Robust Characterization of Leakage Errors

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Leakage errors arise when the quantum state leaks out of some subspace of interest, for example, the two-level subspace of a multi-level system defining a computational ‘qubit’ or the logical code space defined by some quantum error-correcting code or decoherence-free subspace. Leakage errors pose a distinct challenge to quantum control relative to the more well-studied decoherence errors and can be a limiting factor to achieving fault-tolerant quantum computation. Here we present scalable and robust randomized benchmarking protocols for quickly estimating the rates of both coherent and incoherent leakage due to an arbitrary Markovian noise process, allowing for practical minimization of the leakage rate by varying over control methods. We illustrate the reliability of the protocol through numerical simulations.

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In order to build a practical and universal quantum computer, the rate of decoherence and other errors must be below certain fault-tolerant thresholds. One way of determining these error rates is to completely characterize the noise on quantum gates using quantum process tomography (QPT) [1, 2]. However, QPT scales exponentially in the number of qubits and is sensitive to state preparation and measurement (SPAM) errors, which can be on the same order as (or even orders of magnitude greater than) the error on the gate operations of interest [3].

An alternative to QPT is a characterization toolkit called randomized benchmarking (RB) [4–13]. These RB protocols scale favorably with the number of qubits at the cost of obtaining only partial information about the decoherence and control errors. Many of these protocols offer the additional advantage of being insensitive to SPAM errors by applying random sequences of quantum operations drawn from a group and extracting average error parameters from the observed fidelity decay curves. These protocols have consequently become an important tool in the validation and verification of quantum operations and have provided an efficient method to optimize over experimental implementations [14, 16].

An important error mechanism in many experimental implementations is leakage outside of the Hilbert space under consideration. Such leakage errors can be a substantial obstacle to fault-tolerant computation [19, 20]. For example, the surface code may not be used directly if there is any probability of losing a qubit, while for the topological cluster states, leakage rates of less than 1% are required to avoid impractical overheads [25].

However, standard RB only provides limited information about leakage rates [17]. There are platform-dependent methods for characterizing leakage in many of the leading experimental approaches to quantum computation, such as ion trap qubits [18], superconducting qubits [19, 20] and quantum dots [21]. However, these approaches do not have all the advantages of RB, in particular, scalability with the number of qubits, robustness to SPAM and no assumptions about the underlying error process beyond the assumption of Markovianity.

Furthermore, there are two distinct types of leakage, which we refer to as incoherent and coherent. In many physical implementations, incoherent leakage can be broadly categorized as the probabilistic but permanent loss of the system (through some process such as photon absorption, etc.); while coherent leakage can be considered as a coherent transition to an extra dimension (e.g., an electron excitation to an energy level outside the Hilbert space being considered) which later transitions back to the Hilbert space under consideration. These transitions back to the Hilbert space make coherent leakage fundamentally non-Markovian.

We present a protocol that provides an estimate of the average leakage rate for both coherent and incoherent leakage over a given set of quantum gates. We consider computational and leakage spaces of arbitrary dimensions, so that our protocol can be applied to both physical and logical qudit systems. We demonstrate that our protocol produces reliable estimates of leakage rates through numerical simulations of our protocol for specific error models.

Defining survival and leakage rates—Within the broad framework of time-dependent Markovian noise, any experimental implementation of a unitary \(g\) at a time step \(t\) can be written as \(g \circ \mathcal{E}_{g,t}\) for some completely positive (CP) map \(\mathcal{E}_{g,t} : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{H})\) where \(\circ\) denotes composition (i.e., \(A \circ B\) means apply \(B\) then apply \(A\)) and \(\mathcal{B}(\mathcal{H})\) is the set of density operators acting on \(\mathcal{H}\) and \(\mathcal{H}\) is the relevant physical Hilbert space (that is, \(\mathcal{E}_{g,t}\) sends quantum states to quantum states). Note that if, as is often the case, \(g\) acts on a subspace \(\mathcal{H}_1\) where \(\mathcal{H} = \mathcal{H}_1 \oplus \mathcal{H}_2\), then we implicitly extend \(g\) to \(g \oplus I_{\mathcal{H}_2}\) where \(\oplus\) denotes
the direct sum and \( \mathcal{I}_H \) denotes the identity on \( H \).

Many methods for characterizing noise channels \( \mathcal{E}_{H,t} \) assume \( \mathcal{E}_{g,t} \) is trace-preserving. However, an important limitation of many experimental implementations is that errors are not trace-preserving, that is, generally the probability \( \text{Tr}[\mathcal{P}_{H,t}\rho] \) of the system being in a Hilbert space \( H_1 \subseteq H \) can decrease upon applying an operation, where \( \mathcal{P}_{H,t} = \mathcal{I}_{H_1} \oplus 0 \) is the projector onto \( H_1 \) [15].

We define the survival rate of a state \( \rho \in H_1 \) under a CP map \( \mathcal{E} \) to be

\[
s(\rho|\mathcal{E},H_1) = \frac{\text{Tr}[\mathcal{P}_{H_1}\mathcal{E}(\rho)]}{\text{Tr}\rho}. \tag{1}
\]

We will consider survival rates averaged over states in both \( \mathcal{H} \) and in a subspace \( H_1 \) of \( \mathcal{H} \). In order to define these averages, note that any \( \rho \in B(H_1) \) can be written as \( \rho \tau \) for some \( \rho \in [0,1] \) and \( \tau \in B(H) \) such that \( \text{Tr}\tau = 1 \). Substituting this into Eq. (1) gives

\[
s(\rho|\mathcal{E},H_1) = \text{Tr}[\mathcal{P}_{H_1}\mathcal{E}(\tau)], \tag{2}
\]

which is a linear function of \( \tau \). Consequently, the average survival rate in \( H_1 \) over any measure \( d\tau \) over mixed states that is invariant under unitaries acting on \( H_1 \) is

\[
s(\mathcal{E},H_1) = \int d\tau \text{Tr}[\mathcal{P}_{H_1}\mathcal{E}(\tau)] = \text{Tr}[\mathcal{P}_{H_1}\mathcal{E}(d\tau^{-1}\mathcal{P}_{H_1})], \tag{3}
\]

where we have used the fact that \( \int dU U\tau U^\dagger = d\tau^{-1}\mathcal{P}_{H_1} \) for any density operator \( \tau \), where \( d\tau \) is the Haar measure over unitaries acting on \( H_1 \) and \( d_1 \) is the dimension of \( H_1 \).

Since CP maps are linear and all quantum states can be written as \( \rho \rho \) for some \( \rho \in [0,1] \) and \( \rho \in B(H) \) such that \( \text{Tr}\rho = 1 \), the survival rate for \( H_1 = \mathcal{H} \) is strictly non-increasing under composition, that is, \( s(\mathcal{E}_1 \circ \mathcal{E},H_1) \leq s(\mathcal{E},H_1) \) for all CP maps \( \mathcal{E}_1 \). In contrast, if \( H_1 \subseteq \mathcal{H} \), the survival rate can increase if \( \mathcal{E} \) lowers coherences between \( H_1 \) and \( H_2 \). We therefore define the coherent and incoherent survival rates to be

\[
s_{\text{coh}}(\mathcal{E}) = \text{Tr}[\mathcal{I}_{H_1}\mathcal{E}(d_{H_1}^{-1}\mathcal{I}_{H_1})] + \text{Tr}[\mathcal{I}_{H_2}\mathcal{E}(d_{H_2}^{-1}\mathcal{I}_{H_2})], \nonumber
\]

\[
s_{\text{inc}}(\mathcal{E}) = \text{Tr}[\mathcal{E}(d_{H}^{-1}\mathcal{I}_{H})] \tag{4}
\]

respectively. We will generally omit the argument as it will be clear from the context. Incoherent and coherent leakage rates can then be defined as \( l_{\text{inc}}(\mathcal{E}) = 1 - s_{\text{inc}}(\mathcal{E}) \) and \( l_{\text{coh}}(\mathcal{E}) = s_{\text{inc}}(\mathcal{E}) - s_{\text{coh}}(\mathcal{E}) \) respectively.

**Experimental protocol**—We now present a protocol for characterizing the average survival rates

\[
|\mathcal{G}|^{-1} \sum_{g \in \mathcal{G}} s_{\text{inc}}(\mathcal{E}_g) = s_{\text{inc}}(\mathcal{E}) \tag{5}
\]

over a set of operations \( \mathcal{G} = \{g = v \oplus (\pm w) : v \in V, w \in W\} \), where \( V \) and \( W \) are unitary 1-designs [24] on \( H_1 \) and \( H_2 \) respectively, \( \mathcal{E} = |\mathcal{G}|^{-1} \sum_{g \in \mathcal{G}} \mathcal{E}_g \) and the equalities follow from the linearity of the survival rates. Note that for incoherent leakage, \( \mathcal{G} \) is simply a unitary 1-design on \( \mathcal{H} \) such as, for example, the Paulis. (Note that standard RB requires a unitary 2-design, which is a strictly stronger requirement.) To account for weak gate-dependencies, we define

\[
\Delta = |\mathcal{G}|^{-1} \sum_{g \in \mathcal{G}} g \circ \mathcal{E}_g - \mathcal{G} \circ \mathcal{E}. \tag{6}
\]

where \( \mathcal{G} = |\mathcal{G}|^{-1} \sum_{g \in \mathcal{G}} g \), and observe that the average variation of errors over the gate set is bounded by

\[
\epsilon = ||\Delta||_\circ. \tag{7}
\]

Also note that for brevity, we assume that the noise is time-independent, though results for time-dependent noise can be obtained by applying the approaches of Ref. [13].

1. Choose a random sequence \( k = (k_1,\ldots,k_m) \in \mathbb{N}^m \) of \( m \) integers uniformly at random, where \( \mathbb{N}_a = \{1,\ldots,a\} \) and \( a = |\mathcal{G}| \).

2. Estimate the probability \( p_k \) of detecting the system in the subspace \( H_1 \) (i.e., measuring \( \mathcal{I}_{H_1} \)) after preparing the state \( |0\rangle \) and applying the sequence \( g_{k_m}g_{k_{m-1}}\ldots g_{k_1} \) of gates.

(Note that in standard RB, an inverse gate is applied immediately prior to the measurement.)

Averaging the results over a number of random sequences with fixed \( m \) will give an estimate of

\[
\mathbb{E}_k p_k = A s_{\text{inc}}^{-1}(\mathcal{E}) + O(m\epsilon) \tag{8}
\]

for \( H_1 = \mathcal{H} \) or

\[
\mathbb{E}_k p_k = B \lambda_m^{-1} + C \lambda_m^{-1} + O(m\epsilon) \tag{9}
\]

for \( H_1 \subseteq \mathcal{H} \), where the constants \( A, B \) and \( C \) are determined by state-preparation and measurement errors (SPAM) and the \( \lambda_k \) are fit parameters that give the coherent survival probability through \( s_{\text{coh}}(\mathcal{E}) = \lambda_k + \lambda_{k+1} \). If the noise is trace-preserving on \( \mathcal{H} \) (that is, if \( s_{\text{inc}}(\mathcal{E}) = 1 \), then Eq. (9) simplifies to

\[
\mathbb{E}_k p_k = B(s_{\text{coh}}(\mathcal{E}) - 1)m^{-1} + C + O(m\epsilon). \tag{10}
\]

The gate dependent terms in these expressions are negligible provided \( m\epsilon \ll 1 \). Fitting the relevant decay curve then gives an estimate of the survival rates.

**Derivation of the fit models.**—For the remainder of this paper we will work exclusively in the Liouville (or superoperator) representation of quantum channels, which we now briefly review. The Liouville representation...
defined relative to a trace-orthonormal operator basis $A = \{A_1, \ldots, A_d\}$ for the operator space $\mathcal{H}_d$. Density operators $\rho$ and measurement outcomes $M$ are represented by column and row vectors $|\rho\rangle$ and $|M\rangle$ whose $i$th elements are $\text{Tr}(A_i^\dagger \rho)$ and $\text{Tr}(M^\dagger A_i)$, respectively. The Born rule can then be expressed as $\text{Tr} M \rho = \langle M | \rho \rangle$. Quantum channels (that is, completely positive maps) $\mathcal{E} : \mathcal{H}_d \rightarrow \mathcal{H}_d$ are represented by matrices $\mathcal{E}$ such that

$$\mathcal{E}_{ij} = \text{Tr}[A_i^\dagger \mathcal{E}(A_j)],$$

where $\mathcal{E}(|\rho\rangle) = \mathcal{E}(|\rho\rangle)$ for all $\rho$.

The primary advantage of using the Liouville representation is that channels compose via matrix multiplication, so that the probability for a sequence $k$ is

$$p_k = \langle E | g_{k_m} \mathcal{E}_{g_{k_m}} \ldots g_{k_1} \mathcal{E}_{g_{k_1}} | \rho \rangle,$$

where $E$ and $\rho$ are the experimental POVM elements and density matrices respectively. The average probability over all sequences of length $m$ is

$$E_k p_k = |\mathcal{G}|^{-m} \sum_{g \in \mathcal{G}^m} \langle E | g_{k_m} \mathcal{E}_{g_{k_m}} \ldots g_{k_1} \mathcal{E}_{g_{k_1}} | \rho \rangle = \langle E | \mathcal{G} \mathcal{E} + \Delta \rangle^m |\rho\rangle,$$

so the average probability simplifies to

$$E_k p_k = \langle E | \mathcal{G} \mathcal{E} + \Delta \rangle^m |\rho\rangle + \delta,$$

where $\rho' = \mathcal{E}(|\rho\rangle)$ and $\delta$ is the sum of all terms with nonzero powers of $\Delta$ obtained by expanding Eq. (13). Given $\epsilon$ as defined above, $\delta = O(m \epsilon)$, which will be negligible in practice provided $m \epsilon \ll 1$.

In order to complete the derivations, we now appeal to special properties of the groups $\mathcal{G}$ chosen to characterize incoherent and coherent leakage rates respectively.

To characterize incoherent leakage, $\mathcal{G}$ is chosen to be a unitary 1-design, so that (see, e.g., Proposition 1 of Ref. [13]),

$$\mathcal{G} = |\mathcal{G}|^{-1} \sum_{g \in \mathcal{G}} g = |A_1\rangle\langle A_1|,$$

where $A_1 = d^{-1/2} \mathbb{1}_d$, which is obtained by noting that the only operators invariant under conjugation by a unitary 1-design (which correspond to a 1-dimensional irreducible representation) are scalar matrices. Therefore

$$\mathcal{G} \mathcal{E} \mathcal{G} = |A_1\rangle\langle A_1| \mathcal{E} |A_1\rangle\langle A_1| = \text{Tr}[A_1 \mathcal{E}(A_1)] |A_1\rangle\langle A_1| = s_{\text{inc.}}(|\mathcal{E}| |A_1\rangle |A_1|),$$

and so the expectation over random sequences is

$$E_k p_k = A s_{\text{inc.}}^{-1} |\mathcal{E}| + O(m \epsilon),$$

as claimed,

$$A = (\mathcal{E}(A_1) |A_1\rangle \langle A_1|)^{-1} = \frac{1}{d} \text{Tr} \mathcal{E}(\rho),$$

To characterize coherent leakage, $\mathcal{G}$ is chosen so that any element $g \in \mathcal{G}$ can be written as $g = v \otimes \mu w$ for $\mu \in \{+,-\}$, where $v$ and $w$ are elements of unitary 1-designs $\mathcal{V}$ and $\mathcal{W}$ on $\mathcal{H}_1$ and $\mathcal{H}_2$ respectively. Then, using the matrix basis $|i\rangle$ for the operator space, so that $U = U \otimes U^*$ where * denotes complex conjugation, we have (again by Proposition 1 of Ref. [13])

$$\mathcal{G} = |\mathcal{G}|^{-1} \sum_{\mu,v,w} (v \otimes \mu w) \otimes (v \otimes \mu w)^* = (|\mathcal{V}|^{-1} \sum_v v \otimes v^*) \oplus 0 \oplus 0 \oplus (|\mathcal{W}|^{-1} \sum_w w \otimes w^*)$$

$$= |d_1|^{-1/2} \mathcal{P}_{\mathcal{H}_1} |d_2|^{-1/2} \mathcal{P}_{\mathcal{H}_1} + |d_2|^{-1/2} \mathcal{P}_{\mathcal{H}_1} |d_2|^{-1/2} \mathcal{P}_{\mathcal{H}_1}.$$ (20)

Setting $A_1 = d_1^{-1/2} \mathcal{P}_{\mathcal{H}_1}$ and $A_2 = d_2^{-1/2} \mathcal{P}_{\mathcal{H}_2}$, we then have

$$\mathcal{G} \mathcal{E} \mathcal{G} = s \oplus 0,$$ (21)

where $s$ is a $2 \times 2$ matrix. We can easily take powers of $s$ by putting it in lower-triangular form, so that

$$E_k p_k = B \lambda_{+}^{-m} + C \lambda_{-}^{-m} + O(m \epsilon),$$ (22)

where

$$\lambda_{\pm} = \frac{s_{1,1} + s_{2,2}}{2} \pm \frac{1}{2} \sqrt{(s_{1,1} - s_{2,2})^2 + 4s_{1,2}s_{2,1}}.$$ (23)

are the eigenvalues of $s$ and $B$ and $C$ are constants (which absorb both the SPAM and the unitary that makes $s$ lower-triangular).

The sum of the eigenvalues is equal to $s_{1,1} + s_{2,2} = s_{\text{coh.}}(|\mathcal{E}|)$ since

$$s_{1,1} = \text{Tr} \mathcal{P}_{\mathcal{H}_1} \mathcal{E} \mathcal{P}_{\mathcal{H}_1} \mathcal{E} \mathcal{P}_{\mathcal{H}_1} = \text{Tr} \mathcal{P}_{\mathcal{H}_2} \mathcal{E} \mathcal{P}_{\mathcal{H}_2} \mathcal{E} \mathcal{P}_{\mathcal{H}_2},$$ (24)

If the noise is trace-preserving, then one of the eigenvalues must be one (corresponding to $\mathbb{1}_{d+\epsilon}$), and the other must then be $s_{\text{coh.}}(|\mathcal{E}|) - 1$.

**Numerical simulations.**—Results of numerical simulations of our protocol for two specific models of incoherent and coherent leakage are illustrated in figures 1 and 2 respectively, demonstrating robust performance with a model of (weakly) gate-dependent errors.
For the numerical simulations of our protocol for incoherent leakage, the set of operations \( \mathcal{G} \) is the set of single-qubit Paulis and we modeled the gate-dependent error \( \mathcal{E}_i \) for each \( g_i \) as

\[
\mathcal{E}_i(\rho) = \frac{p_i}{4}(\mathbb{1} + r_i \cdot \vec{\sigma})(\mathbb{1} + r_i \cdot \vec{\sigma}) + (1 - p_i) \rho, \tag{25}
\]

where \( \vec{\sigma} = (X, Y, Z) \) is the vector of Paulis and \( p_i \in [0, 0.05] \) and \( r_i \in S^2 \) (the unit sphere) were chosen independently and uniformly from the appropriate measures. The channels \( \mathcal{E}_i \) correspond to channels that weakly filter out (that is, absorb) the component of a state orthogonal to some randomly-chosen state with Bloch vector \( r_i \). When \( r_i \) is fixed, this corresponds to loss from a particular energy level. However, we chose \( r_i \) randomly to accentuate the statistical fluctuations as much as possible.

For numerical simulations of our protocol for coherent leakage, we adopted a noise model that is motivated by experimental techniques that use an auxiliary level (e.g., “shelving” in ion trap experiments [27]) to protect certain states while performing another operation. The ideal shelving gate is a Pauli \( X \) rotation between the second and third level, that is, \( V_{\text{ideal}} = 1 \oplus X \). The group \( \mathcal{G} \) of operations is \( \{ P \oplus \pm 1 : P = I, X, Y, Z \} \). Our model of coherent leakage at each time step is

\[
\mathcal{E}_X = V_{\gamma_2} \circ \delta U_2 \circ V_{\gamma_1} \circ \delta U_1, \tag{26}
\]

where

\[
V_{\gamma} = 1 \oplus \begin{pmatrix} i \sin \gamma & \cos \gamma \\ \cos \gamma & i \sin \gamma \end{pmatrix} \quad \delta U = e^{i \phi UXU^+} \oplus 1. \tag{27}
\]

That is, our noise model consists of imperfect shelving \((V_{\gamma_1})\) and unshelving \((V_{\gamma_2})\) gates, together with some small coherent noise on the code space \((\delta U_1 \text{ and } \delta U_2)\). The channel \( \mathcal{E}_X \) is trace-preserving on the combined code and leakage space, but is trace-decreasing when restricted to the code space. We sampled \( U \) from the Haar measure on the code space with \( \phi = 0.01 \) fixed and \( \gamma \) from the normal distribution with zero mean and \( \sigma = 0.06 \), where each variable is sampled independently each time the relevant gate is applied.

Conclusion—In this paper, we have presented a protocol for characterizing average survival rates under incoherent leakage and coherent leakage to an orthogonal subspace. Experimentally implementing our protocol yields a decay curve which can be fitted to our analytical expressions to obtain the average probability of a leakage event occurring. If the experimental data deviates significantly from our decay curves, then the experimental noise is either strongly gate-dependent or non-Markovian. We have also demonstrated that the decay can be observed and fitted in practice through numerical simulations of leakage for specific error models.

Our protocol is scalable and robust against state-preparation and measurement errors. Our current protocol can also be applied in conjunction with standard
RB to determine both the average leakage rate and the average gate infidelity over a unitary 2-design such as the Clifford group.

As with standard RB, obtaining rigorous confidence intervals on the parameters obtained from our protocol is still an open problem, though techniques bounding the number of sequences to be sampled [13] and using Bayesian methods to refine prior information [28] should also be applicable to our protocol.

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