is well-approximated by a linear combination of (matrix) exponentials in m . Every matrix $M_\lambda \in \mathbb{C}^{n_\lambda \times n_\lambda}$ in the expansion is associated with an irreducible representation λ of the reference representation ω and n_λ is the multiplicity of σ_λ in the decomposition of ω . From the collected data, a RB protocol subsequently extracts decay parameters that describe the exponential decay. The decay parameters associated with a matrix M_λ are its eigenvalues

$\text{spec}(M_\lambda) = \{z_i^{(\lambda)}\}_{i=1}^{n_\lambda}$. If M_λ is diagonalizable, then

$$\text{Tr}(A_\lambda M_\lambda^m) = \sum_i^{n_\lambda} a_i^{(\lambda)} (z_i^{(\lambda)})^m \quad (142)$$

with coefficients $a_i^{(\lambda)}$ depending on the overlap of A_λ with the eigenspaces. More generally, let $M_\lambda = S^{-1}JS$ be the Jordan normal decomposition of M_λ with Jordan blocks $J = \text{diag}(J_1, J_2, \dots)$, $J_i \in \mathbb{R}^{\mu_i \times \mu_i}$ and $\{z_i^{(\lambda)}\}$ being the corresponding eigenvalues. For $m \geq \mu_i$, the j th diagonal of the m th power of the i th Jordan block contains the entry $\binom{m}{j} z_i^{m-j}$. Therefore, the matrix exponential takes the form

$$\text{Tr}(A_\lambda M_\lambda^m) = \sum_i \sum_{j \in [\mu_i]} a_i^{(\lambda, j)} \binom{m}{j} (z_i^{(\lambda)})^{m-j} \quad (143)$$

with real coefficients $a_i^{(\lambda, j)}$. Note that $\binom{m}{j}$ are falling polynomials in m . Thus, the function space of $\text{Tr}(A_\lambda M_\lambda^m)$ is in general spanned by exponential function parametrized by the eigenvalues modulated by falling polynomials.

With the pole-finding techniques, which we discuss in the next section, one can extract the set of all poles

$$\mathcal{Q} = \bigcup_{\lambda \in \Lambda} \{z_i^{(\lambda)} \mid i \in [n_\lambda]\} \quad (144)$$

from RB output data. Thus, the general postprocessing task of RB is the following: *given a data-series $\hat{p}(m)$ that is approximately described by linear combinations of polynomial modulated decays, extract the set \mathcal{Q} of all poles.*

Loosely speaking, estimating \mathcal{Q} is typically possible, provided that the coefficients of all representations are sufficiently large and the poles are sufficiently spaced. In the remainder of this section, we assess this statement quantitatively using analytical and numerical methods.

In practice, one might operate under additional assumptions and does not need to extract all poles individually. For example, if one expects multiple poles in the data series that are all more or less aligned, the data-processing problem becomes equivalent to extracting a single pole. The general form of the data-processing task, however, stays the same, namely extracting the poles in the data series. Without additional assumptions or postprocessing, the resulting poles are *unlabeled*, in the sense that one does not know which pole is associated with which irreducible presentation. This issue is addressed when we turn our attention to techniques that filter the RB data for specific representations in Sec. VIII.

B. Data-processing algorithms and guarantees

1. Fitting single decays

Many proposals for RB derive a data model that is well approximated by a single decay curve. This is, for example, the case when the group is a unitary 2-design, the reference representation ω is the adjoint representation and the actual implementation is close to being trace-preserving [24]. The adjoint representation of a unitary 2-group acts irreducible on the space of traceless matrices and yields a single dominant decay curve.

A single dominant decay parameter can be extracted using nonlinear least-squares fitting algorithms such as Levenberg-Marquardt, see, e.g., Ref. [73, Chapter 3.2]. In Ref. [56] it has been shown that in RB for the Clifford group the variance of the data points is expected to strongly vary with the sequence length m . This observed heteroskedasticity motivates us to use iteratively reweighted variants of least-squares fitting algorithms.

Reference [74] analyzes a simplified fitting procedure that estimates the decay parameter from the ratio of the data for two sufficiently separated sequence lengths. In the regime of high fidelity, it establishes a multiplicative error in the deviation of the decay parameter from an efficient number of samples. Relatedly, Ref. [45] gives an estimation scheme for a RB procedure that estimates, in parallel, multiple single exponential decays with multiplicative accuracy. This scheme makes use of postprocessing techniques to guarantee the “single-exponential” shape of the data. We discuss this more in Sec. VIII.

2. Fitting multiple decay with pole-finding algorithms: MUSIC and ESPRIT

Algorithms for simultaneously identifying multiple poles (frequencies and decay parameters) from a discrete series of data points date back to at least the work of Prony [75]. A zoo of modern algorithmic approaches has been developed in the context of direction-of-angle estimation in array signaling. In principle, these techniques can extract poles that are closer together than the grid spacing defined by the finite sampling rate, a phenomenon dubbed *superresolution*. The theoretical framework to derive guarantees for these algorithms that go beyond a perturbative analysis of special noise models or very simple configurations, was only developed recently [76,77], first focusing on convex optimization.

Here, we analyze the performance of the MUSIC algorithm [78] and the ESPRIT [79] algorithm on RB data. Performance guarantees for these two subspace algorithms were derived in Refs. [80–83] for the multiplicity-free case. Furthermore, the ESPRIT algorithm was extended to polynomially modulated exponentials of the type we encounter in RB data with multiplicities in Refs. [84,85]. We summarize the required modification in Sec. VII B 5.

For the sake of clarity, we now start reviewing the algorithms for identifying multiple poles without polynomial modulation. This corresponds to the case of RB with a multiplicity-free reference representation. For the rest of this section we denote the output data as y_m instead of $\hat{p}(m)$, in keeping with the signal-processing literature. We also assume equidistant spacing of the available sequence lengths m . As we point out in Sec. VII B 5, this requirement can be relaxed by running a low-rank completion algorithm on incomplete data and thereby infer equidistantly spaced data y_m . When clear from the context, we write the data series simply as a vector y , dropping the explicit dependence on m .

The strategy of both algorithms, MUSIC and ESPRIT, is to identify the range of the subspaces associated with the dominant singular values of the Hankel matrix of the data series $\{y_m\}_m$. The crucial observation is that from this subspace the poles can be extracted. Let $y \in \mathbb{R}^M$ be the RB data with M the maximal sequence length. The *Hankel matrix* for $1 \leq L < M$ is given by

$$\text{Hankel}_L(y) = \begin{pmatrix} y_0 & y_1 & \cdots & y_{M-L} \\ y_1 & y_2 & \cdots & y_{M-L+1} \\ \vdots & \vdots & \ddots & \vdots \\ y_L & y_{L+1} & \cdots & y_M \end{pmatrix}. \quad (145)$$

We denote the Vandermonde matrix of size $n \times M$ for poles $z = (z_1, \dots, z_n)$ by

$$W_M(z) = W_M(z_1, \dots, z_n) = \begin{pmatrix} 1 & z_1 & z_1^2 & \cdots & z_1^{M-1} \\ 1 & z_2 & z_2^2 & \cdots & z_2^{M-1} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & z_n & z_n^2 & \cdots & z_n^{M-1} \end{pmatrix}. \quad (146)$$

If $n = 1$, and thus $z \in \mathbb{C}$ we refer to $W_M(z)$ as the Vandermonde vector of length M and pole z .

With this notation, the data vector y , without noise, is in the range of $W_M(z)^T$. Furthermore, cyclically shifting the entries of y amounts to multiplication of the summands with the respective poles. In effect, the Hankel matrix has a Vandermonde decomposition

$$\text{Hankel}_L(y) = W_L^T(z) \text{diag}(a) W_{M-L}(z) + \text{Hankel}_L(\alpha), \quad (147)$$

where we denote by α the deviation of y from an ideal linear combination of exponentials due to the perturbative error $\epsilon(m)$ and finite statistics and where a is the vector of prefactors given in Eq. (143).

To identify the signal subspace and distinguish it from the noise subspace, the MUSIC and ESPRIT algorithms employ a singular value decomposition (SVD) of the Hankel matrix, $\text{Hankel}_L(y) = U \Sigma V^T$. In the absence of noise

and perturbation, i.e., $\alpha = 0$, $\text{Hankel}_L(y)$ has n nonvanishing singular values and the corresponding singular vectors form an orthonormal basis of the signal space $\text{span } W_M^T(z)$. Let U_{signal} be the matrix consisting of the singular vectors of the nontrivial singular values as columns and let U_{noise} be the matrix consisting of an orthonormal basis of the complement. It is convenient to define associated noise space (P_{noise}) and signal space (P_{signal}) projectors as $P_{\text{noise}} = U_{\text{noise}}U_{\text{noise}}^\dagger$ and $P_{\text{signal}} = U_{\text{signal}}U_{\text{signal}}^\dagger$. In the presence of noise, analogously choosing the singular vectors of the n largest singular values yields an estimate of the signal space.

From the *noise-space projector* $P_{\text{noise}} = U_{\text{noise}}U_{\text{noise}}^\dagger$, the MUSIC algorithm defines the inverse noise-space correlation function $R_{\text{noise}}^{-1} : \mathbb{C} \rightarrow \mathbb{R}$,

$$R_{\text{noise}}^{-1}(z) = \frac{\|W_L(z)\|_2}{\|P_{\text{noise}}W_L(z)\|_2}. \quad (148)$$

The poles z can then be identified as the peaks of $R_{\text{noise}}^{-1}(z)$. These can be found by a continuous scan of the values of $R_{\text{noise}}^{-1}(z)$, which can be done numerically.

A slightly different approach that avoids the continuous search for poles is taken by the ESPRIT algorithm. The ESPRIT algorithm exploits a so-called ‘‘rotational invariance’’ property. To this end, let $W_L^\downarrow(z)$ and $W_L^\uparrow(z)$ be the submatrices of the Vandermonde matrix $W_L^T(z)$ that omit the last and first column, respectively. These submatrices are related via

$$W_L^\downarrow(z) = W_L^\uparrow(z)\text{diag}(z). \quad (149)$$

This rotational invariance property is inherited by U_{signal} . In consequence, let H^\downarrow and H^\uparrow be the submatrix of the Hankel matrix H that omits the last and first rows, respectively. Then, in the noiseless case, a solution matrix Ψ of the equation

$$H^\downarrow = H^\uparrow\Psi \quad (150)$$

has nonzero eigenvalues z , which are the poles contained in the data. It is given explicitly by the pseudoinverse of H^\uparrow applied to H^\downarrow . Again noisy signals can be considerably denoised by projecting H^\uparrow to the signal space before inversion. Altogether we find the algorithmic strategy of ESPRIT to be (i) calculate the SVD of the Hankel matrix of y and determine $P_{\text{signal}} = U_{\text{signal}}U_{\text{signal}}^\dagger$, (ii) calculate $\Psi = (P_{\text{signal}}H^\uparrow)^\dagger H^\downarrow$, and (iii) determine z as the eigenvalues of Ψ .

3. Performance guarantees

Nonperturbative analysis of the performance of MUSIC has been conducted in Refs. [80,82]. Therein, the following bound for the deviation of the noise-correlation function $R_{\text{noise}}(z)$ from the ideal noiseless counterpart $R_{\text{signal}}(z)$

[defined similarly to Eq. (148) but using P_{signal}] has been derived for poles z of unit absolute value (sinusoids).

The argument, however, holds verbatim for all $z \in \mathbb{C}^n$.

Theorem 11: (Noise-correlation function bound [82], Proposition 4.2). *Let $E = \text{Hankel}_L(\alpha)$ denote the Hankel matrix of the perturbation and noise of the signal vector y . Let ε_{min} be the smallest singular value of the Hankel matrix of the noise-free signal. Suppose $L \geq n$, $M - L + 1 \geq n$ and $2\|E\|_\infty < \varepsilon_{\text{min}}$. Then,*

$$|R_{\text{noise}}(z) - R_{\text{signal}}(z)| \leq \frac{2\|E\|_\infty}{\varepsilon_{\text{min}}} \quad (151)$$

for all $z \in \mathbb{C}$.

We observe that the bound on $R_{\text{noise}}(z)$ is proportional to the spectral norm of the noise in the signal but in addition is decorated by a *noise-enhancing* factor inversely proportional to the smallest singular value ε_{min} of the Hankel matrix. The bound on $R_{\text{noise}}(z)$ can thus not be directly translated into a bound on the precision in recovering the poles z without further assumptions, see Ref. [80, Theorem 4] in this context. Nonetheless, the peaks of $R_{\text{noise}}^{-1}(z)$ are typically very sharp, and the bound on $R_{\text{noise}}(z)$ indicates a regime where one can typically expect MUSIC to accurately work. For the ESPRIT algorithm, similar bounds can be found in Refs. [81,83]. The bounds for ESPRIT additionally involve the minimum singular value of the truncation (as defined above) of the Hankel matrix.

4. Conditioning of Vandermonde matrices

The performance guarantees for MUSIC (and ESPRIT) show a noise enhancement inversely proportional to the minimum singular value ε_{min} of the Hankel matrix of the ideal signal. The minimum singular value ε_{min} in turn can be regarded as a measure for the conditioning of the Vandermonde matrices into which the Hankel matrix decomposes. This conditioning depends on the system parameters and on the configuration of poles. Given expected values for the poles and the maximal sequence length, it is straightforward to calculate the minimum singular value numerically. This can provide valuable information in the design of RB experiments.

More systematically, it is informative to understand the scaling behavior of the conditioning of the Vandermonde matrices with the help of theoretical bounds. One such bound that allows us to study its asymptotic behavior is briefly reviewed in this section. A lot of work has been devoted to study the often surprisingly favorable conditioning of Vandermonde matrices for poles on the unit circle, which describe sinusoidal oscillations, see, e.g., Ref. [83] and references therein for a discussion of the phenomenon of superresolution.

In the context of RB, we are conversely interested in poles that are on the real line. A more general characterization of the conditioning of Vandermonde matrices with poles inside the unit circle (allowing for decays beyond oscillations) has been studied in Ref. [86]. The conditioning obviously depends on the set of poles z and the size M of the Vandermonde matrix. To state the result given in Ref. [86] we define several quantities. To the set of poles $z = (z_1, \dots, z_n)$, we associate $\check{z} := \max_j |z_j|$, $\hat{z} := \min_j |z_j|$ and $\tilde{z} := \min_{j \neq k} |z_j - z_k|$. Furthermore, let us define

$$Q_M(z) = [W_M(z)W_M^\dagger(z)]^{-1/2}. \quad (152)$$

Note that $W_M(z)W_M^\dagger(z)$ is the frame operator of the frame defined by the rows of the Vandermonde matrix and $Q_M(z)$ is the orthogonalizing matrix arising in symmetric orthogonalization. With the help of $Q_M(z)$, we define the matrix

$$F_M(z) := Q_M(z) \text{diag}(z) Q_M^{-1}(z), \quad (153)$$

which will play a prominent role for analyzing the Vandermonde conditioning. In particular, its departure from normality as measured by $D^2[F_M(z)] = \|F_M(z)\|_F^2 - \|z\|_{\ell_2}^2$ will appear.

In Ref. [86] a bound is derived for the 2-norm condition number $\kappa_2(W_M) = \|W_M\|_\infty \|W_M^+\|_\infty$ through the bounding of the Frobenius norm condition number $\kappa_F(W_M) = \|W_M\|_2 \|W_M^+\|_2$. Here X^+ denotes the (Moore-Penrose) pseudoinverse of a matrix X . The condition number of a linear map A gives a worst-case bound on the relative reconstruction error in ℓ_2 norm induced by an additive error in ℓ_2 norm for a linear inverse problem. But here we are more concerned with how it enters into the accuracy of identifying poles in the MUSIC and ESPRIT algorithms. For the analysis of the MUSIC and ESPRIT algorithm, we want to upper bound the minimum singular value ε_{\min}^{-1} . By means of the Vandermonde decomposition (147) and the submultiplicativity of the spectral norm, we have $\varepsilon_{\min}^{-1} \leq \|W_{M-L}^+\|_\infty \|W_L^+\|_\infty \hat{z}^{-1}$. Since $\|W_M\|_\infty \geq 1$, we conclude that

$$\varepsilon_{\min}^{-1} \leq \kappa_2(W_{M-L})\kappa_2(W_L)\hat{z}^{-1}. \quad (154)$$

For the condition number the following bound holds.

Theorem 12: (Conditioning of Vandermonde matrices [86], Theorem 6). *For $M > n \geq 2$, for a Vandermonde matrix $W_M(z)$, it holds that*

$$\frac{\varepsilon_1[F_M(z)]}{\tilde{z}} \leq \kappa_2[W_M(z)] \leq \frac{1}{2} \left(\rho + \sqrt{\rho^2 - 4} \right) \quad (155)$$

with

$$\rho = n \left[1 + \frac{D^2[F_M(z)]}{(n-1)\tilde{z}^2} \right]^{\frac{n-1}{2}} \frac{\|\phi_L(\check{z})\|_{\ell_2}}{\|\phi_L(\hat{z})\|_{\ell_2}} - n + 2. \quad (156)$$

Most interesting in our context is the asymptotic scaling in the limit of large maximal sequence length M , for poles inside the unit disc $|z_i| < 1$ for all i . In this limit, the above bounds become tight and the following holds true.

Lemma 13: (Asymptotics of condition number [86], Lemma 8). *Let $z = (z_1, \dots, z_n) \in \mathbb{C}^n$ with $|z_i| < 1$ for all $i \in [n]$. Define $C(z) \in \mathbb{C}^{n \times n}$ as the matrix with entries*

$$C_{ij}(z) = \frac{1}{1 - z_i \bar{z}_j}. \quad (157)$$

Then,

$$\lim_{M \rightarrow \infty} \kappa_2[W_M(z)] = \sqrt{\kappa_2[C(z)]}. \quad (158)$$

Later in this section we use this bound to perform numerical investigations of the resolving power of the MUSIC and ESPRIT algorithms and to give a sampling complexity bound for general RB.

5. Extensions of the algorithms

a. Incomplete data or logarithmic grids. So far the presented algorithms and analysis relied on having an equidistant grid of sequence length. It is well known that a low-rank matrix can under fairly general assumptions be completed from the knowledge of just a subset of their entries [87]. Thus, given only data y_m for values m on an irregular subset regular grid, one can attempt at completing the Hankel matrix for the regular grid using a low-rank matrix completion algorithm. This preprocessing step can be combined with MUSIC or ESPRIT to arrive at pole-finding algorithms that do not rely on complete data from an equidistant grid [80]. In particular, we suspect that for exponential decays a logarithmic grid can potentially yield improved recovery similar to the multiplicative error bounds for the fitting of single exponentials derived in Ref. [74], but we leave formally verifying this to future work.

b. Generalization of ESPRIT to matrix exponentials. References [84,85] have generalized the ESPRIT algorithm to signal spaces spanned by products of falling polynomials and exponentials. This is exactly the signal model, Eq. (143), that we encountered for RB output data, when the reference representation has multiplicities. The key insight in this generalization is that the Hankel matrix of such signals admits a decomposition analogous to the Vandermonde decomposition (147) in terms of *Pascal-Vandermonde matrices*. These Pascal-Vandermonde matrices feature the same rotational invariance property underlying the ESPRIT algorithm.

Thus, one can show that when applying the standard ESPRIT algorithm to data of this form, the vector of eigenvalues of the matrix Ψ is still the vector of poles z with the eigenvalues appearing in multiplicities according to the maximal degree of the associated falling polynomial. Hence, ESPRIT can be directly applied to estimate matrix-exponential data series. Noise in the signal will generically break the degeneracy of the eigenvalue spectrum, corresponding to the fact that a generic matrix has nondegenerate eigenvalues. Searching for regular polygons of poles allows for matching groups of perturbed poles corresponding to the same unperturbed pole. We refer to Refs. [84,85] for further details.

C. Randomized benchmarking sampling complexity—estimation of the Hankel matrix

The performance bounds on the pole-finding algorithms, such as Theorem 11, depend on the deviation of the Hankel matrix from ideal data in spectral norm. In RB protocols this error has two contributions:

1. The finite sampling statistics of the measurements, which yields a statistical error of the mean estimator $\hat{p}(m)$.
2. The perturbative error that comes from neglecting subdominant eigenvalues, which is controlled by our Theorems 8, 9, and 10.

For the finite sampling error, we provide the following bound. To this end, we model the individual measurement performed during the RB protocol by a random variable \hat{Y}_m . To simplify the notation in the proof, we assume that the number of different sequence lengths is even and use a square Hankel matrix.

Lemma 14: (Statistical estimation). *Let M be even and $L = M/2$. For $m \in [M]$, let \hat{Y}_m be a random variable taking values in $[0, 1]$ with $\text{Var}[\hat{Y}_k] \leq \epsilon^2$. Furthermore, let $\hat{p}(m) = 1/N \sum_{i=1}^N \hat{Y}_m^{(i)}$ the corresponding mean estimator of N independent identically distributed (IID) copies $\hat{Y}_m^{(i)}$ of \hat{Y}_m . We denote with $\text{Hankel}_L(\hat{p})$ the Hankel matrix of the vector $\hat{p} = [\hat{p}(m)]_{m \in [M]} \in \mathbb{R}^M$. Then,*

$$\|\text{Hankel}_L(\hat{p}) - \mathbb{E}\text{Hankel}_L(\hat{p})\|_\infty \leq \epsilon \quad (159)$$

with probability $1 - \delta$ provided that

$$N \geq 4 \max \left\{ \frac{M\epsilon^2}{\epsilon^2}, \frac{2}{3\epsilon} \right\} \log \frac{M}{\delta}. \quad (160)$$

Combining Lemma 14 with the performance bound for MUSIC, Theorem 11, and Eq. (154) we can state the following result for the overall sampling complexity of random benchmarking experiments.

Corollary 15: (Sampling complexity). *Let M be even and $L = M/2$. And $z = (z_i)_{i=1}^n$ be a set of poles. For $m \in [M]$ let $\hat{p}(m)$ be the mean estimator of IID copies of random variables with variance bounded by ϵ^2 . Choose $\tilde{\epsilon}, \delta > 0$, provided that the total number of random trials is*

$$N_{\text{total}} \geq 8\kappa_2^4 [W_{M/2}(z)] \hat{z}^{-2} \frac{M\epsilon^2}{\tilde{\epsilon}^2} \log \frac{M}{\delta} \quad (161)$$

and

$$N_{\text{total}} \geq \frac{16}{3} \kappa_2^2 [W_{M/2}(z)] \hat{z}^{-1} \frac{1}{\tilde{\epsilon}} \log \frac{M}{\delta} \quad (162)$$

for the noise-space correlation function (148) defined by the MUSIC algorithm with input data \hat{p} it holds that $|R_{\text{noise}}(z') - R_{\text{signal}}(z')| \leq \tilde{\epsilon}$ with probability δ .

We state this bound in terms of the condition number of the Vandermonde matrix, which allows us to make analytic claims about the behavior of the sampling complexity in various regimes. However, one can state an equivalent bound in terms of the smallest singular value, which will often be significantly smaller. It is, however, difficult to work with analytically.

For the application of Corollary 15 to RB data processing, one has to additionally control the perturbative error appearing in Theorems 8, 10, and 9. The perturbative error ϵ per RB data point, see, e.g., Eq. (73), yields an additive error in the noise correlation function of order of $M\hat{z}^{-1}\kappa_2^2[W_{M/2}(z)]\epsilon$. The scaling with $M\epsilon$ originate from the spectral norm of the Hankel matrix and the factor of $z^{-1}\kappa_2^2[W_{M/2}(z)]$ captures the noise enhancement.

Lemma 14 follows from the matrix Bernstein bound [88,89] that requires us to control the spectral norm and matrix variance statistics in order to provide a tail bound for sums of matrices. We follow the same strategy as presented in Ref. [88] for Toeplitz matrices.

Proof of Lemma 14. With the help of the $L \times L$ exchange matrix

$$J_{i,j} = \begin{cases} 1 & j = L - i + 1 \\ 0 & \text{else} \end{cases} \quad (163)$$

and the $L \times L$ (noncyclic) shift matrix X that has ones its first upper off-diagonal and zeros everywhere else we can write

$$\text{Hankel}_L(\hat{p}) = \sum_{k=-L+1}^{L-1} \hat{p}_k X^k J, \quad (164)$$

where we identify the elements of p cyclically. We define

$$S_k^{(i)} := \frac{1}{N} (\hat{Y}_k^{(i)} - \mathbb{E}[\hat{Y}_k^{(i)}]) X^k J \quad (165)$$

such that $\text{Hankel}_L(\hat{P}) - \mathbb{E}\text{Hankel}_L(\hat{P}) = \sum_{i=1}^N \sum_{k=-L+1}^{L-1} S_k$ is the sum of the random matrices $S_k^{(i)}$. Since

$$\|X\|_\infty = \|J\|_\infty = 1 \quad (166)$$

and \hat{Y}_k takes values in $[0, 1]$, we have that

$$\|S_k^{(i)}\|_\infty \leq 2/N \quad (167)$$

for all i, k . For the matrix variance we calculate that

$$\begin{aligned} \sum_{k=-L+1}^{L-1} \mathbb{E}[S_k^{(i)}(S_k^{(i)})^\dagger] &= \frac{1}{N^2} \sum_{k=-L+1}^{L-1} \text{Var}[\hat{Y}_k] X^k X^{-k} \\ &= \frac{1}{N^2} \sum_{k=-L+1}^{L-1} \text{Var}[\hat{Y}_k] P_k, \end{aligned} \quad (168)$$

with P_k a diagonal projector having k ones on the diagonal and zeros everywhere else. One finds the same structure for $\sum_{k=-L+1}^{L-1} \mathbb{E}[(S_k^{(i)})^\dagger S_k^{(i)}]$ analogously. By the assumption of the lemma $\text{Var}[\hat{Y}_k] \leq \varepsilon^2$. Therefore, matrix variance statistics is dominated as

$$\begin{aligned} \max \left\{ \left\| \sum_{i=1}^N \sum_{k=-L+1}^{L-1} \mathbb{E}(S_k S_k^\dagger) \right\|_\infty, \left\| \sum_{i=1}^N \sum_{k=-L+1}^{L-1} \mathbb{E}(S_k^\dagger S_k) \right\|_\infty \right\} \\ \leq \frac{M\varepsilon^2}{N}. \end{aligned} \quad (169)$$

The matrix Bernstein inequality [88] yields

$$\begin{aligned} \mathbb{P} \left[\left\| \sum_{i=1}^N \sum_{k=-L+1}^{L-1} S_k \right\|_\infty \geq \epsilon \right] \\ \leq M \exp \left(- \min \left\{ \frac{\epsilon^2 N}{4M\varepsilon^2}, \frac{3\epsilon N}{8} \right\} \right). \end{aligned} \quad (170)$$

Requiring the right-hand side to be dominated by δ and solving for N yields the lemma's assertion. \blacksquare

D. Vandermonde conditioning for randomized benchmarking decays

The noise-enhancement factor in the performance guarantee for the tone-finding algorithms MUSIC and ESPRIT is given by the inverse of the minimum singular value ε_{\min}^{-1} of the Hankel matrix of the ideal, noise-free signal. This minimum singular value, Eq. (154), is in turn controlled by the minimal absolute value of the poles and the conditioning of the Vandermonde matrix $W_L(z)$ associated with the poles and the signal length. Here we numerically investigate this conditioning in various scenarios relevant to RB. We express all data in terms of the dimension of the Hankel matrix L , which one can generally take as being about half of the maximal sequence length M .

When the RB data model is described by many poles that are close in value the noise enhancement due to bad conditioning can be the limiting factor rendering the extraction of poles infeasible.

Increasing the sequence length improves the conditioning of $W_L(z)$, see Fig. 3. But Theorem 12 shows that the condition number of $W_L(z)$ is even in the asymptotic limit $W_\infty(z)$ for large L bounded away from zero. Thus, increasing the length of observed RB series only improves the conditioning up to a certain point.

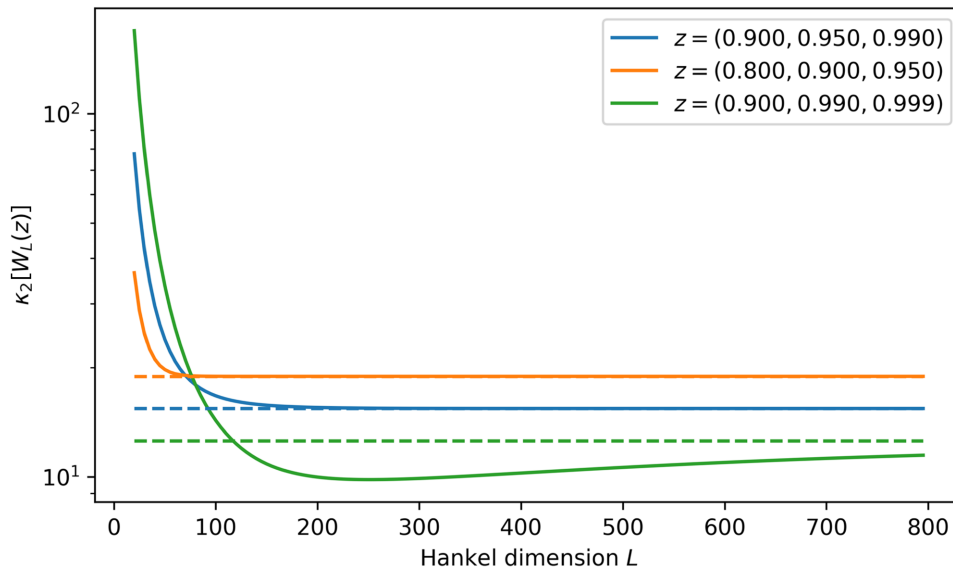


FIG. 3. The condition number of the Vandermonde matrix for different Hankel matrix dimensions (\propto RB sequence length) for three different sets of poles. The dashed lines indicate the asymptotic expression of Lemma 13. Note that the minimum for the green line is due to the scaling of the maximal eigenvalue of W_{M-L} . We observe (not depicted here) that the minimum singular value of the Hankel matrix, as appearing in Theorem 11, is monotonically increasing in L for all three sets of poles.

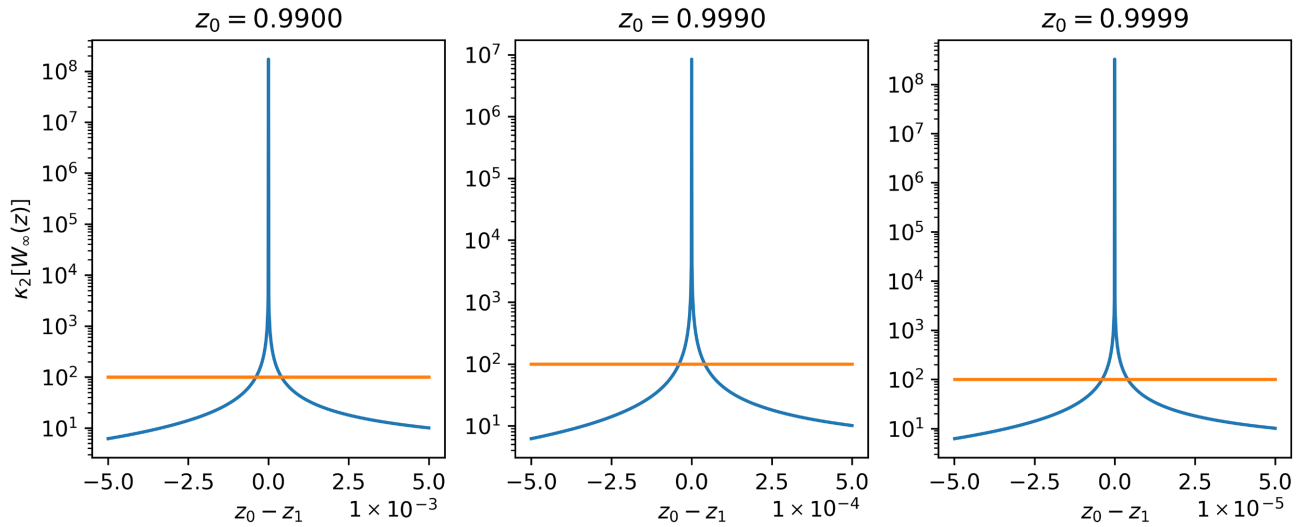


FIG. 4. Here we show the dependency of the conditioning number of the Vandermonde matrix on the spacing of two poles z_0, z_1 , for infinite sequence length. We see that the conditioning depends drastically on the distance between the two poles, but not on the absolute location of the poles on the real line. The orange line at 10^2 is added for the purpose of comparison.

The explicit expressions of the upper and lower bounds on the condition number in Theorem 12 have a rather complicated dependency on the geometrical constellation of the poles. One can argue that for RB data with poles on the real line there are roughly speaking two effects coming into play: (1) the spacing of the poles and (2) the number of poles.

To illustrate the dependency on the spacing of the poles, we numerically evaluate the $\kappa_2[W_\infty(z)]$ for different pairs of poles as they might appear in RB data. The result is shown in Fig. 4. The first pole is chosen to deviate from 1 by a value $r \in \{10^{-2}, 10^{-3}, 10^{-4}\}$, the second pole is chosen at different values around the first one. We observe that as both poles move together the condition number diverges. Importantly, the size of the interval in which the condition number grows over a certain threshold scales with r . Correspondingly, we expect that poles closer to 1 can be still resolved with a smaller spacing compared to poles that deviate considerably from 1.

Secondly, even if the poles are spaced such that the ratio of the departure from normality and the minimum spacing are fixed the upper bound in Theorem 12 exhibits an exponential dependency on the number of poles. We numerically evaluate this dependency for different families of poles that each defines a set of poles for every

cardinality, see Table I. These families include linearly spaced poles within the interval $(\alpha, 1)$ and the pole families $F_a(n) = (z_i = 1 - 10^{-i/a} \mid i \in [n])$ for positive real a . For example, $F_1(n) = (.9, .99, .999, \dots)$, which can be regarded as featuring exponentially spaced “infidelities”.

Figure 5 depicts the dependency of $\kappa_2[W_\infty(z)]$ on the number of poles n for different families. We find that due to a typically exponential dependency, the conditioning indicates that the reconstruction of multiple poles becomes demanding for already small numbers n .

Note that the conditioning is significantly improved if the poles are not exclusively on the real line but also have nonvanishing imaginary parts. Such pole sets, for example, arise in the RB variant of Ref. [9] focusing on individual gates.

E. Performance evaluation

After collecting evidence that the reconstruction of multiple poles quickly becomes a demanding task. We here show that for moderate configurations (i.e., not too many poles, not too close together) the ESPRIT algorithm is suitable for the postprocessing of RB data. To this end, we implement the ESPRIT algorithm in Python. For a fixed set of poles the ideal data series (constructed from

TABLE I. Examples of pole families for different numbers of poles n .

n	2	4	6
Lin. $\alpha = .9$	(0.9, 0.95)	(0.9, 0.925, 0.95, 0.975)	(0.9, 0.9167, 0.9333, 0.95, 0.9667, 0.9833)
Lin. $\alpha = .5$	(0.5, 0.75)	(0.5, 0.625, 0.75, 0.875)	(0.5, 0.5833, 0.6667, 0.75, 0.8333, 0.9167)
F_1	(.9, .99)	(.9, .99, .999, .9999)	(.9, .99, .999, .9999, .99999, .999999)
F_2	(0.9, 0.9684)	(0.9, 0.9684, 0.99, 0.9968)	(0.9, 0.9684, 0.99, 0.9968, 0.999, 0.9997)

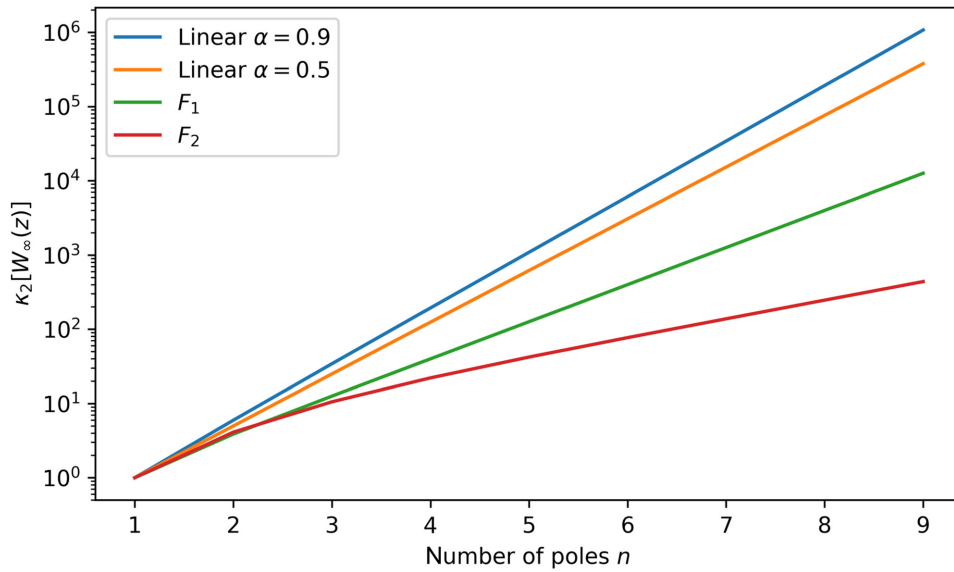


FIG. 5. The dependency of the condition number in the limit of infinite sequence length on the number of poles for different families of poles. These families are defined in Table I.

the poles and a fixed identical prefactor) is made noisy by randomly sampling binomial distributions. This simulates the random noise due to finite statistics for a certain number of samples per sequence length. Subsequently, the set of poles is reconstructed from the noisy data using the ESPRIT algorithms. We compare the reconstructed set of poles with the ideal set of poles using the symmetric Hausdorff distance. Let $z \in \mathbb{C}^n$ and $z' \in \mathbb{C}^{n'}$

$$d_H(z, z') = \max\{d_{dH}(z'; z), d_{dH}(z; z')\},$$

$$d_{dH}(z, z') = \max_{k \in [n]} \min_{k' \in [n']} |z_k - z'_{k'}|. \quad (171)$$

Figure 6 displays the mean Hausdorff distance for a different number of samples. Each data point is averaged over 100 repetitions. Figure 7 depicts the mean Hausdorff distance for different numbers of samples and maximal

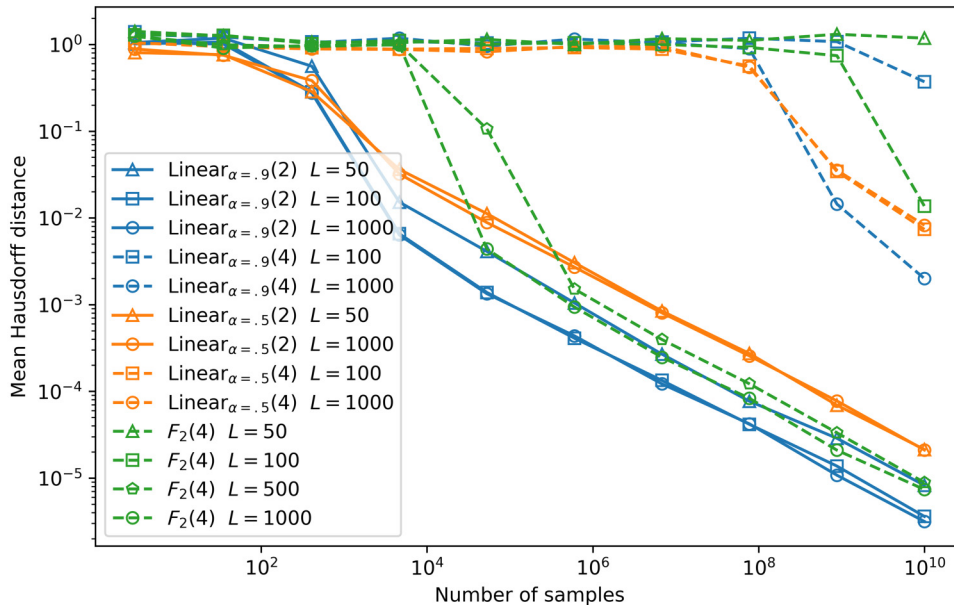


FIG. 6. Mean Hausdorff distance between the real set of poles and the reconstructed set of poles (via ESPRIT) for different families of poles (as defined in Table I) and Hankel dimension L (\propto maximal RB sequence length M) versus the number of samples used per expectation value estimation. Each data point is averaged over 100 repetitions. For all families we see that the reconstruction essentially fails until a sampling threshold is reached, after this threshold the accuracy of the estimation increases rapidly with increased number of samples. This threshold increases strongly with the number of poles in the family across all families and also depends on the maximal sequence length. This latter dependence is mediated by the actual locations of the poles in the complex plane, which is as expected.

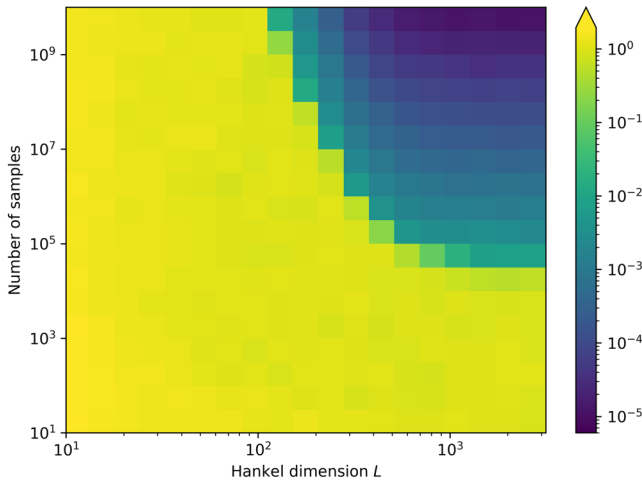


FIG. 7. Mean Hausdorff distance of the reconstruction (via ESPRIT) for poles $z = F_2(4) = (0.9, 0.968, 0.99, 0.997)$ for different number of samples and Hankel dimension L (\propto maximal RB sequence length M). Each data point is averaged over 100 repetitions. We see again that reconstruction essentially fails, until a threshold is reached both in the number of samples and in maximal sequence length after which the accuracy of reconstruction increases with increasing number of samples and in L .

sequence lengths. In both of these plots we note a threshold effect where the reconstruction of the poles essentially fails until a threshold of samples and maximal sequence length is reached, after which reconstruction accuracy increases with increasing number of samples. This phenomenon is observed for different families of poles and the location of the threshold depends strongly on the number of poles in the signal. It is interesting to note in Fig. 7 that the minimal number of samples needed for reconstruction is dependent on the maximal sequence length. Since increasing the maximal sequence length has an implicit sampling cost, this points to a nontrivial optimization problem in allocating resources. We leave further investigation of the optimal point for a family of poles for further research. The conclusion from these numerical investigations is that the RB decay-rate recovery problem is feasible using modern methods when the number of poles is small but rapidly becomes impractical as the number of poles grows.

VIII. ISOLATING MATRIX EXPONENTIALS ASSOCIATED WITH A REPRESENTATION

We have seen in Sec. VI that for uniform randomized benchmarking the output data is well described by a linear combination of (matrix) exponential decays associated with irreducible subrepresentations of a reference representation. The decay rates can, in principle, be extracted by the methods described in Sec. VII. However, two issues crop up here: (1) the sample complexity of extraction is strongly dependent on the number of decays present in the

RB output data, limiting RB to groups with reference representations containing at most a few irreducible subrepresentations, and (2) upon successful extraction of decay constants, it is not clear *a priori* how they are related to the different irreducible subrepresentations present, making it hard to relate the decay constants to the average fidelity.

A data-processing technique that addresses this problem was proposed in various papers (marked with a * in Fig. 2) such as the dihedral benchmarking scheme [37] for the single-qubit dihedral group, the character benchmarking scheme [39], which works for general groups (with some technical constraints on the reference representation) and the Pauli channel tomography scheme [45] and cycle benchmarking [13] for the Pauli group (in Ref. [45] multiple decays are actually estimated in parallel). The unifying theme in all of these procedures is that one estimates RB output data $p(i, m, g_{\text{end}})$ for different ending gates $g_{\text{end}} \in \mathbb{G}$, and then correlates the resulting vector of signals $[p(i, m, g_{\text{end}})]_{g_{\text{end}}}$ with a scalar function $f_\lambda(g_{\text{end}})$ (which can be thought of as a dual vector) that depends on an irreducible subrepresentation σ_λ of the reference representation ω .

In this section we take this idea and generalize it as far as possible. In particular, we propose a postprocessing method that, for any group \mathbb{G} and reference representation ω , takes in RB output data $p(i, m, g_{\text{end}})$ (for all $g_{\text{end}} \in \mathbb{G}$) and an irreducible subrepresentation σ_λ of the reference representation ω , and outputs postprocessed data $k_\lambda(m)$ that depends only on the (matrix) exponential decay associated with σ_λ . We state theorems for uniform RB, but the discussion below generalizes to the other types of RB.

We note that all examples of RB schemes without inversion gates (marked with a ** in Fig. 2) can be seen as special cases of the procedure given below, where the output data $[p(i, m, g_{\text{end}})]_{g_{\text{end}}}$ is simply averaged over g_{end} . We would also like to note that the procedure defined here obviates the need for explicitly implementing the inversion gate (as it can be simply absorbed by redefining g_{end}). This makes the protocol more experimentally practical.

A. The postprocessing procedure

We begin by defining *filter functions* α_λ (associated with a representation σ_λ)

$$\alpha_\lambda : \mathbb{G} \times I \rightarrow \mathbb{C} : g, i \mapsto \langle \langle \Pi_i | \mathcal{P}_\lambda \bar{\omega}(g) | \rho_0 \rangle \rangle, \quad (172)$$

where $\mathcal{P}_\lambda : \mathcal{S}_d \rightarrow \mathcal{S}_d$ is the projection onto the subrepresentation $\sigma_\lambda^{\oplus n_\lambda}$ of the reference representation ω . This is (up to normalization) the matrix element of the subrepresentation $\sigma_\lambda^{\oplus n_\lambda}$ corresponding to the vectors $|\rho_0\rangle$ and $\langle \langle \Pi_i |$. From the RB data and the above matrix element function we can now compute the following quantity we call the

λ -filtered RB output data:

$$k_\lambda(m) = \frac{1}{|\mathbb{G}|} \sum_{\mathbf{g}_{\text{end}} \in \mathbb{G}} \sum_{i \in I} N_\lambda^{-1} \alpha_\lambda(i, \mathbf{g}_{\text{end}}) p(i, m, \mathbf{g}_{\text{end}}), \quad (173)$$

where the normalization constant is given by

$$N_\lambda = \frac{1}{|\mathbb{G}|} \sum_{g \in \mathbb{G}} \sum_{i \in I} \alpha_\lambda(g, i) \langle \Pi_i | \omega(g) | \rho_0 \rangle. \quad (174)$$

One can think of this quantity as measuring the presence of the subrepresentation σ_λ in the data $p(i, \mathbf{g}_{\text{end}}, m)$. We make this more precise in the following theorem.

Theorem 16: (Measuring subrepresentations in the data). *Let \mathbb{G} be a finite group and $\omega : \mathbb{G} \rightarrow \mathcal{S}_d$ a reference representation of \mathbb{G} with decomposition $\omega = \bigoplus_{\lambda' \in \Lambda} \sigma_{\lambda'}^{\oplus n_{\lambda'}}$. Moreover, let ϕ be an implementation of ω for which Theorem 8 holds. For a fixed $\lambda \in \Lambda$ consider the λ -filtered data $k_\lambda(m)$ as defined in Eq. (173). As a function of m we now have that*

$$|k_\lambda(m) - \text{Tr}(B_\lambda M_\lambda^m)| \leq 8K \left(\delta \left[1 + \frac{2\delta}{1-5\delta} \right] \right)^m, \quad (175)$$

where B_λ is an $n_\lambda \times n_\lambda$ matrix encoding SPAM terms, M_λ is given by the projection onto the subspace associated with the n_λ largest eigenvalues of $\mathcal{F}(\phi)[\sigma_\lambda]$ (as given in Theorem 8), and K is some constant independent of m .

Proof. We know from Theorem 8 that

$$|p(i, m, \mathbf{g}_{\text{end}}) - \sum_{\lambda' \in \Lambda} \text{Tr}(A_{\lambda'} M_{\lambda'}^m)| \leq 8 \left(\delta \left[1 + \frac{2\delta}{1-5\delta} \right] \right)^m, \quad (176)$$

with $A_{\lambda'}$ given in Eq. (101). From the definition of $k_\lambda(m)$, we can thus compute

$$k_\lambda(m) = \frac{1}{|\mathbb{G}|} \sum_{\mathbf{g}_{\text{end}} \in \mathbb{G}} \sum_{i \in I} N_\lambda^{-1} \alpha_\lambda(i, \mathbf{g}_{\text{end}}) \sum_{\lambda' \in \Lambda} \text{Tr}(A_{\lambda'} M_{\lambda'}^m) \quad (177)$$

$$+ \frac{1}{|\mathbb{G}|} \sum_{\mathbf{g}_{\text{end}} \in \mathbb{G}} \sum_{i \in I} N_\lambda^{-1} \alpha_\lambda(i, \mathbf{g}_{\text{end}}) \times \left(p(i, \mathbf{g}_{\text{end}}, m) - \sum_{\lambda' \in \Lambda} \text{Tr}(A_{\lambda'} M_{\lambda'}^m) \right). \quad (178)$$

Considering only the first term, and inserting the definition of $\alpha_\lambda(i, \mathbf{g}_{\text{end}})$ we are interested in the SPAM operator quantity

$$B_{\lambda, \lambda'} = \frac{1}{|\mathbb{G}|} \sum_{\mathbf{g}_{\text{end}} \in \mathbb{G}} \sum_{i \in I} \langle \Pi_i | \mathcal{P}_\lambda \bar{\omega}(\mathbf{g}_{\text{end}}) | \rho_0 \rangle A_{\lambda'} \quad (179)$$

for $\lambda' \in \Lambda$. From the proof of Theorem 8 [Eq. (101)], we can recover an expression for the $n_{\lambda'} \times n_{\lambda'}$ matrix $A_{\lambda'}$:

$$\begin{aligned} [A_{\lambda'}]_{j, j'} &= d_{\sigma_{\lambda'}} \langle \mathcal{E}_M(\Pi_i) | \text{Tr}_{V_{\sigma_{\lambda'}}} \\ &\times \left[\bar{\sigma}_{\lambda'}(\mathbf{g}_{\text{end}}^{-1}) \otimes \mathbb{1} \right] R_1^{\lambda'} F(\mathcal{P}_{\lambda'}^j \omega \mathcal{P}_{\lambda'}^{j'}) L_1^{\lambda' \dagger} \\ &\times |\mathcal{E}_{\text{SP}}(\rho_0)\rangle, \end{aligned} \quad (180)$$

where $\mathcal{P}_{\lambda'}^j$ is the projector onto the j 'th copy of $\sigma_{\lambda'}$ in the reference representation ω and $R_1^{\lambda'}, L_1^{\lambda'}$ encode the deviation of ϕ from ω (their precise shape is not relevant for our argument). By linearity, we can now consider

$$[B_{\lambda, \lambda'}]_{j, j'} \quad (181)$$

$$= \sum_{i \in I} d_{\sigma_{\lambda'}} \langle \Pi_i \otimes \mathcal{E}_M(\Pi_i) | \frac{1}{|\mathbb{G}|} \sum_{\mathbf{g}_{\text{end}} \in \mathbb{G}} [\mathcal{P}_\lambda \bar{\omega}(\mathbf{g}_{\text{end}}^{-1})] \otimes \text{Tr}_{V_{\sigma_{\lambda'}}} \left[\bar{\sigma}_{\lambda'}(\mathbf{g}_{\text{end}}^{-1}) \otimes \mathbb{1} \right] R_1^{\lambda'} F(\mathcal{P}_{\lambda'}^j \omega \mathcal{P}_{\lambda'}^{j'}) L_1^{\lambda' \dagger} | \rho_0 \otimes \mathcal{E}_{\text{SP}}(\rho_0) \rangle \rangle \quad (182)$$

$$= \sum_{i \in I} d_{\sigma_{\lambda'}} \langle \Pi_i \otimes \mathcal{E}_M(\Pi_i) | \text{Tr}_{V_{\sigma_{\lambda'}}} \left[\delta_{\lambda, \lambda'} [\mathcal{F}(\omega)[\sigma_\lambda] \otimes \mathbb{1}] \mathbb{1} \otimes [R_1^{\lambda'} F(\mathcal{P}_{\lambda'}^j \omega \mathcal{P}_{\lambda'}^{j'}) L_1^{\lambda' \dagger}] \right] | \rho_0 \otimes \mathcal{E}_{\text{SP}}(\rho_0) \rangle \rangle, \quad (183)$$

where we use that

$$\frac{1}{|\mathbb{G}|} \sum_{\mathbf{g}_{\text{end}} \in \mathbb{G}} \mathcal{P}_\lambda \omega(\mathbf{g}_{\text{end}}) \otimes \sigma_{\lambda'}(\mathbf{g}_{\text{end}}) = \frac{1}{|\mathbb{G}|} \sum_{\mathbf{g}_{\text{end}} \in \mathbb{G}} \sigma_\lambda^{\oplus n_\lambda}(\mathbf{g}_{\text{end}}) \otimes \sigma_{\lambda'}(\mathbf{g}_{\text{end}}) = \delta_{\lambda, \lambda'} \mathcal{F}(\omega)[\sigma_{\lambda'}], \quad (184)$$

which is the Fourier transform analog of the orthogonality of characters of irreducible representations. Hence $B_{\lambda,\lambda'} = \delta_{\lambda,\lambda'} B_{\lambda,\lambda'} := B_{\lambda}$.

Plugging this back into the expression for k_{λ} we get

$$k_{\lambda}(m) = \text{Tr}(B_{\lambda} M_{\lambda}^m) + \frac{1}{|\mathbb{G}|} \sum_{\mathbf{g}_{\text{end}} \in \mathbb{G}} \sum_{i \in I} N_{\lambda}^{-1} \alpha_{\lambda}(i, \mathbf{g}_{\text{end}}) \times \left(\sum_{\lambda' \in \Lambda} \text{Tr}[A(\Pi_i, \mathbf{g}_{\text{end}})_{\lambda'} M_{\lambda'}^m] - p(i, \mathbf{g}_{\text{end}}, m) \right). \quad (185)$$

We can thus upper bound the difference $k_{\lambda}(m) - \text{Tr}(B_{\lambda} M_{\lambda})$ by considering the magnitude of the difference term. Note that we know from Theorem 8 that $\{\sum_{\lambda' \in \Lambda} \text{Tr}[A(\Pi, \mathbf{g}_{\text{end}})_{\lambda'} M_{\lambda'}^m] - p(i, m, \mathbf{g}_{\text{end}})\} \leq O(\delta^m)$. It follows that there exists a K such that

$$\left| \frac{1}{|\mathbb{G}|} \sum_{\mathbf{g}_{\text{end}} \in \mathbb{G}} \sum_{i \in I} N_{\lambda}^{-1} \alpha_{\lambda}(i, \mathbf{g}_{\text{end}}) \times \left(\sum_{\lambda' \in \Lambda} \text{Tr}[A(\Pi, \mathbf{g}_{\text{end}})_{\lambda'} M_{\lambda'}^m] - p(i, m, \mathbf{g}_{\text{end}}) \right) \right| \leq 8K \left(\delta \left[1 + \frac{2\delta}{1-5\delta} \right] \right)^m. \quad (186)$$

■

Hence, the λ -filtered output data has essentially the same behavior as regular RB data, except that only the Fourier mode associated with σ_{λ} is included in the signal. One can think of the λ filter function α_{λ} as placing a δ -peak filter function centered on the “frequency” σ_{λ} . Note that by linearity we get essentially the same result if one defines a filter function associated with nonirreducible representations (via a direct sum of irreducible representations). This can be thought of as placing a frequency comb on the RB data. Finally, it is interesting to explicitly write down the form of the SPAM matrix B_{λ} in the limit of no SPAM and

perfect gates. In the case of a multiplicity-free reference representation ω we have

$$B_{\lambda} = N_{\lambda}^{-1} \sum_{i \in I} \langle \langle \Pi_i^{\otimes 2} | \mathcal{F}(\omega) [\sigma_{\lambda}] | \rho_0^{\otimes 2} \rangle \rangle, \quad (187)$$

which emphasizes the importance of the normalization constant (on which more later), but also the importance of choosing ρ and $\{\Pi_i\}_{i \in I}$ such that B_{λ} is nonzero.

B. Statistical estimation

When computing the filtered output data $k_{\lambda}(m)$ in the previous section we assumed we had access to the RB output data $p(i, \mathbf{g}_{\text{end}}, m)$ for all $i \in I$ and $\mathbf{g}_{\text{end}} \in \mathbb{G}$. This is not realistic since both the size of the POVM $\{\Pi_i\}_{i \in I}$ and the size of the group $|\mathbb{G}|$ can be exponential in the number of qubits. In practice, we need to construct a statistical estimator \hat{k}_{λ} for k_{λ} , and argue that \hat{k}_{λ} is a good approximation for a reasonable number of samples. This we do in this section.

Note that the normalization factor N_{λ} is essential in lower bounding the magnitude of the filtered function k_{λ} (i.e., making sure that the number k_{λ} is not too small). However, this normalization factor can be proportional to the Hilbert-space dimension d , making it tricky to set up an estimator for k_{λ} that has a sampling complexity that does not grow with d (which would make sampling practically impossible for more than a few qubits). This is the task we turn to now. We can construct an estimator for $k_{\lambda}(m)$ essentially directly from its definition.

It is easy to see that the mean of this estimator is equal to the λ -filtered output data $k_{\lambda}(m)$. However, this does not mean that the associated estimation procedure is efficient. *A priori* the variance of the estimator could scale with Hilbert-space dimension d , since the magnitude of the filter function $N_{\lambda}^{-1} \alpha_{\lambda}$ does so in general. We cannot prove that this estimator is efficient for all groups \mathbb{G} and POVMs $\{\Pi_i\}_{i \in I}$. We can, however, make some partial statements. In particular, we can prove that the estimator is efficient as long as the POVM $\{\Pi_i\}_{i \in I}$ is generated by a

-
- 1 **for** $l \in \{1, \dots, L\}$ **do**
 - 2 Choose $\mathbf{g}_{\text{end}l} \in \mathbb{G}$ uniformly at random
 - 3 Perform the RB protocol Algorithm 1 to obtain frequencies $\{f_i(\mathbf{g}_{\text{end}l})\}_{i \in I}$ from the distribution $\{p(i, \mathbf{g}_{\text{end}l}, m)\}_{i \in I}$
 - 4 Compute λ -filter function values for the nonzero frequencies: $\{\alpha_{\lambda}(i, \mathbf{g}_{\text{end}l}) \parallel i \in I, f_i(\mathbf{g}_{\text{end}l})\}$
 - 5 **end**
 - 6 Compute the empirical weighted average

$$\hat{k}_{\lambda}(m) = \frac{1}{L} \sum_{l=1}^L N_{\lambda}^{-1} \alpha_{\lambda}(i, \mathbf{g}_{\text{end}l}) f_i(\mathbf{g}_{\text{end}l}) \quad (188)$$

Algorithm 2. An estimator for $k_{\lambda}(m)$

3-design. This is a restrictive condition, but not impossible to fulfill. We discuss how to implement such a POVM after stating and proving the following theorem, which essentially states that under the 3-design condition, the variance of the estimator $\hat{k}_\lambda(m)$ does not scale with the Hilbert-space dimension d . This means that the sampling resources required by the protocol do not depend on the number of qubits in the system, making the postprocessing step scalable (at least with respect to sampling). We note that this theorem gives an extremely crude bound on the variance, and the actual variance is liable to be substantially smaller. For simplicity, we assume that there is no SPAM or gate noise, but the conclusions made here easily generalize.

Theorem 17: (Efficient estimators). *Consider a uniform RB experiment of sequence length m , with group \mathbb{G} , reference representation ω , measurement POVM $\{\Pi_i\}_{i \in I}$, and initial state ρ_0 , and further assume that the POVM $\{\Pi_i\}_{i \in I}$ is an (exact) 3-design, that is $\Pi_i = d/|I| |\chi_i\rangle\langle\chi_i|$ with states $|\chi_i\rangle$ and $1/|I| \sum_{i \in I} |\chi_i\rangle\langle\chi_i|^{\otimes 3} = \int d\psi |\psi\rangle\langle\psi|^{\otimes 3}$. Then for all $\lambda \in \Lambda$ the variance of the estimator $\hat{k}_\lambda(m)$ is asymptotically independent of the Hilbert-space dimension d .*

Proof. First we calculate the effect of the 3-design condition on the normalization factor of the correlation function $\alpha(i, \cdot)$, by direct calculation we have

$$N_\lambda = \frac{1}{|\mathbb{G}|} \sum_{g \in \mathbb{G}} \sum_{i \in I} \alpha_\lambda(i, g) \langle \Pi_i | \omega(g) | \rho_0 \rangle, \quad (189)$$

$$= \frac{d^2}{|I| |\mathbb{G}|} \sum_{g \in \mathbb{G}} \int d\psi \langle \psi^{\otimes 2} | \omega(g)^{\otimes 2} \mathcal{P}_\lambda \otimes \mathbb{1} | \rho_0^{\otimes 2} \rangle, \quad (190)$$

$$= \frac{d^2}{|I|} \left[\frac{1}{d^2 - 1} \text{Tr}[\rho_0 \mathcal{P}_\lambda(\rho_0)] + \frac{\text{Tr}[\mathcal{P}_\lambda(\rho_0)] \text{Tr}(\rho_0)}{d^2} \right], \quad (191)$$

$$= \frac{1}{|I|} \left[\frac{d^2}{d^2 - 1} \text{Tr}[\rho_0 \mathcal{P}_\lambda(\rho_0)] + \text{Tr}[\mathcal{P}_\lambda(\rho_0)] \right], \quad (192)$$

where we use the fact that the Haar measure is invariant under unitary action to absorb the $\omega(g)$ dependence, as well as a standard formula for the second moment of a Haar average over the unitary group, see, e.g., Ref. [55, Proposition 37] or Ref. [54] [and that $\text{Tr}(\rho_0) = 1$]. We can now calculate the variance. We denote by $\hat{k}_\lambda(m, \mathbf{g}_{\text{end}})$ the estimator of $\sum_{i \in I} N_\lambda^{-1} \alpha(i, \mathbf{g}_{\text{end}}) p(i, m, \mathbf{g}_{\text{end}})$ for a fixed $\mathbf{g}_{\text{end}} \in \mathbb{G}$. By the law of total variation we can write

$$\mathbb{V}[\hat{k}_\lambda(m)] = \frac{1}{|\mathbb{G}|} \sum_{\mathbf{g}_{\text{end}} \in \mathbb{G}} \mathbb{V}[\hat{k}_\lambda(m, \mathbf{g}_{\text{end}})] + \mathbb{V}_{\mathbb{G}} \left[\sum_{i \in I} \alpha(i, \mathbf{g}_{\text{end}}) p(i, m, \mathbf{g}_{\text{end}}) \right] \quad (193)$$

$$\leq \frac{1}{|\mathbb{G}|} \sum_{\mathbf{g}_{\text{end}} \in \mathbb{G}} \sum_{i \in I} N_\lambda^{-2} \alpha(i, \mathbf{g}_{\text{end}})^2 p(i, m, \mathbf{g}_{\text{end}}) + \frac{1}{|\mathbb{G}|} \sum_{\mathbf{g}_{\text{end}} \in \mathbb{G}} \left[\sum_{i \in I} N_\lambda^{-1} \alpha(i, \mathbf{g}_{\text{end}}) p(i, m, \mathbf{g}_{\text{end}}) \right]^2, \quad (194)$$

by dropping the negative terms in the variances. We begin with calculating the second term. For this note that for all $\mathbf{g}_{\text{end}} \in \mathbb{G}$ (again using the invariance of the Haar measure):

$$\sum_{i \in I} N_\lambda^{-1} \alpha(i, \mathbf{g}_{\text{end}}) p(i, m, \mathbf{g}_{\text{end}}) = I \left[\frac{d^2}{d^2 - 1} \text{Tr}[\rho_0 \mathcal{P}_\lambda(\rho_0)] + \text{Tr}[\mathcal{P}_\lambda(\rho_0)] \right]^{-1} \quad (195)$$

$$\times \int d\psi \frac{d^2}{I} \langle \psi^{\otimes 2} | \{ \omega(g) \otimes [\mathcal{E}_M \phi^{*m}(\mathbf{g}_{\text{end}}) \mathcal{E}_{\text{SP}}] \} (\mathcal{P}_\lambda \otimes \mathbb{1}) | \rho_0^{\otimes 2} \rangle \quad (196)$$

$$= \left[\frac{d}{d^2 - 1} \text{Tr} \{ \rho_0 [\mathcal{P}_\lambda \mathcal{E}_M \phi^{*m}(\mathbf{g}_{\text{end}}) \mathcal{E}_{\text{SP}}] (\rho_0) \} + \text{Tr}[\mathcal{P}_\lambda(\rho_0)] \right] \quad (197)$$

$$\times \left[\frac{d^2}{d^2 - 1} \text{Tr}[\rho_0 \mathcal{P}_\lambda(\rho_0)] + \text{Tr}[\mathcal{P}_\lambda(\rho_0)] \right]^{-1}, \quad (198)$$

where we use the expression for $p(i, m, \mathbf{g}_{\text{end}})$ from Eq. (69). Note that this expression is asymptotically independent of the Hilbert-space dimension (depending only on how well the initial state overlaps with the projector \mathcal{P}_λ). Next we discuss the first term, given by

$$\frac{1}{|\mathbb{G}|} \sum_{\mathbf{g}_{\text{end}} \in \mathbb{G}} \sum_{i \in I} N_\lambda^{-2} \alpha(i, \mathbf{g}_{\text{end}})^2 p(i, m, \mathbf{g}_{\text{end}}) \tag{199}$$

$$= N_\lambda^{-2} \frac{d^3}{|I|^2} \frac{1}{|\mathbb{G}|} \sum_{\mathbf{g}_{\text{end}} \in \mathbb{G}} \int d\psi \langle \langle \psi^{\otimes 3} | \{ \omega(\mathbf{g}_{\text{end}})^{\otimes 2} \otimes [\mathcal{E}_M \phi^{*m}(\mathbf{g}_{\text{end}}) \mathcal{E}_{\text{SP}}] \} (\mathcal{P}_\lambda^{\otimes 2} \otimes \mathbb{1}) | \rho_0^{\otimes 3} \rangle \rangle \tag{200}$$

$$= N_\lambda^{-2} \frac{d^3}{|I|^2} \int d\psi \langle \langle \psi^{\otimes 3} | \{ \mathcal{P}_\lambda^{\otimes 2} \otimes [\mathcal{E}_M \phi^{*m}(e) \mathcal{E}_{\text{SP}}] \} | \rho_0^{\otimes 3} \rangle \rangle. \tag{201}$$

Here appears a third moment of a Haar average, which can be evaluated using Weingarten calculus (see, for instance, Eqs. S35 and S36 in Ref. [54], Ref. [55] or Ref. [90] more generally). In this particular instance, we get

$$\int d\psi \langle \psi | \mathcal{P}_\lambda(\rho_0) | \psi \rangle \langle \psi | \mathcal{P}_\lambda(\rho_0) | \psi \rangle \langle \psi | [\mathcal{E}_M \phi^{*m}(e) \mathcal{E}_{\text{SP}}](\rho_0) | \psi \rangle \tag{202}$$

$$= \frac{\text{Tr}[\mathcal{P}_\lambda(\rho_0)|_I^2] + 2 \text{Tr}\{\mathcal{P}_\lambda(\rho_0)|_I^2 [\mathcal{E}_M \phi^{*m}(e) \mathcal{E}_{\text{SP}}](\rho_0)\}}{(d+2)(d+1)d} \tag{203}$$

$$+ \frac{\text{Tr}[\mathcal{P}_\lambda(\rho_0)] \text{Tr}\{\mathcal{P}_\lambda(\rho_0)|_I [\mathcal{E}_M \phi^{*m}(e) \mathcal{E}_{\text{SP}}](\rho_0)\}}{d^2(d+1)} + \frac{\text{Tr}[\mathcal{P}_\lambda(\rho_0)]^2}{d^3}, \tag{204}$$

where $A|_I = A - \text{Tr}(A)\mathbb{1}$ for matrices A . By isolating a common d^{-3} factor and plugging back in, we get

$$\frac{1}{|\mathbb{G}|} \sum_{\mathbf{g}_{\text{end}} \in \mathbb{G}} \sum_{i \in I} N_\lambda^{-2} \alpha(i, \mathbf{g})^2 p(i, m, \mathbf{g}_{\text{end}}) \tag{205}$$

$$= \left[\frac{2 \text{Tr}[\mathcal{P}_\lambda(\rho_0)|_I^2] \text{Tr}\{\mathcal{P}_\lambda(\rho_0)|_I^2 [\mathcal{E}_M \phi^{*m}(e) \mathcal{E}_{\text{SP}}](\rho_0)\}}{(d+2)(d+1)d^{-2}} \tag{206}$$

$$+ \frac{\text{Tr}[\mathcal{P}_\lambda(\rho_0)] \text{Tr}\{\mathcal{P}_\lambda(\rho_0)|_I [\mathcal{E}_M \phi^{*m}(e) \mathcal{E}_{\text{SP}}](\rho_0)\}}{d^{-1}(d+1)} + \text{Tr}[\mathcal{P}_\lambda(\rho_0)]^2 \right] \tag{207}$$

$$\times \left[\frac{d^2}{d^2-1} \text{Tr}[\rho_0 \mathcal{P}_\lambda(\rho_0)] + \text{Tr}[\mathcal{P}_\lambda(\rho_0)] \right]^{-2}, \tag{208}$$

which is again asymptotically independent of the Hilbert-space dimension. \blacksquare

Measurement POVMs that are proportional to 3-designs are not very common. However, when considering a system of q qubits it is possible to construct one by considering computational basis measurements conjugated by a random element of the q -qubit Clifford group \mathbb{C}_q . That is, we consider the POVM

$$\{\Pi_{x,C}\} = \left\{ \frac{1}{|\mathbb{C}_q|} C|x\rangle\langle x|C^\dagger \mid x \in \{0,1\}^q, C \in \mathbb{C}_q \right\}. \tag{209}$$

It is easy to see that this is a POVM

$$\sum_{C \in \mathbb{C}_q} \sum_{x \in \{0,1\}^q} \frac{1}{|\mathbb{C}_q|} C|x\rangle\langle x|C^\dagger = \frac{1}{|\mathbb{C}_q|} \sum_{C \in \mathbb{C}_q} CC^\dagger = \mathbb{I} \tag{210}$$

and it is also proportional to a 3-design, because the multiqubit Clifford group is a unitary 3-design [91,92], and hence every orbit $\{C|x\rangle\langle x|C^\dagger\}_{C \in \mathbb{C}_q}$ is a state 3-design (and thus so is the union over x).

We emphasize that the 3-design condition is only a sufficient condition for a controlled variance of the estimator for the filtered output data, which works for any group \mathbb{G} and subrepresentation σ_λ . For particular choices of \mathbb{G} and σ_λ the estimator $\hat{k}_\lambda(m)$ might be efficient for other choices of the POVM $\{\Pi_i\}_{i \in I}$. It is, for instance, easy to see that the variance will also be controlled if the degree d_λ of the irrep σ_λ is small. This follows from the fact that the normalization factor N_λ can be written as

$$N_\lambda = \frac{1}{d_\lambda} \sum_{i \in I} \text{Tr}[\Pi_i \mathcal{P}_\lambda(\Pi_i)] \text{Tr}[\rho_0 \mathcal{P}_\lambda(\rho_0)] \tag{211}$$

so assuming the POVM $\{\Pi_i\}_{i \in I}$ and the initial state ρ_0 can be chosen to have sufficient (larger than $1/d$) overlap with the subrepresentation σ_λ the magnitude of the inverse normalization factor N_λ^{-1} , and hence the size of the support of the probability distribution $\{N_\lambda^{-1}\alpha(i, \mathbf{g}_{\text{end}})\}_{p(i, m, \mathbf{g}_{\text{end}})}$ is controlled by $1/d_\lambda$. Hence, if d_λ is small, the estimator $\hat{k}_\lambda(m)$ is efficient. This follows because it is constructed by sampling from a $[O(1) \text{ in } d]$ bounded random variable. Examples of this behavior have been noted in the literature [37, 39, 45].

Alternatively, there are situations where the dimension of the representation σ_λ scales with the total Hilbert-space dimension d but the estimator $\hat{k}_\lambda(m)$ is still efficient because the group \mathbb{G} under consideration is sufficiently randomizing (roughly, it spans its own 3-design due to the randomization over the ending gate \mathbf{g}_{end}). An example of this is the recently introduced *linear-cross-entropy benchmarking procedure*, which we discuss in the next section.

Finally, we would like to add that if one reuses the same experimental data $p(m, \mathbf{g}_{\text{end}})$ to estimate $k_\lambda(m)$ for different λ , the resulting estimates for $k_\lambda(m)$ (and consequently the associated decay rates) will be correlated. This must be taken into account when performing joint statistical inferences on estimates for several M_λ . This can of course be remedied by gathering new data for each representation label λ .

C. Example: linear cross-entropy benchmarking

Recently, Ref. [29] has introduced a RB-like protocol referred to as *linear-cross-entropy benchmarking*, in short *XEB*. We see in this section that this protocol falls into the framework of the benchmarking schemes introduced here. In fact, it can be seen as uniform RB with \mathbb{G} the full unitary group, together with a postprocessing scheme that is a special case of the above filtering scheme. Let $\phi : U(2^q) \rightarrow \mathcal{S}_d$ be an implementation map of the unitary group, also let $\{\Pi_x\}_{x \in \{0,1\}^q}$ be the computational basis POVM, and $\rho_0 = |0\rangle\langle 0|$. The linear cross-entropy fidelity is now given by

$$\mathcal{F}_{\text{XEB}} = d \int_{\text{Haar}} dU \sum_{x \in \{0,1\}^q} |\langle x | U | 0 \rangle|^2 \langle \Pi_x | \mathcal{E}_M \phi(U) \mathcal{E}_{\text{SP}} | \rho_0 \rangle \rangle \quad (212)$$

with $\mathcal{E}_M, \mathcal{E}_{\text{SP}}$ being the usual SPAM error channels. Setting $\alpha(x, U) = |\langle x | U | 0 \rangle|^2 = \langle \Pi_x | \omega(U) | \rho_0 \rangle \rangle$ we see that \mathcal{F}_{XEB} can be interpreted as a RB experiment of sequence length “0” with $\mathbf{g}_{\text{end}} = U$ together with postprocessing by correlation with the adjoint representation $\omega(U) = U \cdot U^\dagger$. Note that the dimensional factor almost precisely serves as the

correct normalization factor for $\alpha(x, U)$, since

$$\int dU \sum_x |\langle x | U | 0 \rangle|^4 = \frac{2d}{d+1}. \quad (213)$$

We can extend this interpretation by considering the linear cross entropy of a sequence of m random unitaries (this is done implicitly in Ref. [29]). This gives

$$\mathcal{F}_{\text{XEB}, m} = d \int_{\text{Haar}} dU_1 \dots U_m \sum_{x \in \{0,1\}^q} |\langle x | U_m \dots U_1 | 0 \rangle|^2 \times \langle \Pi_x | \mathcal{E}_M \phi(U_1 \dots U_m) \mathcal{E}_{\text{SP}} | \rho_0 \rangle \rangle. \quad (214)$$

Using the invariance of the Haar measure and the linearity of the trace and the tensor product we can rewrite this as

$$\begin{aligned} \mathcal{F}_{\text{XEB}, m} &= d \int_{\text{Haar}} dU_m \sum_{x \in \{0,1\}^q} |\langle x | U_m | 0 \rangle|^2 \\ &\quad \times \langle \Pi_x | \mathcal{E}_M \phi^{*m}(U_m) \mathcal{E}_{\text{SP}} | \rho_0 \rangle \rangle \quad (215) \\ &= d \int_{\text{Haar}} dU_m \sum_{x \in \{0,1\}^q} |\langle x | U_m | 0 \rangle|^2 p(x, U_m, m) \end{aligned} \quad (216)$$

with $p(x, U_m, m)$ the output probability of a regular RB experiment. Now noting that $\omega(U)$ decomposes into the trivial representation (on the space $\{a|\mathbb{1}\} \mid a \in \mathbb{C}\}$) and the adjoint representation [on the space $\{|A\rangle \mid \text{Tr}(A) = 0\}$] we apply Theorem 8 to the above to get

$$\mathcal{F}_{\text{XEB}, m} = A_{\text{tr}} s_{\text{tr}}^m + A_{\text{adj}} f_{\text{adj}}^m \quad (217)$$

up to a correction exponentially small in m , where $s_{\text{tr}} (f_{\text{adj}})$ is the largest eigenvalue of the Fourier transform of ϕ evaluated at the trivial (adjoint) representation. Recall that $s_{\text{tr}} = 1$ if $\phi(U)$ is trace preserving for all U , and that we can moreover interpret f_{adj} as affinely related to the average fidelity (certainly in the gate-independent noise setting). Hence, through Theorem 8 and our general postprocessing scheme the linear-cross-entropy benchmarking procedure inherits both the stability and interpretation of uniform RB.

It is notable that the estimator $\hat{k}_\lambda(m)$, which in this case estimates the linear cross entropy fidelity $\mathcal{F}_{\text{XEB}, m}$ is actually efficient, in the sense of Theorem 17. We can sketch an argument for this by directly estimating the variance of the estimator. For this argument we assume gate-independent noise [i.e., $\phi(U) = \mathcal{A}\omega(U)$ for some completely positive \mathcal{A}]. Following Theorem 17, we have

$$\mathbb{V}[\hat{k}_\lambda(m)] \leq d^2 \sum_{x \in \{0,1\}^q} \int_{\text{Haar}} dU |\langle x | U | 0 \rangle|^4 \langle \Pi_x | \mathcal{E}_M \phi^{*m}(U) \mathcal{E}_{\text{SP}} | \rho_0 \rangle \rangle \quad (218)$$

$$+ d^2 \int_{\text{Haar}} dU \left[\sum_{x \in \{0,1\}^q} |\langle x | U | 0 \rangle|^2 \langle \Pi_x | \mathcal{E}_M \phi^{*m}(U) \mathcal{E}_{\text{SP}} | \rho_0 \rangle \rangle \right]^2 \quad (219)$$

$$\leq d^3 \max_{x \in \{0,1\}^q} \int_{\text{Haar}} dU |\langle x | U | 0 \rangle|^4 \langle \Pi_x | \mathcal{E}_M \phi^{*m}(U) \mathcal{E}_{\text{SP}} | \rho_0 \rangle \rangle \quad (220)$$

$$+ d^4 \max_{x, x' \in \{0,1\}^q} \int_{\text{Haar}} dU |\langle x | U | 0 \rangle|^2 |\langle x' | U | 0 \rangle|^2 \quad (221)$$

$$\times \langle \Pi_x | \mathcal{E}_M \phi^{*m}(U) \mathcal{E}_{\text{SP}} | \rho_0 \rangle \rangle \langle \Pi_{x'} | \mathcal{E}_M \phi^{*m}(U) \mathcal{E}_{\text{SP}} | \rho_0 \rangle \rangle. \quad (222)$$

Using the gate-independent noise assumption and the fact that $\omega(U)(\rho) = U\rho U^\dagger$, the rhs is a Haar integral of a degree-3 homogeneous polynomial in the entries of U , \bar{U} , and the second term is a Haar integral of a degree-4 homogeneous polynomial. The asymptotic behavior of such integrals (in the limit of large d) is well known [90] and evaluates to $O(d^{-3})$ and $O(d^{-4})$, respectively. Hence, the overall variance is $O(1)$ in d . One could fill in the exact constants by evaluating the Haar integrals (like we did in Theorem 17), but we do not pursue this here.

IX. RANDOMIZED BENCHMARKING AND AVERAGE FIDELITY

To date, we have treated the information extracted from RB procedures, and in particular the decay rates, as figures of merit in their own right, without establishing a direct connection to other well-known quantities such as the average gate fidelity. Indeed, this latter object is often portrayed as the conclusive result of an RB protocol.

In this section, we provide a series of arguments to validate the interpretation of the RB parameters as standalone information, by showing that connecting RB decays to the average gate fidelity presents complications that are hard to overcome. The underlying reason for this incompatibility is due to the gauge-dependent nature of the average gate fidelity (as argued in Ref. [26]) that cannot be established nor controlled under RB. More precisely, in Sec. IX A we provide an explicit example showing that adopting a gauge to match the average gate fidelity gives rise to a channel that is not physical. In Sec. IX B, we substantiate our argument with an analysis of the expression of the entanglement fidelity—a quantity closely related to the average fidelity—in terms of RB decay parameters and the adopted gauge. Observing this expression we conclude that RB parameters and fidelity can be linked only if there is a close overlap between the dominant eigenvector of the ideal operator and the dominant, gauge-dependent left and

right eigenvectors of its implemented version; the critical point is that ascertaining whether this requirement is met is not possible with a RB procedure. We want to highlight that this intricacy in connecting RB to other well-established quantities does not mean RB protocols are inherently flawed, but only that the information they provide have to be regarded independently, with decay rates as the defining quantities to characterize the accuracy of experimentally implemented sets of gates.

A. The depolarizing gauge and in-between noise average fidelity

In an attempt to resolve the apparent disconnect between fidelity and RB decay parameters in the gate-dependent noise setting, in Refs. [24] and [25] proposals have been made for the precise connection between RB decay rates and average fidelity. In Ref. [24], it has been noted that the output data of Clifford RB could be exactly fitted to a single exponential whose decay rates are exactly interpreted as the average fidelity of the “noise in between gates,” a manifestly gauge invariant quantity. Similarly in Ref. [25], it has been argued that the decay of Clifford RB can be regarded as the average fidelity of the implementation with regard to a particular gauge choice, namely the one in which the average implementation inverted with the reference representation is precisely a depolarizing channel. We show here that (1) both of these statements can be generalized to RB with arbitrary groups, (2) both statements in fact say the exact same thing, and (3) both interpretations suffer from the same problem, namely that the channel of which the average fidelity is measured by RB is not necessarily a completely positive (CP) map (i.e., physical), even if the implementation map ϕ is.

In Ref. [24], the RB decay rate is interpreted as measuring the fidelity of “the noise in between gates.” (A general version of) this construction goes as follows. For an implementation ϕ of a group \mathbb{G} , close to some reference representation $\omega = \bigoplus_{\lambda \in \Lambda} \sigma_\lambda$ we can pick the dominant

eigenvectors $\text{vec}(\mathcal{R}_\lambda)$ of the Fourier transform $\mathcal{F}(\phi)$ evaluated at the irreducible subrepresentation $\sigma_\lambda \subset \omega$ (for now assuming no multiplicities, this easily generalizes). We can devectorize these eigenvectors and sum them up to create a superoperator \mathcal{R} with the property

$$\frac{1}{|\mathbb{G}|} \sum_{g \in \mathbb{G}} \phi(g) \mathcal{R} \omega(g)^\dagger = \mathcal{R} \text{dep}, \quad (223)$$

where dep is the generalized depolarizing channel $\text{dep} = \sum_{\lambda \in \Lambda} f_\lambda \mathcal{P}_\lambda$ with f_λ the eigenvalue corresponding to \mathcal{R}_λ . Without loss of generality we can assume that \mathcal{R} is invertible (as a matrix). Note also that for any ϕ we can write $\phi(g) = \mathcal{R} \omega(g) \mathcal{L}(g)$, where $\mathcal{L}(g)$ is some implementation map (not necessarily completely positive).

With this parametrization the noise between two gates g, g' (which in this parametrization only depends on g) is given by $\mathcal{L}(g) \mathcal{R}$. The entanglement fidelity with regards to the identity averaged over all $g \in \mathbb{G}$ of this map is

$$\begin{aligned} & \frac{1}{|\mathbb{G}|} \sum_{g \in \mathbb{G}} F_{\text{avg}}[\mathcal{L}(g) \mathcal{R}, \mathbb{1}] \\ &= \frac{1}{|\mathbb{G}|} \sum_{g \in \mathbb{G}} F_{\text{avg}}[\mathcal{R}^{-1} \mathcal{R} \omega(g) \mathcal{L}(g) \mathcal{R} \omega(g)^\dagger, \mathbb{1}] \\ &= F_{\text{avg}}(\text{dep}, \mathbb{1}), \end{aligned} \quad (224)$$

where we use the linearity and unitary invariance of the average fidelity. Note that $F_{\text{avg}}(\text{dep}, \mathbb{1}) = 1/d^2 - 1 \sum_{\lambda \in \Lambda} f_\lambda d_\lambda - 1$ is precisely the average fidelity one would obtain by plugging the RB decay rates f_λ into Eq. (242).

On the other hand, Ref. [25] connects the RB decay rates to the average fidelity of the implementation map ϕ in a particular gauge, that is a particular choice of invertible superoperators such that

$$\frac{1}{|\mathbb{G}|} \sum_{g \in \mathbb{G}} F_{\text{avg}}[S^{-1} \phi(g) S, \omega(g)] = F_{\text{avg}}(\text{dep}, \mathbb{1}). \quad (225)$$

This map $\phi_{\text{dep}} = S^{-1} \phi S$ is called the depolarizing gauge. According to Ref. [25] the correct interpretation of the RB decay rates is that they measure the fidelity of the implementation map ϕ in the depolarizing gauge with respect to the reference implementation ω . It turns out that the correct choice for S is precisely the operator R mentioned above, which can be easily seen by explicit computation

$$\begin{aligned} & \frac{1}{|\mathbb{G}|} \sum_{g \in \mathbb{G}} F_{\text{avg}}[\mathcal{R}^{-1} \phi(g) \mathcal{R}, \omega(g)] \\ &= F_{\text{avg}} \left(\mathcal{R}^{-1} \frac{1}{|\mathbb{G}|} \sum_{g \in \mathbb{G}} \phi(g) \mathcal{R} \omega(g)^\dagger, \mathbb{1} \right) \\ &= F_{\text{avg}}(\mathcal{R}^{-1} \mathcal{R} \text{dep}, \mathbb{1}). \end{aligned} \quad (226)$$

We can connect the above two interpretations by inserting the parametrization $\phi(g) = \mathcal{R} \omega(g) \mathcal{L}(g)$ into the expression for ϕ_{dep} as

$$\phi_{\text{dep}}(g) = \mathcal{R}^{-1} \mathcal{R} \omega(g) \mathcal{L}(g) \mathcal{R} = \omega(g) \mathcal{L}(g) \mathcal{R}. \quad (227)$$

Hence, the depolarizing gauge is precisely the gauge in which each superoperator $\phi_{\text{dep}}(g)$ is viewed as the ideal superoperator $\omega(g)$ preceded by the noise in between gates $\mathcal{L}(g) \mathcal{R}$ (in the sense of Ref. [24]). Hence, these two interpretations of the RB decay rates as corresponding to an average fidelity of “something” neatly map to each other.

A central open question in both the above constructions is whether the noise in between gates, or equivalently the noise in the implementation in the depolarizing gauge, can always be chosen to be a completely positive implementation map. This is essential if we want to consider these interpretations as actual descriptions of reality. Here we answer this question in the negative by giving an example (an adaptation of a construction given in Ref. [26]) of a pointwise CP implementation map ϕ where the noise in between gates (the implementation in the depolarizing gauge) is not completely positive. Let \mathbb{G} be the single-qubit Clifford group, and consider, in the Pauli basis, the following superoperators:

$$\begin{aligned} T(\gamma) &= \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \sqrt{\gamma} & 0 & 0 \\ 0 & 0 & \sqrt{\gamma} & 0 \\ 1 - \gamma & 0 & 0 & \gamma \end{pmatrix}, \\ M_1(\alpha) &= \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \alpha & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \\ M_2(\alpha) &= \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & \alpha^{-1} \end{pmatrix}. \end{aligned} \quad (228)$$

From these we can construct the implementation $\phi(g) = T(\gamma) M_1(\alpha) \omega(g) M_2(\alpha)$, with $\omega(g)(\rho) = U_g \rho U_g^\dagger$ the standard reference representation. It is easy to see that the transformation to the depolarizing gauge is given by $M_2(\alpha) \phi(g) M_2(\alpha)^{-1} = M_2(\alpha) T(\gamma) M_1(\alpha) \omega(g)$. Equivalently, the noise in between gates is given by $M_2(\alpha) T(\gamma) M_1(\alpha)$. The claim is now that there exists pairs α, γ such that $\phi(g)$ is completely positive for all $g \in \mathbb{G}$ but $M_2(\alpha) T(\gamma) M_1(\alpha)$ is not. An easy pathological example

can be obtained by setting $\gamma = 0$. In this case we have

$$\phi(g) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix},$$

$$M_2(\alpha)T(1)M_1(\alpha) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ \alpha^{-1} & 0 & 0 & 0 \end{pmatrix}. \quad (229)$$

Hence, for all $\alpha < 1$ the maps $\phi(g)$ are CP while the map $M_2(\alpha)T(0)M_1(\alpha)$ is not (this can be verified by using the complete positivity conditions for qubit channels from Ref. [93]). For $\gamma < 1$ one can always construct interval conditions on α such that the same holds. Hence, the interpretations [24,25] both suffer from a problem, namely that in order to imagine RB as “measuring the average fidelity” of some object, this object has to be chosen in a way that is not necessarily physical. This possibility was already indicated by both papers, but no explicit example was given. It is unclear how to resolve this problem: one could, for instance, try to find natural conditions on ϕ such that the noise in between gates, or equivalently the implementation in the depolarizing gauge, is always completely positive. Alternatively one could adopt the framework of Ref. [27] where one relaxes the problem by asking for

a positive-gauged implementation map that has a fidelity approximately given by the RB decay rates (with approximate meaning small relative to $1 - f_\lambda$). This can be done for Clifford RB on a single qubit [27] but generalizing to higher dimensions seems difficult (although some work in this direction has been done [94]).

B. Connecting average fidelity and randomized benchmarking decay rates

In the previous subsection we showed that the depolarizing gauge does not always give rise to a CP implementation map, and hence, cannot be connected in all cases to the average fidelity of a physical process. Here we want to investigate the link between fidelity and the RB decay parameters under a general gauge choice S . We do this using the tools of perturbation theory we have used earlier to establish Theorem 8.

1. The randomized benchmarking measurement outcome

Let us consider a special case of Theorem 8 corresponding to reference representations ω that are multiplicity-free (for simplicity), and making the gauge freedom S explicit. In this situation, we can write the Fourier operator $F(\omega)$ as a direct sum of rank-1 orthogonal projections, since from Eqs. (29) and (30) it follows that for each unitary irreducible representation σ_λ of \mathbb{G}

$$\mathcal{F}(\pi)[\sigma_\lambda] = \begin{cases} |z(\sigma_\lambda)\rangle\langle z(\sigma_\lambda)| & \text{rank-1 orthogonal projection if } \pi \text{ and } \sigma_\lambda \text{ are equivalent irreducible representations,} \\ 0 & \text{otherwise.} \end{cases} \quad (230)$$

Furthermore, we also assume that the Fourier transform $\mathcal{F}(\sigma_\lambda)$ is a diagonalizable operator. Since the set of diagonalizable matrices is dense [95], it is always possible to find such a diagonalizable matrix at arbitrary proximity of any given operator. We can thus write the Fourier transform of the implementation map on the irreducible representation appearing in the decomposition of ω as the perturbation $\widehat{E}(\sigma_\lambda) := \mathcal{F}(S\phi S^{-1} - \omega)[\sigma_\lambda]$ of the rank-1 operator $\mathcal{F}(\omega)[\sigma_\lambda]$,

$$\mathcal{F}(S\phi S^{-1})[\sigma_\lambda] = \mathcal{F}(\omega)[\sigma_\lambda] + \widehat{E}(\sigma_\lambda) \quad (231)$$

$$= \mathcal{F}(\omega)[\sigma_\lambda] + \widehat{E}(\sigma_\lambda) \quad (232)$$

$$= f_{\max}(\sigma_\lambda) |r_{\max}(\sigma_\lambda)\rangle\langle \ell_{\max}(\sigma_\lambda)| + \sum_{j_\lambda=1}^{d_\lambda-1} f_{j_\lambda}(\sigma_\lambda) |r_{j_\lambda}(\sigma_\lambda)\rangle\langle \ell_{j_\lambda}(\sigma_\lambda)|, \quad (233)$$

where $f_{\max}(\sigma_\lambda)$ is the largest eigenvalue of $\mathcal{F}(S\phi S^{-1})[\sigma_\lambda]$ and $\{f_{j_\lambda}\}_{j_\lambda=1}^{d_\lambda-1}$ are the other eigenvalues. The sets of left and right eigenvectors form a biorthogonal system, that is, $\langle \ell_{\max}(\sigma_\lambda) | r_{\max}(\sigma_\lambda) \rangle = \langle \ell_{j_\lambda}(\sigma_\lambda) | r_{j_\lambda}(\sigma_\lambda) \rangle = 1$ and $\langle \ell_{\max}(\sigma_\lambda) | r_{j_\lambda}(\sigma_\lambda) \rangle = \langle \ell_{j_\lambda}(\sigma_\lambda) | r_{\max}(\sigma_\lambda) \rangle = \langle \ell_{j_\lambda}(\sigma_\lambda) | r_{k_\lambda}(\sigma_\lambda) \rangle = 0$, for $j_\lambda \neq k_\lambda$. The important remark that we should make here is that this basis of eigenvectors reflects the gauge transformation $S\phi S^{-1}$.

In this scenario, we can thus write Eq. (75) in the proof of Theorem 8 for $g_{\text{end}} = \mathbb{1}$

$$p(i, m) = \sum_{\lambda \in \text{Irr}(\mathbb{G})} d_\lambda \langle \langle \mathcal{E}_M(\Pi_i) | \text{Tr}_{V_\lambda} \{ \mathcal{F}(S\phi S^{-1})^{m+1} [\sigma_\lambda][\overline{\sigma_\lambda}(\mathbb{1}) \otimes \mathbb{1}] \} | \mathcal{E}_{\text{SP}}(\rho_0) \rangle \rangle \quad (234)$$

$$= \sum_{\lambda \in \Lambda} \left\{ d_\lambda [f_{\max}(\sigma_\lambda)]^{m+1} \langle \langle \mathcal{E}_M(\Pi_i) | \text{Tr}_{V_\lambda} [|r_{\max}(\sigma_\lambda)\rangle \langle \ell_{\max}(\sigma_\lambda) |] | \mathcal{E}_{\text{SP}}(\rho_0) \rangle \rangle \right. \quad (235)$$

$$+ \sum_{j_\lambda} d_\lambda [f_{j_\lambda}(\sigma_\lambda)]^{m+1} \langle \langle \mathcal{E}_M(\Pi_i) | \text{Tr}_{V_\lambda} [|r_{j_\lambda}(\sigma_\lambda)\rangle \langle \ell_{j_\lambda}(\sigma_\lambda) |] | \mathcal{E}_{\text{SP}}(\rho_0) \rangle \rangle \left. \right\} \quad (236)$$

$$+ \sum_{\nu \notin \Lambda} d_\nu \langle \langle \mathcal{E}_M(\Pi_i) | \text{Tr}_{V_\nu} \{ \mathcal{F}(S\phi S^{-1})^{m+1} [\sigma_\nu][\overline{\sigma_\nu}(\mathbb{1}) \otimes \mathbb{1}] \} | \mathcal{E}_{\text{SP}}(\rho_0) \rangle \rangle. \quad (237)$$

By Eq. (62), it follows that $f_{\max}(\sigma_\lambda)$ for each σ_λ in the irreducible decomposition of ω is lower bounded by $1 - \|\widehat{E}(\sigma_\lambda)\|_2$, while the subdominant eigenvalues, correspond to perturbations of the kernel of $\mathcal{F}(\omega)[\sigma_\lambda]$, are upper bounded by $\|\widehat{E}(\sigma_\lambda)\|_2$. Moreover, by Theorem 18 presented in Sec. X, the eigenvalues in those subspaces not related to irreducible representations appearing in decomposition are again dominated by $\|\widehat{E}(\sigma_\lambda)\|_2$. Hence, we can choose m large enough such that $f_{\max}^m(\lambda) \gg f_{j_\lambda}^m(\sigma_\lambda)$ for all $f_{j_\lambda}(\sigma_\lambda)$ and for each irreducible representations σ_λ occurring in the decomposition of ω , and such that the leakage of the perturbation in nonoccurring irreducible subspaces is suppressed.

For these values of m , we then retrieve the formula for the power law in Eq. (63), but here with respect to 1-dim parameters,

$$p(i, m) \approx \sum_{\lambda \in \Lambda} [f_{\max}(\lambda)]^{m+1} \xi(S, \sigma_\lambda, \Pi_i, \rho_0), \quad (238)$$

where $\xi(S, \sigma_\lambda, \Pi_i, \rho_0) := d_\lambda \langle \langle \mathcal{E}_M(\Pi_i) | \text{Tr}_{V_\lambda} [|r_{\max}(\sigma_\lambda)\rangle \langle \ell_{\max}(\sigma_\lambda) |] | \mathcal{E}_{\text{SP}}(\rho_0) \rangle \rangle$.

2. Average gate fidelity and entanglement fidelity

The first RB protocols based on the Clifford group [5,34] linked a single decay parameter f to the average fidelity of a quantum channel \mathcal{R} , under the assumption of gate-independent noise, i.e., $\phi(g) = \mathcal{R}\omega(g)$. The relation is given by

$$F_{\text{avg}}(\mathcal{R}) = f + \frac{1-f}{d}. \quad (239)$$

This formula generalizes to uniform RB with an arbitrary group \mathbb{G} with reference representation $\omega = \bigoplus_{\lambda \in \Lambda} \sigma_\lambda^{\oplus n_\lambda}$, again under the assumption of gate-independent noise. However, it is more convenient to express it in terms of

the *entanglement fidelity*, defined as

$$F_e(\mathcal{R}) := \langle \langle \Psi | (\mathbb{1} \otimes \mathcal{R}) | \Psi \rangle \rangle = \frac{1}{d^2} \text{Tr}(\mathcal{R}), \quad (240)$$

where the trace is taken over the superoperators, and related to the average gate fidelity by

$$F_{\text{avg}}(\mathcal{R}) = \frac{dF_e(\mathcal{R}) + 1}{d + 1}. \quad (241)$$

In particular, we have (first formally written down in Ref. [14])

$$F_{\text{avg}}(\mathcal{R}) = \frac{1}{d^2} \sum_{\lambda \in \Lambda} d_\lambda \text{Tr}(M_\lambda) \quad (242)$$

with M_λ again an $n_\lambda \times n_\lambda$ matrix.

The connection between the RB decay rates and the fidelity has been challenged in Ref. [26], where it has been argued that the average fidelity and the output of RB are not related in a unique way. In doing so they introduced the concept of gauge freedom into the RB literature.

In the context of RB, gauge freedom is the observation that two implementation maps ϕ and ϕ' give rise to the same RB output data $p(m)$ if they are related by a similarity transformation S , i.e., $\phi' = S\phi S^{-1}$. However, the average fidelity of these implementation maps (relative to some reference implementation) will generally differ. Note that this an issue even with the assumption of gate-independent noise, however, in this case there is a ‘‘canonical’’ choice of gauge for which the RB decay rates and the fidelity are related. In the gate-dependent noise scenario there is no such obvious gauge choice. The rest of this section will be concerned with this question.

The entanglement fidelity—averaged over \mathbb{G} —can be expressed in terms of Fourier transforms (as has first been

noted in Ref. [25]). Indeed, we have

$$\begin{aligned} & \mathbb{E}_g F_e[S\phi S^{-1}(g), \omega(g)] \\ &= \mathbb{E}_g F_e[\omega^\dagger(g) S\phi S^{-1}(g)] \end{aligned} \quad (243)$$

$$= \frac{1}{d^2} \mathbb{E}_g \text{Tr}[\omega^\dagger(g) S\phi S^{-1}(g)] \quad (244)$$

$$= \frac{1}{d^2} \sum_{\lambda \in \text{Irr}(\mathbb{G})} d_\lambda \text{Tr}(\{\mathcal{F}(\omega)[\sigma_\lambda]\}^\dagger \mathcal{F}(S\phi S^{-1})[\sigma_\lambda]), \quad (245)$$

where we use the second Parseval identity (28).

At this point we can again use of the property in Eq. (230) for $\mathcal{F}(\omega)[\sigma_\lambda]$ and the reformulation in Eq. (233) for $\mathcal{F}(S\phi S^{-1})[\sigma_\lambda]$ and write

$$\begin{aligned} & \mathbb{E}_g F_e[S\phi S^{-1}(g), \omega(g)] \\ &= \frac{1}{d^2} \sum_{\lambda \in \Lambda} d_\lambda \text{Tr} \left[|z(\sigma_\lambda)\rangle\langle z(\sigma_\lambda)| \right. \\ & \quad \times \left. [f_{\max}(\sigma_\lambda) |r_{\max}(\sigma_\lambda)\rangle\langle \ell_{\max}(\sigma_\lambda)| \right. \end{aligned} \quad (246)$$

$$\left. + \sum_{j_\lambda} f_{j_\lambda}(\sigma_\lambda) |r_{j_\lambda}(\sigma_\lambda)\rangle\langle \ell_{j_\lambda}(\sigma_\lambda)| \right] \quad (247)$$

$$\begin{aligned} &= \frac{1}{d^2} \sum_{\lambda \in \Lambda} d_{\sigma_\lambda} f_{\max}(\sigma_\lambda) \langle z(\sigma_\lambda)|r_{\max}(\sigma_\lambda)\rangle \\ & \quad \times \langle \ell_{\max}(\sigma_\lambda)|z(\sigma_\lambda)\rangle + \alpha_{\text{res}}, \end{aligned} \quad (248)$$

where we define the residuum term

$$\alpha_{\text{res}} := \frac{1}{d^2} \sum_{\lambda \in \Lambda} d_{\sigma_\lambda} \sum_{j_\lambda} f_{j_\lambda}(\sigma_\lambda) \langle z(\sigma_\lambda)|r_{j_\lambda}(\sigma_\lambda)\rangle \langle \ell_{j_\lambda}(\sigma_\lambda)|z(\sigma_\lambda)\rangle. \quad (249)$$

This establishes a connection between the decay parameters $f_{\max}(\sigma_\lambda)$ retrieved from Eq. (238) and the entanglement fidelity as expressed in Eq. (248).

We observe that this connection is complicated by two factors. Firstly, it depends on the gauge-dependent overlap $\langle z(\sigma_\lambda)|r_{\max}(\sigma_\lambda)\rangle \langle \ell_{\max}(\sigma_\lambda)|z(\sigma_\lambda)\rangle$ between the rank-1 projection and the perturbed dominant eigenvectors—a quantity that we cannot retrieve from RB data—which might deviate significantly from 1 depending on the gauge choice. Secondly, the residuum α_{res} may be large, constituting a non-negligible part of the entanglement fidelity. The rest of the section is concerned with analyzing these gauge-dependent connective factors.

We begin by deriving a bound on α_{res} , showing that this term is small, more precisely, of third order in the gauge-dependent perturbation term $\widehat{E}(\sigma_\lambda)$. For this, we use Corollary 7, where in this specific case $a_1 = 1$ and $A_2 = 0_{(d^2-1), (d^2-1)}$ and where

$$Q_{z(\sigma_\lambda)} := X_2 X_2^\dagger = \mathbb{1} - |z(\sigma_\lambda)\rangle\langle z(\sigma_\lambda)| \quad (250)$$

is the orthogonal complement of the projection $|z(\sigma_\lambda)\rangle\langle z(\sigma_\lambda)|$. Then, the relations between unperturbed and perturbed dominant eigenvectors is given by

$$\begin{aligned} |r_{\max}(\sigma_\lambda)\rangle &= |z(\sigma_\lambda)\rangle + Q_{z(\sigma_\lambda)} \widehat{E}(\sigma_\lambda) |z(\sigma_\lambda)\rangle \\ & \quad + O[\|\widehat{E}(\sigma_\lambda)\|_2^2], \end{aligned} \quad (251)$$

$$\begin{aligned} \langle \ell_{\max}(\sigma_\lambda)| &= \langle z(\sigma_\lambda)| + \langle z(\sigma_\lambda)| \widehat{E}(\sigma_\lambda) Q_{z(\sigma_\lambda)} \\ & \quad + O[\|\widehat{E}(\sigma_\lambda)\|_2^2]. \end{aligned} \quad (252)$$

Furthermore, let us define the matrix

$$\widehat{K}(\sigma_\lambda) := \sum_{j_\lambda} f_{j_\lambda}(\sigma_\lambda) |r_{j_\lambda}(\sigma_\lambda)\rangle\langle \ell_{j_\lambda}(\sigma_\lambda)|, \quad (253)$$

where we have

$$\widehat{K}(\sigma_\lambda) |r_{\max}(\sigma_\lambda)\rangle = |0\rangle \quad \text{and} \quad \langle \ell_{\max}(\sigma_\lambda)| \widehat{K}(\sigma_\lambda) = \langle 0|, \quad (254)$$

and the bound on the 2-norm

$$\|\widehat{K}(\sigma_\lambda)\|_2 = \|\mathcal{F}(S\phi S^{-1})[\sigma_\lambda] - f_{\max}(\sigma_\lambda) |r_{\max}(\sigma_\lambda)\rangle\langle \ell_{\max}(\sigma_\lambda)|\|_2 \quad (255)$$

$$= \||z(\sigma_\lambda)\rangle\langle z(\sigma_\lambda)| + \widehat{E}(\sigma_\lambda) - f_{\max}(\sigma_\lambda) |r_{\max}(\sigma_\lambda)\rangle\langle \ell_{\max}(\sigma_\lambda)|\|_2 \quad (256)$$

$$= \||z(\sigma_\lambda)\rangle\langle z(\sigma_\lambda)| + \widehat{E}(\sigma_\lambda) - f_{\max}(\sigma_\lambda) (|z(\sigma_\lambda)\rangle\langle z(\sigma_\lambda)| + Q_{z(\sigma_\lambda)} \widehat{E}(\sigma_\lambda) |z(\sigma_\lambda)\rangle\langle z(\sigma_\lambda)|) \|_2 \quad (257)$$

$$+ |z(\sigma_\lambda)\rangle\langle z(\sigma_\lambda)| \widehat{E}(\sigma_\lambda) Q_{z(\sigma_\lambda)} + Q_{z(\sigma_\lambda)} \widehat{E}(\sigma_\lambda) |z(\sigma_\lambda)\rangle\langle z(\sigma_\lambda)| \widehat{E}(\sigma_\lambda) Q_{z(\sigma_\lambda)} \|_2 \quad (258)$$

$$\leq |1 - f_{\max}(\sigma_\lambda)| \||z(\sigma_\lambda)\rangle\langle z(\sigma_\lambda)|\|_2 + O[\|\widehat{E}(\sigma_\lambda)\|_2] \quad (259)$$

$$\leq O[\|\widehat{E}(\sigma_\lambda)\|_2], \quad (260)$$

where we use the fact that $|1 - f_{\max}(\sigma_\lambda)| \leq \|\widehat{E}(\sigma_\lambda)\|_2$.

Now, inserting Eqs. (251)–(253) into Eq. (249) and using the Cauchy-Schwarz inequality, we obtain the following bound on the residuum:

$$|\alpha_{\text{res}}| = \frac{1}{d^2} \sum_{\lambda \in \Lambda} d_{\sigma_\lambda} |\langle \ell_{\text{max}}(\sigma_\lambda) | [\mathbb{1} - \widehat{E}(\sigma_\lambda) \mathcal{Q}_{z(\sigma_\lambda)} + O[\|\widehat{E}(\sigma_\lambda)\|_2^2]] \widehat{K}(\sigma_\lambda) [\mathbb{1} - \mathcal{Q}_{z(\sigma_\lambda)} \widehat{E}(\sigma_\lambda)] + O(\|\widehat{E}(\sigma_\lambda)\|_2^2) |r_{\text{max}}(\sigma_\lambda)\rangle| \quad (261)$$

$$\leq \frac{1}{d^2} \sum_{\lambda \in \Lambda} d_{\sigma_\lambda} |\langle \ell_{\text{max}}(\sigma_\lambda) | \widehat{E}(\sigma_\lambda) \mathcal{Q}_{z(\sigma_\lambda)} \widehat{K}(\sigma_\lambda) \mathcal{Q}_{z(\sigma_\lambda)} \widehat{E}(\sigma_\lambda) |r_{\text{max}}(\sigma_\lambda)\rangle| \quad (262)$$

$$+ \frac{1}{d^2} \sum_{\lambda \in \Lambda} d_{\sigma_\lambda} O[\|\widehat{E}(\sigma_\lambda)\|_2^3] \|\widehat{K}(\sigma_\lambda)\|_2 \|\ell_{\text{max}}(\sigma_\lambda)\| \|r_{\text{max}}(\sigma_\lambda)\| + O[\|\widehat{E}(\sigma_\lambda)\|_2^4] \quad (263)$$

$$\leq \frac{1}{d^2} \sum_{\lambda \in \Lambda} d_{\sigma_\lambda} O[\|\widehat{E}(\sigma_\lambda)\|_2^3] \|\ell_{\text{max}}(\sigma_\lambda)\| \|r_{\text{max}}(\sigma_\lambda)\| + O[\|\widehat{E}(\sigma_\lambda)\|_2^4]. \quad (264)$$

This bound for α_{res} has a significant implication: it means that the residuum will not cover the leading term in Eq. (248) if the latter is $\Omega(\|\widehat{E}(\sigma_\lambda)\|_2^2)$, for all gauge choices S that yield $\|\ell_{\text{max}}(\sigma_\lambda)\| \cdot \|r_{\text{max}}(\sigma_\lambda)\|$ smaller than $1/\|\widehat{E}(\sigma_\lambda)\|_2$.

Note that it is important to compare α_{res} to the difference between 1 (the value of the entanglement fidelity of a perfect implementation) and the dominant eigenvalues in Eq. (248). This distance is indeed what RB protocols are designed to detect, and in order for the connection between fidelity and decay rates to be meaningful we require α_{res} to be negligible in comparison. To analyze this further, we first write

$$\Delta_{\text{max}} := \frac{1}{d^2} \sum_{\lambda \in \Lambda} d_{\sigma_\lambda} |1 - f_{\text{max}}(\sigma_\lambda) \langle z(\sigma_\lambda) | r_{\text{max}}(\sigma_\lambda) \rangle \langle \ell_{\text{max}}(\sigma_\lambda) | z(\sigma_\lambda) \rangle|, \quad (265)$$

and we calculate deviation of the absolute of the overlap from 1, which is remarkably only in second order in perturbation,

$$\langle z(\sigma_\lambda) | r_{\text{max}}(\sigma_\lambda) \rangle \langle \ell_{\text{max}}(\sigma_\lambda) | z(\sigma_\lambda) \rangle \quad (266)$$

$$= \left| \left(\langle z(\sigma_\lambda) | \mathbb{1} + \mathcal{Q}_{z(\sigma_\lambda)} \widehat{E}(\sigma_\lambda) + O[\|\widehat{E}(\sigma_\lambda)\|_2^2] |z(\sigma_\lambda)\rangle \right) \left(\langle z(\sigma_\lambda) | \mathbb{1} + \widehat{E}(\sigma_\lambda) \mathcal{Q}_{z(\sigma_\lambda)} + O[\|\widehat{E}(\sigma_\lambda)\|_2^2] |z(\sigma_\lambda)\rangle \right) \right| \quad (267)$$

$$\leq \left| 1 + O[\|\widehat{E}(\sigma_\lambda)\|_2^2] \right|^2 \quad (268)$$

$$\leq 1 + O[\|\widehat{E}(\sigma_\lambda)\|_2^2]. \quad (269)$$

This bound on the overlap, together with the one on the residuum, implies that the parameters $f_{\text{max}}(\sigma_\lambda)$ obtained from the fitting of the RB model in Eq. (238) yield a meaningful characterization of the fidelity on the condition when they are $\Omega[\|\widehat{E}(\sigma_\lambda)\|_2]$.

Having derived a bound on the residuum we can consider Eq. (248) in different regimes [always assuming small perturbations, i.e., $\|\widehat{E}(\sigma_\lambda)\|_2 \ll 1$]. In the first regime we make the assumption

$$\Omega[\|\widehat{E}(\sigma_\lambda)\|_2^2] = |1 - f_{\text{max}}(\sigma_\lambda)| \gg |1 - \langle z(\sigma_\lambda) | r_{\text{max}}(\sigma_\lambda) \rangle \langle \ell_{\text{max}}(\sigma_\lambda) | z(\sigma_\lambda) \rangle|, \quad (270)$$

corresponding to the situation where the parameters $\{f_{\text{max}}(\sigma_\lambda)\}_{\lambda \in \Lambda}$ are more sensitive to the perturbation than the overlap of the dominant eigenvectors. As we mentioned before, this is indeed the regime where RB provides a meaningful estimation of the fidelity. Indeed, we have

$$\Delta_{\text{max}} \geq \frac{1}{d^2} \sum_{\lambda \in \Lambda} d_{\sigma_\lambda} \left\{ |f_{\text{max}}(\sigma_\lambda) - 1| \cdot |\langle z(\sigma_\lambda) | r_{\text{max}}(\sigma_\lambda) \rangle \langle \ell_{\text{max}}(\sigma_\lambda) | z(\sigma_\lambda) \rangle| \right. \quad (271)$$

$$\left. - |1 - \langle z(\sigma_\lambda) | r_{\text{max}}(\sigma_\lambda) \rangle \langle \ell_{\text{max}}(\sigma_\lambda) | z(\sigma_\lambda) \rangle| \right\} \quad (272)$$

$$\geq \frac{1}{d^2} \sum_{\lambda \in \Lambda} d_{\sigma_\lambda} \left\{ |f_{\max}(\sigma_\lambda) - 1| \left(1 - O[\|\widehat{E}(\sigma_\lambda)\|_2^2] \right) - |1 - \langle z(\sigma_\lambda) | r_{\max}(\sigma_\lambda) \rangle \langle \ell_{\max}(\sigma_\lambda) | z(\sigma_\lambda) \rangle| \right\} \quad (273)$$

$$= \frac{1}{d^2} \sum_{\lambda \in \Lambda} d_{\sigma_\lambda} \Omega[\|\widehat{E}(\sigma_\lambda)\|_2^2] \quad (274)$$

$$\gg |\alpha_{\text{res}}|. \quad (275)$$

In a second regime we can assume the converse, namely that

$$|1 - f_{\max}(\sigma_\lambda)| \ll |1 - \langle z(\sigma_\lambda) | r_{\max}(\sigma_\lambda) \rangle \langle \ell_{\max}(\sigma_\lambda) | z(\sigma_\lambda) \rangle| = \Theta[\|\widehat{E}(\sigma_\lambda)\|_2^2] \quad (276)$$

holds true. This case is analogous, since we now have

$$\Delta_{\max} \geq \frac{1}{d^2} \sum_{\lambda \in \Lambda} d_{\sigma_\lambda} \left\{ |1 - \langle z(\sigma_\lambda) | r_{\max}(\sigma_\lambda) \rangle \langle \ell_{\max}(\sigma_\lambda) | z(\sigma_\lambda) \rangle| \right. \quad (277)$$

$$\left. - |f_{\max}(\sigma_\lambda) - 1| \cdot |\langle z(\sigma_\lambda) | r_{\max}(\sigma_\lambda) \rangle \langle \ell_{\max}(\sigma_\lambda) | z(\sigma_\lambda) \rangle| \right\} \quad (278)$$

$$\geq \frac{1}{d^2} \sum_{\lambda \in \Lambda} d_{\sigma_\lambda} \left\{ |1 - \langle z(\sigma_\lambda) | r_{\max}(\sigma_\lambda) \rangle \langle \ell_{\max}(\sigma_\lambda) | z(\sigma_\lambda) \rangle| - |f_{\max}(\sigma_\lambda) - 1| \left(1 + O[\|\widehat{E}(\sigma_\lambda)\|_2^2] \right) \right\} \quad (279)$$

$$= \frac{1}{d^2} \sum_{\lambda \in \Lambda} d_{\sigma_\lambda} \Theta[\|\widehat{E}(\sigma_\lambda)\|_2^2] \quad (280)$$

$$\gg |\alpha_{\text{res}}|. \quad (281)$$

This situation is, however, problematic, since RB gives us no information in this regime about a significant quantity: the vector overlap $\langle z(\sigma_\lambda) | r_{\max}(\sigma_\lambda) \rangle \langle \ell_{\max}(\sigma_\lambda) | z(\sigma_\lambda) \rangle$.

The last regime we consider is when $|1 - f_{\max}(\sigma_\lambda)|$ is close to the deviation of the vector overlap from 1, that is,

$$|1 - f_{\max}(\sigma_\lambda)| \approx |1 - \langle z(\sigma_\lambda) | r_{\max}(\sigma_\lambda) \rangle \langle \ell_{\max}(\sigma_\lambda) | z(\sigma_\lambda) \rangle|, \quad (282)$$

which is troublesome not only for the fact that we cannot retrieve the overlap but also because in this case Δ_{\max} may be of the same magnitude or smaller than $|\alpha_{\text{res}}|$. Indeed, in this regime the residuum can then play a significant role in the characterization of the average gate fidelity.

The conclusion we draw from this analysis is that the overlap $\langle z(\sigma_\lambda) | r_{\max}(\sigma_\lambda) \rangle \langle \ell_{\max}(\sigma_\lambda) | z(\sigma_\lambda) \rangle$ is the key factor to consider when relating RB decays to the fidelity. This overlap must be sufficiently close to 1 under the adopted gauge relative to the difference $|1 - f_{\max}(\sigma_\lambda)|$.

Finally, we wish to relate $\{\|\widehat{E}(\sigma_\lambda)\|_2\}_\lambda$ to a promise on a physical quantity related to the perturbation of the ideal gate implementation ω . We recall that $\widehat{E}(\sigma_\lambda) = \mathcal{F}(S\phi S^{-1} - \omega)[\sigma_\lambda]$ and consider that $\|\cdot\|_2 \leq \|\cdot\|_F$ such

that

$$\sum_{\lambda \in \text{Irr}(\mathbb{G})} d_\lambda \|\widehat{E}(\sigma_\lambda)\|_2^2 = \sum_{\lambda \in \text{Irr}(\mathbb{G})} d_\lambda \|\mathcal{F}(S\phi S^{-1} - \omega)[\sigma_\lambda]\|_2^2 \quad (283)$$

$$\leq \sum_{\lambda \in \text{Irr}(\mathbb{G})} d_\lambda \|\mathcal{F}(S\phi S^{-1} - \omega)[\sigma_\lambda]\|_F^2 \quad (284)$$

$$= \mathbb{E}_G \|S\phi S^{-1}(g) - \omega(g)\|_F^2, \quad (285)$$

where we apply Parseval's identity. Note, however, that the lhs of this expression runs over all irreducible representations of \mathbb{G} and not the only ones decomposing ω .

X. RANDOMIZED BENCHMARKING UNDER DIAMOND NORM AND FIDELITY CONSTRAINTS

In Theorem 8, we have argued that randomized benchmarking output data associated with an implementation of a group \mathbb{G} could be approximated as a sum of (matrix) exponentials provided the implementation map ϕ was close to a reference representation ω with respect to the diamond norm (averaged over all group elements). Here we argue that this is a natural condition to demand in the

context of RB. In particular, we show that this condition is stable, in the sense that it is impossible to be close [in the sense of Eq. (72)] to two inequivalent representations at once, and, moreover, we show that this requirement cannot be replaced with a weaker one involving the average fidelity, resolving an open question in Ref. [25].

A. Stability of representations under diamond norm

First, we prove that “closeness to a representation” is a stable concept, that is, it is impossible to be close to two representations at once (in a suitable sense).

Theorem 18: (Stability of representations). *Let ϕ be an implementation map of a group \mathbb{G} taking values in \mathcal{S}_d such that*

$$\frac{1}{|\mathbb{G}|} \sum_{g \in \mathbb{G}} \|\mathbb{1} - \phi(g)\phi(g^{-1})\|_{\diamond} \leq \delta \quad (286)$$

and let ω, ω' be representations of G on $V_n, V_{n'}$ with embedding maps $\mathcal{L} : V_n \rightarrow V_n, \mathcal{L}' : V_{n'} \rightarrow V_{n'}$ and $\mathcal{R} : V_n \rightarrow V_n, \mathcal{R}' : V_{n'} \rightarrow V_{n'}$ such that

$$\frac{1}{|\mathbb{G}|} \sum_{g \in \mathbb{G}} \|\phi(g) - \mathcal{R}\omega(g)\mathcal{L}\|_{\diamond} \leq \epsilon, \quad (287)$$

$$\frac{1}{|\mathbb{G}|} \sum_{g \in \mathbb{G}} \|\phi(g) - \mathcal{R}'\omega'(g)\mathcal{L}'\|_{\diamond} \leq \epsilon'. \quad (288)$$

Moreover, assume that there exists K such that $\|\mathcal{R}\omega(g)\mathcal{L}\|_{\diamond} \leq K, \|\mathcal{R}'\omega'(g)\mathcal{L}'\|_{\diamond} \leq K$ for all $g \in \mathbb{G}$. If the inequality $K(\epsilon + \epsilon') + 3\delta + 2\epsilon + \epsilon^2 < 1$ holds then the representations ω, ω' are equivalent on a subspace of dimension at least d^2 .

Proof. Consider the map $\mathcal{L}\mathcal{R}' : V_{n'} \rightarrow V_n$, as well as its twirled version

$$T = \frac{1}{|\mathbb{G}|} \sum_{g \in \mathbb{G}} \omega(g)\mathcal{L}\mathcal{R}'\omega'(g)^{\dagger}. \quad (289)$$

We would like to argue that T is a map of rank at least d^2 , as then we can decide the theorem by application of Schur’s lemma. To do this, consider the distance to the identity of the natural pullback of T to \mathcal{S}_d , namely $\mathcal{R}T\mathcal{L}'$. We can calculate

$$\|\mathbb{1} - \mathcal{R}T\mathcal{L}'\|_{\diamond} \leq \left\| \mathbb{1} - \frac{1}{|\mathbb{G}|} \sum_{g \in \mathbb{G}} \mathcal{R}\omega(g)\mathcal{L}\mathcal{R}\omega(g)^{\dagger}\mathcal{L}' \right\|_{\diamond} + \left\| \frac{1}{|\mathbb{G}|} \sum_{g \in \mathbb{G}} \mathcal{R}\omega(g)\mathcal{L}\mathcal{R}\omega(g)^{\dagger}\mathcal{L}' - \mathcal{R}T\mathcal{L}' \right\|_{\diamond} \quad (290)$$

$$\leq \frac{1}{|\mathbb{G}|} \sum_{g \in \mathbb{G}} \|\mathbb{1} - \mathcal{R}\omega(g)\mathcal{L}\mathcal{R}\omega(g)^{\dagger}\mathcal{L}'\|_{\diamond} + \|\mathcal{R}\omega(g)\mathcal{L}\mathcal{R}\omega(g)^{\dagger}\mathcal{L}' - \mathcal{R}\rho(g)\mathcal{L}\mathcal{R}'\omega'(g)^{\dagger}\mathcal{L}'\|_{\diamond}. \quad (291)$$

We upper bound these two terms separately. For the first term, consider

$$\frac{1}{|\mathbb{G}|} \sum_{g \in \mathbb{G}} \|\mathbb{1} - \mathcal{R}\omega(g)\mathcal{L}\mathcal{R}\omega(g)^{\dagger}\mathcal{L}'\|_{\diamond} \quad (292)$$

$$\leq \frac{1}{|\mathbb{G}|} \sum_{g \in \mathbb{G}} \|\mathbb{1} - \phi(g)\phi(g^{-1})\|_{\diamond} + \|\mathbb{1} - \phi(g)\mathcal{R}\omega(g^{-1})\mathcal{L}'\|_{\diamond} + \|\mathbb{1} - \mathcal{R}\omega(g)\mathcal{L}\phi(g^{-1})\|_{\diamond} + \|[\phi(g) - \mathcal{R}\omega(g)\mathcal{L}][\phi(g^{-1}) - \mathcal{R}\omega(g^{-1})\mathcal{L}']\|_{\diamond} \quad (293)$$

$$\leq \delta + \epsilon^2 + \frac{1}{|\mathbb{G}|} \sum_{g \in \mathbb{G}} \|\mathbb{1} - \phi(g)\phi(g^{-1})\|_{\diamond} + \|\phi(g)[\phi(g^{-1}) - \mathcal{R}\omega(g^{-1})\mathcal{L}']\|_{\diamond} \quad (294)$$

$$+ \|\mathbb{1} - \phi(g)\phi(g^{-1})\|_{\diamond} + \|[\phi(g) - \mathcal{R}\omega(g)\mathcal{L}]\phi(g^{-1})\|_{\diamond} \quad (295)$$

$$\leq 3\delta + 2\epsilon + \epsilon^2, \quad (296)$$

where we exploit the submultiplicativity of the diamond norm and the fact that $\|\phi(g)\|_{\diamond} = 1$ for all $g \in \mathbb{G}$. Similarly, for the second term we get

$$\frac{1}{|\mathbb{G}|} \sum_{g \in \mathbb{G}} \|\mathcal{R}\omega(g)\mathcal{L}\mathcal{R}\omega(g)^\dagger\mathcal{L} - \mathcal{R}\omega(g)\mathcal{L}\mathcal{R}'\omega'(g)^\dagger\mathcal{L}'\|_\diamond = \frac{1}{|\mathbb{G}|} \sum_{g \in \mathbb{G}} \|\mathcal{R}\omega(g)\mathcal{L}[\mathcal{R}\omega(g)^\dagger\mathcal{L} - \mathcal{R}'\omega'(g)^\dagger\mathcal{L}']\|_\diamond \quad (297)$$

$$\leq \frac{1}{|\mathbb{G}|} \sum_{g \in \mathbb{G}} \|\mathcal{R}\omega(g)\mathcal{L}\|_\diamond \|\mathcal{R}\omega(g)^\dagger\mathcal{L} - \mathcal{R}'\omega'(g)^\dagger\mathcal{L}'\|_\diamond \quad (298)$$

$$\leq K(\epsilon + \epsilon'). \quad (299)$$

Combining all of this we get

$$\|\mathbb{1} - \mathcal{R}T\mathcal{L}'\|_\diamond \leq (K + \epsilon)\epsilon' + 3\delta + (2 + K)\epsilon < 1, \quad (300)$$

by the assumptions of the theorem. Now assume that T has an image of dimension strictly less than d^2 . This means there exists a Hermitian $X \in \mathcal{M}_d$ such that $\mathcal{R}T\mathcal{L}'(X) = 0$. But this implies that

$$\|\mathbb{1} - \mathcal{R}T\mathcal{L}'\|_\diamond \geq \frac{\|X - \mathcal{R}T\mathcal{L}'(X)\|_1}{\|X\|_1} = 1, \quad (301)$$

which is a contradiction. Hence, the rank of T is at least d^2 . Since T by construction commutes with the representations ω, ω' we can decide that there exists a representation ω'' of degree at least d^2 which is a subrepresentation of both ω and ω' and moreover that both $\mathcal{R}\omega''\mathcal{L}(g)$ and $\mathcal{R}'\omega''\mathcal{L}'(g)$ are of rank at least d^2 for all $g \in \mathbb{G}$. ■

Next, we state a complementary theorem, saying that closeness to a representation is a concept stable under perturbations of the implementation. This is just a trivial consequence of the triangle inequality.

Theorem 19: (Stability of the closeness to a representation). *Let ϕ, ϕ' be implementations of a group \mathbb{G} on the superoperators \mathcal{S}_d such that*

$$\frac{1}{|\mathbb{G}|} \sum_{g \in \mathbb{G}} \|\phi(g) - \phi'(g)\|_\diamond \leq \delta \quad (302)$$

and let ω be a representation of \mathbb{G} on V_n with associated maps $\mathcal{L} : \mathcal{S}_d \rightarrow V_n$ and $\mathcal{R} : V_n \rightarrow \mathcal{S}_d$ such that

$$\frac{1}{|\mathbb{G}|} \sum_{g \in \mathbb{G}} \|\phi(g) - \mathcal{R}\omega(g)\mathcal{L}\|_\diamond \leq \epsilon \quad (303)$$

then

$$\frac{1}{|\mathbb{G}|} \sum_{g \in \mathbb{G}} \|\mathcal{R}\omega(g)\mathcal{L} - \phi'(g)\|_\diamond \leq \delta + \epsilon. \quad (304)$$

B. Randomized benchmarking under fidelity constraints

In this subsection, we argue that the condition Eq. (72) is in some sense necessary for the correct behavior of RB, in the sense that it cannot be replaced with a natural weaker condition. Given the worst-case nature of the diamond norm Eq. (72) is rather restrictive, and one might wonder if it is possible to replace this diamond-norm constraint with a more congenial constraint based on the average fidelity. That is, one can imagine replacing Eq. (72) with a constraint of the form

$$\frac{1}{|\mathbb{G}|} \sum_{g \in \mathbb{G}} F_{\text{avg}}[\phi(g), \omega(g)] \geq 1 - \delta' \quad (305)$$

for some $\delta' > 0$. Indeed, this is the assumption made in Ref. [25] to prove a version of Theorem 8 for the Clifford group. Here, it has been noted that in order to guarantee correct behavior the constant δ' must be chosen inversely proportional to the Hilbert-space dimension ($\delta' \sim 1/d$). It has been speculated that this dimensional scaling could perhaps be an artifact of the proof techniques used.

We argue that this scaling is in fact real, by providing an explicit family (inspired by example 8.1 in Ref. [96]) of examples of implementations ϕ_L (where L is an integer independent of d) of a group \mathbb{G} with

$$\frac{1}{|\mathbb{G}|} \sum_{g \in \mathbb{G}} F_{\text{avg}}[\phi(g), \omega(g)] \geq 1 - \frac{2L}{d} \quad (306)$$

relative to a reference implementation ω but with associated RB output data that is not even qualitatively of the form Eq. (63). In fact, by choosing L large (but constant in d) we can obtain almost arbitrary nonexponential behavior in the RB output data associated with ϕ_L .

Example 1: Real scaling. Choose \mathbb{G} to be the q -qubit Clifford group with standard reference implementation $\omega(g) = U_g \cdot U_g^\dagger$. Now let Λ_L^μ be a superoperator indexed by an integer L and a real number $0 \leq \mu \leq 1$, defined by its action on the basis matrices $|i\rangle\langle j|$ as

$$\Lambda_L^\mu(|i\rangle\langle j|) = \sum_{k=1}^d \delta_{i,j} [S_L^\mu]_{i,k} |k\rangle\langle k| \quad (307)$$

with S^μ a $d \times d$ stochastic matrix of the form

$$[S_L^\mu] = \begin{cases} \mu & \text{if } i = j \leq L - 1 \\ 1 & \text{if } i = j \geq L \\ 1 - \mu & \text{if } i = j - 1 \leq L \\ 0 & \text{otherwise.} \end{cases} \quad (308)$$

For convenience we write Λ for Λ_L^μ in the following. It is easy to see that Λ is a quantum channel and moreover that if $i, j \leq L$ then $\Lambda(|i\rangle\langle j|) \in \text{Span}\{|i'\rangle\langle j'| \mid i', j' \leq L\}$.

Consider now the following implementation map defined by its action on $X \in \mathcal{M}_d$:

$$\phi(g)(X) = \Lambda(P_L X P_L) + U_g(I - P_L)X(I - P_L)U_g^\dagger, \quad (309)$$

where P_L is the projection onto the space $\text{Span}\{|i\rangle \mid i \leq L\}$. This map can be seen as checking whether a state is in the support of P_L (though a measurement) and then applying Λ or U_g depending on the outcome. We can calculate the average fidelity $F_{\text{avg}}[\phi(g), \omega(g)]$ directly as

$$F_{\text{avg}}[\phi(g), \omega(g)] = \int d\psi \text{Tr}[\phi(g)(|\psi\rangle\langle\psi|)\omega(g)^\dagger(|\psi\rangle\langle\psi|)] \quad (310)$$

$$= \int d\psi \text{Tr}[U_g|\psi\rangle\langle\psi|U_g^\dagger\Lambda(P_L|\psi\rangle\langle\psi|P_L)] + \int d\psi \text{Tr}[|\psi\rangle\langle\psi|(I - P_L)|\psi\rangle\langle\psi|(I - P_L)] \quad (311)$$

$$= \int d\psi \text{Tr}[U_g|\psi\rangle\langle\psi|U_g^\dagger\Lambda(P_L|\psi\rangle\langle\psi|P_L)] + \int d\psi [1 - 2\langle\psi|P_L|\psi\rangle + (\langle\psi|P_L|\psi\rangle)^2] \quad (312)$$

$$\leq 1 - 2 \int d\psi \langle\psi|P_L|\psi\rangle \quad (313)$$

$$\leq 1 - \frac{2L}{d}, \quad (314)$$

where we make use of the fact that $\Lambda(P_L|\psi\rangle\langle\psi|P_L) \geq 0$, since Λ is CP. Note that for constant L we can make the fidelity arbitrarily high by choosing $d = 2^q$ large enough. Now consider RB with input state $\rho = |1\rangle\langle 1|$ and measurement POVM $\{|1\rangle\langle 1| + |L\rangle\langle L|, \mathbb{1} - |1\rangle\langle 1| - |L\rangle\langle L|\}$ and implementation map ϕ_L as defined above. The RB probability for the POVM element $|1\rangle\langle 1| + |L\rangle\langle L|$ is going to be (setting $g_{\text{end}} = e$ and assuming no SPAM errors)

$$p(|1\rangle\langle 1| + |L\rangle\langle L|, m) = \text{Tr}[(|1\rangle\langle 1| + |L\rangle\langle L|)\phi_L^{*m}(|1\rangle\langle 1|)]. \quad (315)$$

Note that since $P_L|1\rangle\langle 1| = |1\rangle\langle 1|P_L$ we have that $\phi_L(g)(|1\rangle\langle 1|) = (\Lambda_L^\mu)^m(|1\rangle\langle 1|)$ for all g . From this it follows that

$$p(|1\rangle\langle 1| + |L\rangle\langle L|, m) = \text{Tr}[(|1\rangle\langle 1| + |L\rangle\langle L|)(\Lambda_L^\mu)^m(|1\rangle\langle 1|)] = [S_L^{\mu^m}]_{1,L} + [S_L^{\mu^m}]_{1,1}. \quad (316)$$

This data shows curious behavior. For small sequence lengths we have $p(|1\rangle\langle 1| + |L\rangle\langle L|, m) \approx \mu^m$, but with increasing sequence length we observe wildly nonexponential behavior.

XI. CONCLUSIONS

In this work, we have introduced a comprehensive theory of RB. As such, it goes beyond a mere classification of known protocols (a task that we also hope to achieve). But at the same time, it provides a deeper understanding, a more precise formulation and interpretation of what the data acquired in RB means, actionable advice to experimentalists and theoretical practitioners and a conceptual platform from which new schemes can be derived. Specifically, we show how RB gives rise to exponential decays under broad classes of Markovian noise models, show—importantly in practical contexts—in what sense RB is robust to deviations from uniform sampling and provides further evidence to the interpretation in terms of average gate fidelities. Maybe most important for our work to serve as a basis for substantial further development of methods and protocols are new conceptual insights into how inversion gates are—in contrast to common belief—not required for RB and into how large classes of groups in RB can become available by means of new filtering techniques. This contributes to overcoming the problem of isolating exponential decays in a fully scalable manner. First steps into exploiting the insights established here when devising new schemes have already been made [57–59]. We hope that this work provides a starting point

of a further rich class of new protocols of quantum certification and benchmarking, providing stringent and rigorous quality criteria, while respecting experimental needs and desiderata.

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