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Implementing Generalized Measurements with Superconducting Qubits

Implementing generalized measurements with superconducting qubits

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We describe a method to perform any generalized purity-preserving measurement of a qubit with techniques tailored to superconducting systems. First, we consider two methods for realizing a two-outcome partial projection: using a thresholded continuous measurement in the circuit QED setup and using an indirect ancilla qubit measurement. Second, we decompose an arbitrary purity-preserving two-outcome measurement into single-qubit unitary rotations and a partial projection. Third, we systematically reduce any multiple-outcome measurement to a sequence of such two-outcome measurements and unitary operations. Finally, we consider how to define suitable fidelity measures for multiple-outcome generalized measurements.

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I. INTRODUCTION

The ability to isolate and control coherent quantum systems has dramatically improved in recent decades. As a consequence, techniques that were previously restricted to thought experiments have recently been promoted to practical laboratory methods. Generalized quantum measurements fall into this category.

The concept of measurement in quantum mechanics has been largely dominated historically by projective measurements, in which an experimenter learns precise information about a quantum system under study [1]. Such projective measurements are commonly called "von Neumann measurements" since von Neumann first formalized the quasi-Boolean lattice of projection operators used to describe the curious logic obeyed by these measurements [2,3]. However, it is worth noting that von Neumann simultaneously introduced the possibility of learning imprecise information about a quantum system by measuring a correlated ancilla that acts as an indirect detector for the system [2]. When such an indirect detector becomes correlated with the system, an experimenter still obtains some information about the system, but the precision of that information depends on the degree of correlation between the ancilla and the system. These imprecise measurements are an example of generalized measurements.

The mathematical description of generalized quantum measurements has been considerably refined since these early observations [4–8], giving rise to the modern formalism of *quantum operations*. This formalism has proven itself invaluable for reasoning about tasks in quantum information and quantum computing [9–13]. However, it is only in the past decade that experimental systems have become sufficiently controllable to make generalized measurements a practical laboratory tool.

Thus far, optical systems have been the primary arena for implementing generalized quantum measurements, with experiments using them to examine nonorthogonal state discrimination [14], nondestructive photon measurements [15–17], feedback control [18,19], entanglement distillation [20], weak-value superoscillation effects [21–23], Leggett-Garg inequality violations [24–26], weak-value amplification [27–33], locally averaged photon trajectories [34], direct wave-function determination [35], error-disturbance complementarity [36,37], conditional measurement reversal [38,39], Hardy's paradox [40,41], and much more. In addition to these specific examples of generalized measurements, there have been several discussions about how to implement any desired measurement on optical qubits [42–44]. Nevertheless, current optical qubit architectures are not easily scalable. Though measuring one or two photonic qubits in a general way is possible using linear optics and parametric downconversion, it is not so easy to reliably entangle and manipulate larger numbers of independent photonic qubits. This scaling difficulty limits the potential applications of generalized measurements.

In contrast, solid-state systems have demonstrated better scalability in recent years and have also implemented a variety of generalized quantum measurements. Experiments with superconducting qubits have used generalized measurements to demonstrate partial collapse [45] and measurement reversal [46], violate Leggett-Garg inequalities [47,48], stabilize Rabi oscillations with quantum feedback control [49], demonstrate quantum backaction in an individual continuous measurement [50], observe single quantum trajectories [51,52], entangle qubits by measurement [53,54], and reduce decoherence via uncollapsing [55]. These systems show promise for realizing scalable architectures that can manipulate many entangled qubits simultaneously. As such, we expect that many more applications of generalized measurements will soon appear. It is thus of particular interest to specify exactly how to implement generalized measurements with these systems in a systematic way [44].

In this paper, we discuss how to use modern superconducting systems to perform any generalized purity-preserving qubit measurement, which is the most commonly discussed (and most useful) type of generalized measurement (see, e.g., [9]). For such a measurement, any pure initial state will collapse to another pure state for each outcome of the measurement process, but the collection of final pure states need not form an orthogonal set. Each outcome of a purity-preserving measurement is characterized by a single Kraus operator (measurement operator), with the traditional projection operators being a special case.

Our strategy will be to reduce an arbitrary n-outcome generalized measurement to a more manageable sequence of two-outcome measurements. Each such two-outcome measurement can be further decomposed into single-qubit unitary rotations

and a standardized partial projection. We discuss two different ways to realize such a partial projection, specifying explicitly the experimentally controllable parameters. For simplicity of discussion in what follows, we consider efficient detectors that naturally perform purity-preserving measurements, with the understanding that real laboratory implementations will also include additional imperfections (like purity-reducing decoherence) that would require multiple Kraus operators per measurement outcome to fully describe. As such, we also examine the issue of how to characterize the fidelity of an experimentally realized many-outcome generalized quantum measurement, as compared to an ideal purity-preserving measurement.

The paper is organized as follows. In Sec. II, we detail two methods of implementing two-outcome partial projections using superconducting qubits. In Sec. III we describe how to implement any generalized measurements by decomposing them into sequences of unitary operations and partial projections. In Sec. IV the ways to characterize the fidelity of a generalized measurement are discussed (with more details in the Appendix). We conclude in Sec. V.

II. TWO-OUTCOME PARTIAL PROJECTIONS

To understand how to implement an arbitrary generalized measurement, we first consider how to implement the simple case of a two-outcome partial projection. We will then be able to construct the general case as an appropriate sequence of these partial projections and additional unitary rotations.

Recall that in a projective two-outcome qubit measurement, the state collapses into an eigenstate of the measurement $|\psi\rangle \to |0\rangle,|1\rangle$. By convention, these eigenstates correspond to the Pauli Z operator $\sigma_z = |0\rangle\langle 0| - |1\rangle\langle 1|$. Formally, the collapse can be understood as the application of a particular projection operator, $|0\rangle\langle 0|$ or $|1\rangle\langle 1|$, followed by state renormalization. The measurement result of 0 or 1 determines which projection operator is applied and thus fully determines the qubit state after the measurement. In the special case when the initial state is either $|0\rangle$ or $|1\rangle$, the measurement result is deterministic, perfectly correlated with the qubit state, and measurement does not change the qubit state.

For a generalized two-outcome measurement, the measurement result can be "noisy." That is, the measurement result of 0 or 1 need not perfectly correlate with the premeasurement qubit state. Instead, the results will correspond to the qubit state only probabilistically. (Note that we assume the simplest case here where the measurement basis of $|0\rangle$ and $|1\rangle$ is unchanged.) If the qubit is in state $|0\rangle$, then there is a probability p that the result will correctly report 0. Similarly, if the qubit is in state $|1\rangle$, then there is a (generally different) probability q that the result will correctly report 1. Since the obtained information is imperfect, the state will only partially collapse toward the eigenstates of the measurement when a result is obtained.

The simplest form of such a partial collapse does not include additional unitary evolution and also does not include decoherence (see [56] for more details). As a result, such a measurement is purity-preserving, meaning that any pure initial state collapses to another pure final state for each measurement outcome. Each outcome (labeled 0 or 1) of such a measurement formally corresponds to partial-projection operators,

$$D_0 = \sqrt{p}\,|0\rangle\langle 0| + \sqrt{1-q}\,|1\rangle\langle 1|,$$
$$D_1 = \sqrt{1-p}\,|0\rangle\langle 0| + \sqrt{q}\,|1\rangle\langle 1|, \tag{1}$$

which depend on the two probability parameters (measurement fidelities) $p,q \in [0,1]$. When a result 0 (or 1) is obtained, the qubit state is updated to the pure state $D_0|\psi\rangle$ (or $D_1|\psi\rangle$) and then renormalized. The probabilities of obtaining results 0 and 1 are $||D_0|\psi\rangle||^2$ and $||D_1|\psi\rangle||^2$, respectively. It is natural to assume (without loss of generality) that $p+q \geqslant 1$, so the stated correspondence between D_0 and 0 (or D_1 and 1) is sensible.

When $p = q = 1$, the projective measurement is recovered as a special case. The case $p = 1, q \neq 1$ is often called a null-result measurement for the outcome 0 (the outcome 1 collapses the state to $|1\rangle$, while the outcome 0 produces only a partial collapse towards $|0\rangle$). The case $p + q = 1$ corresponds to no measurement, with p and q directly indicating the probabilities of the results 0 and 1 independently of the qubit state. Thus, $|p + q - 1|$ characterizes the strength of the measurement (i.e., how well the measurement can discriminate between the states $|0\rangle$ and $|1\rangle$); for example, a "weak" measurement (in the sense of Ref. [7]) satisfies $|p + q - 1| \ll 1$. The difference $p - q$ characterizes the asymmetry between the probabilities of results 0 and 1; in particular, the probability of the result 0 averaged over initial qubit states is $(1 + p - q)/2$, while the averaged probability of the result 1 is $(1 + q - p)/2$.

We now consider two methods available for superconducting qubits to implement such a partial projection for an arbitrary choice of p and q.

A. Thresholded continuous readout

The standard readout of a superconducting qubit in the circuit QED setup [47–50,50–54,57–62] involves a quadrature measurement of the leaked output from a pumped microwave resonator that is dispersively coupled to the qubit. In this case the qubit state evolves stochastically in the process of its continuous measurement [63,64] (see also [11,12,65]).

Let us assume that a quadrature at an angle α from the information-carrying quadrature is amplified by a quantum-limited phase-sensitive amplifier and then measured. The instantaneous output signal (which includes noise) is denoted as $I(t)$. The average of this noisy signal is correlated with the state of the qubit, so that the dimensionless readout $r(t)$ that averages to the σ_z range of $[-1,1]$ is

$$r(t) = 2\,\frac{I(t) - I_c}{\Delta I}, \tag{2}$$

where $I_c = (I_0 + I_1)/2$, $\Delta I = I_0 - I_1$, and the values I_0 and I_1 are the average signals obtained when the qubit is fixed in the states $|0\rangle$ and $|1\rangle$, respectively. The readout $r(t)$ corresponds to the z component of the qubit state on the Bloch sphere. Note that I_c will depend on the quadrature angle α in general. The response ΔI will also depend on α as $\Delta I = \Delta I_{\max}\cos\alpha$, where $\Delta I_{\max}$ is the maximum response at angle $\alpha = 0$.

In the quantum nondemolition (QND) regime [8] with no additional unitary evolution, the integrated readout

$$R = \int_0^T \frac{dt}{\tau}\, r(t) \tag{3}$$

completely determines the partial projection of the qubit [12,64]. Here $\tau = 2S/(\Delta I)^2$ is a characteristic "measurement time" that controls the rate of partial projection (the signal-to-noise ratio of 1 is reached after time τ), while S is the (approximately constant) one-sided spectral density of the noisy signal due to the amplifier noise, which is assumed here to be quantum limited. [The variance of $I(t)$ is related to the spectral density as $\mathrm{Var}(I) = \int_0^\infty S(\omega)\, d\omega/2\pi$.] Notably, the integration duration T in Eq. (3) is arbitrary, so one can wait for a desired integrated readout R to appear and then terminate the measurement (i.e., stop pumping the microwave resonator).

If the output of the microwave resonator is collected efficiently (i.e., without quantum information loss in connectors, transmission lines, and amplifying circuitry), then each integrated readout R corresponds to a purity-preserving measurement that is characterized by a partial-projection operator (see [64]),

$$M_R \propto \exp\left[\frac{R}{2\cos\alpha} e^{-i\alpha}\sigma_z\right] = e^{R/2} e^{-i(R/2)\tan\alpha}|0\rangle\langle 0| + e^{-R/2} e^{i(R/2)\tan\alpha}|1\rangle\langle 1|. \quad (4)$$

After state renormalization, the constant proportionality factor will cancel. Nonzero α increases the typical measurement timescale $\tau = \tau_{\min}/\cos^2\alpha$ and produces z rotations of the qubit state that depend on the integrated result R. For simplicity in what follows, we assume measurement of the optimal quadrature, $\alpha = 0$.

An experimenter can then follow a simple procedure to implement the two-outcome partial projection in Eq. (1).

(1) Set a positive value R_0 and a negative value R_1 [given later in Eq. (7)] as threshold values for the integrated readout R.

(2) Wait for one of the threshold values to appear and then terminate the measurement.

According to Eq. (4), this procedure will produce one of the partial projections,

$$D_{0,1} = \sqrt{C_{0,1}}[e^{R_{0,1}/2}|0\rangle\langle 0| + e^{-R_{0,1}/2}|1\rangle\langle 1|], \quad (5)$$

where the normalization constants $C_{0,1}$ can be obtained either by the first-passage techniques similar to Refs. [66,67] or simply by using the condition $D_0^\dagger D_0 + D_1^\dagger D_1 = \mathbb{1}$, which follows from the fact that at least one of the two thresholds will eventually be reached (in turn, this follows from the fact that at infinite time our continuous measurement would collapse the qubit state to either $|0\rangle$ or $|1\rangle$).

The thresholds $R_{0,1}$ will determine the probabilities p and q in Eq. (1). Squaring the operators in Eq. (5) and comparing them to Eq. (1) produces the relations

$$D_0^\dagger D_0 = C_0[e^{R_0}|0\rangle\langle 0| + e^{-R_0}|1\rangle\langle 1|] = p|0\rangle\langle 0| + (1-q)|1\rangle\langle 1|,$$

$$D_1^\dagger D_1 = C_1[e^{R_1}|0\rangle\langle 0| + e^{-R_1}|1\rangle\langle 1|] = (1-p)|0\rangle\langle 0| + q|1\rangle\langle 1|.$$

It follows by inspection that

$$C_0 = \sqrt{p(1-q)}, \quad C_1 = \sqrt{q(1-p)}, \quad (6)$$

$$R_0 = \frac{1}{2}\ln\left(\frac{p}{1-q}\right), \quad R_1 = -\frac{1}{2}\ln\left(\frac{q}{1-p}\right). \quad (7)$$

Thus, Eq. (7) gives us the threshold values $R_0 > 0$ and $R_1 < 0$ that need to be set to perform the partial projection in Eq. (1) with arbitrary p and q. Note that measuring a different quadrature angle α will require the same thresholds, but will produce additional z rotations that are absent in Eq. (1).

This way of realizing the partial projection in the circuit QED setup is a direct generalization of the "uncollapsing" measurements considered in Refs. [66] and [67]. This measurement technique can also be viewed as an experimental realization of the type of continuous measurement decomposition of a generalized measurement described in [68–70]. For two-outcome measurements on a qubit, only minimal feedback is necessary, that is, determining when the measurement process should terminate. For higher-dimensional systems similar continuous measurement decompositions exist, but, in general, more sophisticated feedback is needed in the measurement process.

From Eq. (7) it is easy to check that a projective measurement ($p = q = 1$) requires $R_0 = -R_1 = \infty$; such a complete measurement can only be realized approximately. The null-result measurement ($p = 1$, $q \neq 1$) requires $R_1 = -\infty$ and finite positive R_0, so that the result 1 gives complete information, while the result 0 is inconclusive. The case of no measurement ($p + q = 1$) gives $R_0 = R_1 = 0$, which means that the measurement is immediately terminated. A weak measurement ($|p + q - 1| \ll 1$, with p and q not too close to 0 or 1) corresponds to small values of the thresholds, $R_0 \ll 1$ and $|R_1| \ll 1$, so that the measurement procedure likely lasts for a short time. A symmetric measurement ($p = q$) requires symmetric thresholds, $R_1 = -R_0$.

There is a significant caveat to this partial projection implementation: The operator M_R in Eq. (4) strictly applies only for a purity-preserving (i.e., efficient) measurement. Experimentally, a quadrature readout typically has imperfect quantum efficiency ($\eta < 1$), which causes additional state decoherence during the readout [64]. For example, recent experiments verifying continuous state collapse showed a quantum efficiency of roughly $\eta \approx 0.5$, meaning that only about half of the observed ensemble dephasing rate could be attributed to information acquisition during the measurement [49–52]. For such an inefficient measurement, the duration T of the integrated readout will matter, since it will determine the extra accumulated decoherence. As such, the thresholding technique will generally produce a fluctuating distribution of measurements with different amounts of additional decoherence and so will only approximate the desired partial projection with imperfect fidelity.

B. Ancilla qubit measurement

As an alternative to thresholding a continuous dispersive readout, one can also realize the partial projection in Eq. (1) with arbitrary p and q as a quantum circuit using an

ancilla qubit measurement. This method does not require a continuous measurement with perfect quantum efficiency, but it does require high-fidelity two-qubit entangling operations and single-qubit gates; it also requires high-fidelity projective measurement of the ancilla qubit. This method can be realized with various types of qubits (not necessarily in circuit QED systems) and at present is easier to implement experimentally for superconducting qubits (e.g., Refs. [48,55]) than the method discussed in the previous subsection.

The procedure requires standard one-qubit and two-qubit gates with adjustable parameters. In particular, the one-qubit gates we will use are the X, Y, and Z rotations around the Bloch sphere [9]:

$$R_x(\phi) = e^{-i\phi\sigma_x/2} = \begin{pmatrix} \cos\frac{\phi}{2} & -i\sin\frac{\phi}{2} \\ i\sin\frac{\phi}{2} & \cos\frac{\phi}{2} \end{pmatrix},$$

$$R_y(\phi) = e^{-i\phi\sigma_y/2} = \begin{pmatrix} \cos\frac{\phi}{2} & -\sin\frac{\phi}{2} \\ \sin\frac{\phi}{2} & \cos\frac{\phi}{2} \end{pmatrix},$$

$$R_z(\phi) = e^{-i\phi\sigma_z/2} = \begin{pmatrix} e^{-i\phi/2} & 0 \\ 0 & e^{i\phi/2} \end{pmatrix}.$$

For most superconducting qubit implementations, X and Y rotations are realized with microwave pulses. The Z rotation can be realized either by changing the qubit frequency or as a composition of X and Y rotations, e.g., $R_z(\phi) = R_x(\pi/2)R_y(\phi)R_x(-\pi/2)$.

The partial-projection procedure also requires a two-qubit entangling gate. The most convenient gate to use for conceptually understanding a partial projection is a Z-controlled Y rotation (or X rotation) of the form

$$R_{y|z}(\phi) = e^{-i\phi(\sigma_z\otimes\sigma_y)/2} = \begin{pmatrix} \cos\frac{\phi}{2} & -\sin\frac{\phi}{2} & 0 & 0 \\ \sin\frac{\phi}{2} & \cos\frac{\phi}{2} & 0 & 0 \\ 0 & 0 & \cos\frac{\phi}{2} & \sin\frac{\phi}{2} \\ 0 & 0 & -\sin\frac{\phi}{2} & \cos\frac{\phi}{2} \end{pmatrix}. \quad (8)$$

This gate rotates the qubit in the Z-X plane of the Bloch sphere by an angle $\pm\phi$ depending on the state of the control qubit. This gate may be produced directly if the qubit implementation admits an effective Z-Y (or Z-X) interaction Hamiltonian of the form $\hbar\Omega(\sigma_z \otimes \sigma_y)$ (e.g., [59,71]). Alternatively, as discussed later, it may be realized by using a controlled-phase gate,

$$\mathrm{CZ}(2\phi) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & e^{i2\phi} \end{pmatrix}, \quad (9)$$

that is properly dressed by $X_{\pi/2}$ rotations of the ancilla (e.g., [48]); the angle in Eq. (9) is 2ϕ because the total phase difference is 2ϕ in the gate (8). Yet another way to realize the gate (8) is by using a fixed controlled-Z gate $\mathrm{CZ}(\pi)$ and one-qubit rotations that depend on ϕ (as we shall see shortly).

Now let us discuss the protocol to implement the partial projection of Eq. (1). Using the Z-controlled Y rotation (8), it can be done via the procedure illustrated in Fig. 1.

(1) Initialize the ancilla qubit in the state $|0\rangle$.

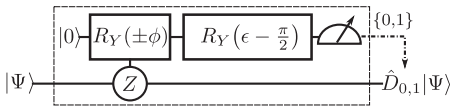

FIG. 1. Quantum circuit implementing the partial projections $D_{0,1}$ using an ancilla qubit. The ancilla is initialized in the state $|0\rangle$ and then a Z-controlled Y rotation of $\pm\phi$ is applied [see Eq. (8)], which creates an angular separation of 2ϕ between the ancilla states coupled to the qubit states of $|0\rangle$ and $|1\rangle$. Finally, the ancilla is Y rotated by the angle $\epsilon - \pi/2$ and measured. For $\epsilon = 0$ this corresponds to measurement in the X basis; the offset ϵ allows for measurement asymmetry. The resulting partial projection of the qubit $D_{0,1}$ depends on the classical outcome 0 or 1 of the ancilla measurement.

(2) Perform a Z-controlled Y rotation (8) of the ancilla by an angle ϕ (to be determined later), which entangles the main qubit with the ancilla.

(3) Perform a Y rotation of the ancilla $R_y(\epsilon - \pi/2)$, with the offset angle ϵ to be determined later.

(4) Measure the ancilla projectively in the computational basis $\{|0\rangle,|1\rangle\}$.

The idea behind this procedure is to first create two states of the ancilla that correspond to the main qubit states $|0\rangle$ or $|1\rangle$ and that are both in the Z-X plane at angles $\pm\phi$ from the Z axis. These ancilla states are then measured along a direction in the same Z-X plane at an angle ϵ from the X axis. The angle ϕ then determines the effective distinguishability of the states $|0\rangle$ and $|1\rangle$ of the main qubit: When $\phi = 0$ the states are indistinguishable. The offset angle ϵ introduces asymmetry between the averaged probabilities of the measurement results, with $\epsilon = 0$ indicating perfect symmetry.

Quantitatively, the results 0 or 1 of the ancilla measurement produce the following partial projections of the main qubit:

$$D_0 = \langle 0|\,[\mathbb{1}\otimes R_y(\epsilon-\pi/2)]\,R_{y|z}(\phi)\,|0\rangle = \sqrt{\frac{1+\sin(\phi+\epsilon)}{2}}\,|0\rangle\langle 0| + \sqrt{\frac{1-\sin(\phi-\epsilon)}{2}}\,|1\rangle\langle 1|, \quad (10)$$

$$D_1 = \langle 1|\,[\mathbb{1}\otimes R_y(\epsilon-\pi/2)]\,R_{y|z}(\phi)\,|0\rangle = \sqrt{\frac{1-\sin(\phi+\epsilon)}{2}}\,|0\rangle\langle 0| + \sqrt{\frac{1+\sin(\phi-\epsilon)}{2}}\,|1\rangle\langle 1|. \quad (11)$$

By comparing the form of Eq. (10) to the standard form of Eq. (1), the parameters p and q are

$$p = \tfrac{1}{2}[1+\sin(\phi+\epsilon)], \quad (12)$$

$$q = \tfrac{1}{2}[1+\sin(\phi-\epsilon)]. \quad (13)$$

Therefore, any desired parameters p and q may be realized by setting the angles of the implementation circuit in Fig. 1 to

$$\phi = \frac{\arcsin(2p-1)+\arcsin(2q-1)}{2}, \quad (14)$$

$$\epsilon = \frac{\arcsin(2p-1)-\arcsin(2q-1)}{2}. \quad (15)$$

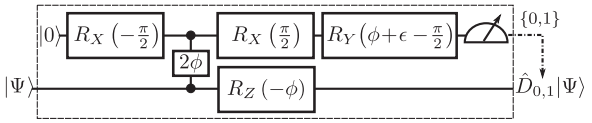

FIG. 2. Quantum circuit using a controlled-phase gate (9) to implement the same partial projections $D_{0,1}$ as in Fig. 1.

It is easy to check that projective measurement ($p = q = 1$) requires $\phi = \pi/2$ and $\epsilon = 0$. The case of no measurement ($p + q = 1$) is realized when $\phi = 0$, and a weak measurement ($|p + q - 1| \ll 1$) requires $|\phi| \ll 1$. The symmetric case ($p = q$) corresponds to $\epsilon = 0$. A null-result measurement ($p = 1$) is realized when $\phi + \epsilon = \pi/2$, so that the qubit state $|0\rangle$ always produces a measurement result of 0.

The realization of the partial projection (1) using a Z-controlled Y rotation (8) is shown in Fig. 1 and Eqs. (14) and (15). Alternatively, Fig. 2 shows how to use a controlled-phase gate (9) instead. In this case, step 2 of the above procedure is further partitioned into the following steps:

(2a) Perform an X rotation of the ancilla by $-\pi/2$.

(2b) Perform a controlled-phase entangling gate by an angle 2ϕ.

(2c) Perform an X rotation of the ancilla by $\pi/2$.

(2d) Perform a Y rotation of the ancilla by ϕ to correct its phase. (This step can be naturally combined with the step 3; see Fig. 2.)

(2e) Perform a Z rotation of the main qubit by $-\phi$ to correct its phase.

This simulation of the Z-controlled Y rotation is useful when a controlled-phase gate is more readily implemented than a direct Z-Y (or Z-X) coupling interaction. Note that the final Z rotation of the main qubit may be omitted if the system will be measured in the Z basis directly after the weak measurement interaction (e.g., [48]).

Similarly, Fig. 3 shows how to replace the Z-controlled Y rotation in the above procedure with a standard controlled-Z gate $\mathrm{CZ}(\pi)$. In this case, step 2 of the above procedure is instead partitioned into the following steps:

(2a) Perform a Y rotation of the ancilla by the angle ϕ.

(2b) Perform a controlled-Z gate to entangle the main qubit with the ancilla.

This implementation has the advantage of using a fixed controlled-Z two-qubit entangling gate, which may be more easily optimized to high fidelity than $\mathrm{CZ}(2\phi)$ (e.g., [62,72]). As such, the implementation will be determined by which two-qubit gate has been optimized; the one-qubit gates typically have high fidelity, even for variable angles such as ϕ and ϵ.

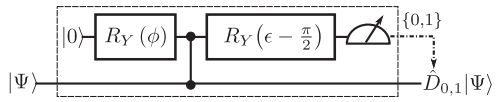

FIG. 3. Quantum circuit using the standard CZ gate to implement the same partial projections $D_{0,1}$ as in Fig. 1. The $R_Y(\phi)$ rotation of the ancilla qubit, followed by the CZ gate, creates an angular separation of 2ϕ between the ancilla states coupled to the qubit states $|0\rangle$ and $|1\rangle$. Then the ancilla qubit is measured in the slanted basis, which becomes the X basis in the symmetric case (when $\epsilon = 0$).

For superconducting qubits, the experimental method discussed in this subsection may suffer from several types of inefficiency, including imperfect fidelities of the gates (e.g., recent two-qubit CZ gates report roughly 0.6% infidelity [72]), decoherence during the procedure (e.g., dephasing times of roughly 10 μs [72]), and imperfect fidelity of the ancilla measurement (e.g., present-day techniques typically permit only up to 99% readout fidelity [73]). Nevertheless, we expect this method to give better overall performance than the thresholded continuous readout for the current implementations of superconducting qubits.

III. GENERALIZED MULTIPLE-OUTCOME MEASUREMENTS

An arbitrary n-outcome purity-preserving measurement can be implemented by reducing it to a sequence of two-outcome measurements, which can be more naturally implemented experimentally. The resulting decomposition is a sequence of unitary gates and standardized two-outcome partial projections [Eq. (1)], each of which can be implemented as discussed in the previous section.

A. Arbitrary two-outcome measurements

First, we decompose an arbitrary two-outcome qubit measurement into the partial projection of Eq. (1) and unitary operations. These partial projections are implementable using either technique described in the previous section, though currently the ancilla method is experimentally simpler. Consider a set of two measurement operators $\{N_0, N_1\}$ that correspond to a single two-outcome purity-preserving measurement [9]. These operators must satisfy the completeness condition $N_0^\dagger N_0 + N_1^\dagger N_1 = \mathbb{1}$. Therefore, the positive operators $|N_{0,1}| \equiv (N_{0,1}^\dagger N_{0,1})^{1/2}$ can be diagonalized simultaneously (with the same unitary operator V), and therefore the singular-value decompositions of $N_{0,1}$ have the form

$$N_{0,1} = U_{0,1} D_{0,1} V^\dagger, \tag{16}$$

where $U_{0,1}$ are unitary operators and $D_{0,1}$ are the (diagonal) partial-projection operators as defined in Eq. (1). Notice that Eq. (16) can be applied to any basis, but we use the natural Z basis, in which the qubit is (partially) measured.

Therefore, one can implement any two-outcome measurement $\{N_0, N_1\}$ of a qubit with the following sequence of operations.

(1) Apply the unitary operation $V^\dagger$ to the qubit.

(2) Perform the partial projection $D_{0,1}$ using specific p and q values [see Eq. (1)]. Record the outcome 0 or 1.

(3) Apply the unitary U_0 or U_1, depending on the obtained outcome.

B. Reduction algorithm

Now we can extend the two-outcome reduction of the previous subsection to an arbitrary n-outcome purity-preserving measurement, with $n > 2$. (See also [43,44] for somewhat similar decompositions.) Consider a set of desired qubit measurement operators $\{M_0, \cdots, M_{n-1}\}$. These operators must satisfy the completeness condition $\sum_{k=0}^{n-1} |M_k|^2 = \mathbb{1}$. (Conceptually, one can imagine these operators as describing

the effects on the quantum state that would be induced by each of the n outcomes of some fictitious laboratory instrument [74].) Note that since $n > 2$, only one of the M_k may be a projection operator satisfying $M_k^2 = M_k$ according to the completeness condition; any such operator will be labeled last as M_{n-1} in what follows.

We can simulate this n-outcome measurement by constructing a sequence of at most $(n-1)$ two-outcome measurements using the following algorithm:

(1) Perform the two-outcome measurement with $N_0^{(0)} = M_0$ and $N_1^{(0)} = \sqrt{\mathbb{1} - |N_0^{(0)}|^2}$. If $N_0^{(0)}$ is seen, then halt: The net effect on the state is then $N_0^{(0)} = M_0$. If $N_1^{(0)}$ is seen, continue to the next step.

(2) Perform the two-outcome measurement with $N_0^{(1)} = M_1[N_1^{(0)}]^{-1}$ and $N_1^{(1)} = \sqrt{\mathbb{1} - |N_0^{(1)}|^2}$. Note that the inverse of $N_1^{(0)}$ must exist by construction, since we have assumed that $N_0^{(0)}$ (and thus $N_1^{(0)}$) is not a projection operator. If $N_0^{(1)}$ is seen, then halt: The net effect on the state is then $N_0^{(1)}N_1^{(0)} = M_1$. If $N_1^{(1)}$ is seen, continue to the next step.

(3) Continue this pattern. At iteration k measure the outcomes $N_0^{(k)} = M_k[N_1^{(0)}]^{-1}\ldots[N_1^{(k-1)}]^{-1}$ and $N_1^{(k)} = \sqrt{\mathbb{1} - |N_0^{(k)}|^2}$. If $N_0^{(k)}$ is seen, then halt: The net effect on the state is then $N_0^{(k)}\ldots N_1^{(1)}N_1^{(0)} = M_k$. If $N_1^{(k)}$ is seen, continue to step $(k+1)$.

(4) Stop at iteration $k = n-2$. A final unitary will in general be necessary to make the net effect for the last outcome $N_1^{(n-2)}$ match M_{n-1}.

Every permutation of the initial set of operators $\{M_k\}$ will produce a different sequence according to this algorithm. Once a particular sequence of two-outcome measurements $\{N_0^{(k)}, N_1^{(k)}\}_{k=0}^{n-2}$ has been constructed theoretically; each set can then be implemented according to Eq. (16). As a technical improvement, note that at any intermediate step of this reduction algorithm the operator $N_1^{(k)}$ can be given an arbitrary unitary degree of freedom: $N_1^{(k)} \to U_{\text{add}}^{(k)}N_1^{(k)}$. This extra unitary may be used to eliminate the unitary rotation $U_1^{(k)}$ from the singular-value decomposition $N_1^{(k)}$ in Eq. (16). Note that in the described algorithm we implicitly assumed $|N_0^{(k)}|^2 \leqslant \mathbb{1}$; this inequality can be proven in a straightforward way.

The described algorithm is general, but it is not the only possible algorithm for realizing an n-outcome generalized quantum measurement (e.g., [43,44]). In practice, it will be useful to optimize the algorithm to produce shorter sequences of measurements.

IV. FIDELITY MEASURES FOR GENERALIZED MEASUREMENT

With the ability to implement generalized quantum measurements comes the necessity of characterizing how well one is implementing them in practice. Currently, there is no standard method for characterizing fidelity of a generalized measurement with multiple possible outcomes. There are, however, standard methods for characterizing the fidelity of individual quantum processes. In this section we extend these existing definitions to multiple-outcome generalized measurements (see the Appendix for more details). In contrast to the previous sections, here we assume an arbitrary number N of qubits, so that the dimension of the Hilbert space is $d = 2^N$.

The standard way [9] of describing a quantum operation $\rho_{\text{in}} \mapsto \rho_{\text{fin}}$ (where ρ denotes a density matrix) is by using the $d^2 \times d^2$ process matrix χ,

$$\rho \mapsto \sum_{i,j} \chi_{ij} E_i \rho E_j^\dagger, \tag{17}$$

where $\{E_i\}$ is the operator basis, which we assume to be the standard Pauli basis, so that $\text{Tr}(E_j^\dagger E_i) = d\delta_{ij}$. For a trace-preserving operation, the matrix χ should satisfy the condition $\sum_{i,j}\chi_{ij}E_j^\dagger E_i = \mathbb{1}$, which in particular implies that $\text{Tr}(\chi) = 1$. If the desired quantum operation χ^{ideal} corresponds to a *unitary* rotation, then the fidelity of an experimental *trace-preserving* operation is usually defined as [75]

$$F = \text{Tr}(\chi^{\text{ideal}}\chi), \tag{18}$$

though sometimes it is defined as the square root of this trace. Note that the process fidelity F is linearly related [76] to the average state fidelity $\overline{F_{\text{st}}}$, which is used in randomized benchmarking and sometimes called [77] "gate fidelity," $1 - F = (1 - \overline{F_{\text{st}}})(1 + 1/d)$. Also note that the definition (18) is inapplicable if two nonunitary operations are compared; see the Appendix.

If a desired unitary operation is experimentally realized by a selective operation (i.e., involving the measurement and selection of a certain measurement result), then the fidelity definition (18) can be modified to [55,78]

$$F = \frac{\text{Tr}(\chi^{\text{ideal}}\chi)}{\text{Tr}(\chi)}. \tag{19}$$

In this case, the actual operation is not trace-preserving, so $\text{Tr}(\chi)$ is the selection probability averaged over all initial pure states (or, equivalently, the selection probability if one prepares the maximally mixed state). Note that the normalized matrix $\chi/\text{Tr}(\chi)$ does not correspond to any physical process, but the definition (19) still satisfies the requirement $0 \leqslant F \leqslant 1$, with $F = 1$ only if $\chi/\text{Tr}(\chi) = \chi^{\text{ideal}}$. Also note that other definitions for fidelity of a selective quantum operation have been considered [55,79,80]; however, here we use Eq. (19) as the starting point for further generalization.

An experimental realization of a generalized multiple-outcome quantum measurement can be described as a set of non-trace-preserving operations, each of them corresponding to a particular outcome k,

$$\rho \mapsto \sum_{i,j} \chi_{ij}^{(k)} E_i \rho E_j^\dagger, \tag{20}$$

so that the total nonselective process, $\chi^\Sigma = \sum_k \chi^{(k)}$, is a trace-preserving operation (we assume that at least one of these outcomes must be reported by the experimental procedure). The probability of an outcome k, averaged over pure initial states, is

$$p_k = \text{Tr}(\chi^{(k)}), \tag{21}$$

such that $\sum_k p_k = 1$. For simplicity, we assume that the desired (ideal) generalized measurement is purity-preserving, $\rho \mapsto M_k \rho M_k^\dagger$ [9], where the measurement (Kraus) operators

M_k satisfy the completeness condition $\sum_k M_k^\dagger M_k = \mathbb{1}$. Therefore,

$$\chi_{ij}^{(k),\,\mathrm{ideal}} = \alpha_i^{(k)} \alpha_j^{(k)*}, \qquad M_k = \sum_i \alpha_i^{(k)} E_i, \tag{22}$$

with $\alpha_i^{(k)}$ being the expansion coefficients of M_k in the basis $\{E_i\}$.

Each outcome k can then be naturally assigned a "partial" fidelity analogous to Eq. (19) [55,78,81,82],

$$F^{(k)} = \frac{\mathrm{Tr}(\chi^{(k),\,\mathrm{ideal}} \chi^{(k)})}{\mathrm{Tr}(\chi^{(k),\,\mathrm{ideal}})\,\mathrm{Tr}(\chi^{(k)})}. \tag{23}$$

Each such fidelity has the proper range, $0 \leqslant F^{(k)} \leqslant 1$, and is unity only if $\chi^{(k)} = \mathrm{const} \times \chi^{(k),\,\mathrm{ideal}}$. Note, however, that this definition is insensitive to the multiplication of $\chi^{(k)}$ by a constant, which affects the average probability p_k of the outcome k. Therefore, to define the overall fidelity F^{tot} of a generalized measurement as a combination of partial fidelities $F^{(k)}$, we must ensure that the definition also penalizes for the difference between the desired probability distribution $p_k^{\mathrm{ideal}} = \mathrm{Tr}(\chi^{(k),\mathrm{ideal}})$ and the actual distribution p_k.

While there is a significant freedom in defining the overall fidelity F^{tot}, here we suggest two different definitions that in our opinion are the most natural (see the Appendix for more discussion on this point). The first definition is

$$F^{\mathrm{tot}} = \sum_k \frac{\mathrm{Tr}(\chi^{(k),\mathrm{ideal}} \chi^{(k)})}{\sqrt{\mathrm{Tr}(\chi^{(k),\mathrm{ideal}})\,\mathrm{Tr}(\chi^{(k)})}}. \tag{24}$$

It is obtained as the weighted sum of the partial fidelities (23), $F^{\mathrm{tot}} = \sum_k \sqrt{p_k^{\mathrm{ideal}} p_k}\, F^{(k)}$, so that the weight factors $\sqrt{p_k^{\mathrm{ideal}} p_k}$ naturally correspond to the outcome probabilities and also automatically penalize the fidelity for unequal probability distributions p_k^{ideal} and p_k.

The second definition we suggest is

$$\tilde{F}^{\mathrm{tot}} = \left[\sum_k \sqrt{\mathrm{Tr}(\chi^{(k),\mathrm{ideal}} \chi^{(k)})} \right]^2, \tag{25}$$

which is obtained from the partial fidelities $F^{(k)}$ as $\tilde{F}^{\mathrm{tot}} = [\sum_k \sqrt{p_k^{\mathrm{ideal}} p_k\, F^{(k)}}]^2$. The square root of this definition is a weighted sum of the square roots of the partial fidelities (23), which in turn are closely related to the Bhattacharyya coefficient defining the fidelity between classical probability distributions (see the Appendix for more details).

For both definitions (24) and (25), the fidelity is between 0 and 1, and the value of 1 is achieved only if $\chi^{(k)} = \chi^{(k),\mathrm{ideal}}$ for all outcomes k. Both definitions are symmetric under exchange of $\chi^{(k)} \leftrightarrow \chi^{(k),\mathrm{ideal}}$. Both of them become inapplicable if the desired generalized measurement includes decoherence (i.e., does not preserve purity). (See the Appendix for the simple generalization that admits decoherence.) It is worth noting that our suggested definitions can also apply in the case that the total nonselective experimental process χ^{Σ} is not trace preserving; the fidelities are then penalized for the missing outcomes.

The fidelity definitions (24) and (25) compare an experimentally implemented generalized quantum measurement to an ideal one, which is characterized both by a desired probability distribution of outcomes (for a given initial state) and by its associated distribution of postmeasurement states. However, in some experiments the generalized measurement may be used only to produce desired probabilities of outcomes, while the postmeasurement state is not important. In this case the fidelity should be defined in a different way.

The probability $P_k(\rho)$ of an outcome k for the initial state ρ is

$$P_k(\rho) = \mathrm{Tr}(\mathcal{P}_k \rho), \quad \mathcal{P}_k = \sum_{i,j} \chi_{ij}^{(k)} E_j^\dagger E_i, \tag{26}$$

where $\mathcal{P}_k$ are so-called POVM elements, which are positive matrices satisfying the completeness condition $\sum_k \mathcal{P}_k = \mathbb{1}$. Note that the average probability p_k introduced earlier is $p_k = P_k(\mathbb{1}/d)$. To define a "probability-only" fidelity F_p (that would be applicable, e.g., to "detector tomography" experiments like [83]), we need to compare the set of POVM elements $\mathcal{P}_k$ with the desired set $\mathcal{P}_k^{\mathrm{ideal}} = M_k^\dagger M_k$. Following the same logic as used above for the process matrices, we define F_p via the weighted sum (with weights $\sqrt{p_k^{\mathrm{ideal}} p_k}$) of the partial fidelities between (normalized) $\mathcal{P}_k$ and $\mathcal{P}_k^{\mathrm{ideal}}$, for which we use either the Uhlmann formula [9] or its square. This leads to the two following definitions

$$F_p = \frac{1}{d} \sum_k \frac{\left(\mathrm{Tr}\sqrt{\sqrt{\mathcal{P}_k^{\mathrm{ideal}}}\,\mathcal{P}_k \sqrt{\mathcal{P}_k^{\mathrm{ideal}}}}\right)^2}{\sqrt{\mathrm{Tr}\left(\mathcal{P}_k^{\mathrm{ideal}}\right)\mathrm{Tr}(\mathcal{P}_k)}}, \tag{27}$$

$$\tilde{F}_p = \left(\frac{1}{d} \sum_k \mathrm{Tr}\sqrt{\sqrt{\mathcal{P}_k^{\mathrm{ideal}}}\,\mathcal{P}_k \sqrt{\mathcal{P}_k^{\mathrm{ideal}}}} \right)^2, \tag{28}$$

which correspond to the logic of Eqs. (24) and (25), respectively. Note that $\mathrm{Tr}(\mathcal{P}_k) = \mathrm{Tr}(\chi^{(k)})\, d = p_k d$, which produces the factors d^{-1} in the definitions of F_p and $\tilde{F}_p$. It is experimentally easier to determine $\mathcal{P}_k$ than $\chi^{(k)}$, because the matrix $\mathcal{P}_k$ has dimension $d \times d$, in contrast to $d^2 \times d^2$ for $\chi^{(k)}$.

V. CONCLUSION

In this paper we have shown that any purity-preserving generalized measurement of a single qubit can be realized by a combination of unitary rotations and two-outcome partial-projection measurements. Two different methods for implementing these partial projections using superconducting qubits were considered: a thresholded continuous measurement using a phase-sensitive amplifier and an indirect ancilla qubit measurement that uses standard unitary gates and projective measurements. The former requires high quantum efficiency of continuous measurement, while the latter requires high-fidelity gates and high-fidelity projective measurements. Both of these methods are already viable experimentally.

The thresholding technique is notable because it realizes a previously proposed decomposition of generalized measurements into continuous measurement procedures. This decomposition is fairly straightforward in the case of qubits; for higher-dimensional systems it can also be done, but will generally require more sophisticated control and feedback of the measurement process.

We have also addressed the issue of characterizing the fidelity of a generalized quantum measurement with multiple possible outcomes, for which there is no established definition in the literature. We proposed two alternative definitions of fidelity for an experimental generalized measurement, each following slightly different logic.

Several special cases of a generalized quantum measurement have already been realized with superconducting qubits, which essentially implement both thresholding-based and ancilla-based techniques similar to those discussed here. We expect that experiments with generalized measurement will become more routine in the future and will continue to attract interest, in particular due to potential practical advantages in applications.

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APPENDIX: DISCUSSION OF FIDELITY MEASURES

In this Appendix we justify the definitions of fidelity presented in Sec. IV of the main text. Let us start with reviewing existing definitions of fidelity for probability distributions, density matrices, and quantum processes, and discuss how they relate to one another.

Suppose that one experimentally determines a classical probability distribution $\{p_k\}$ with $\sum_k p_k = 1$ as a set of measured frequencies. There are several ways to define a characteristic comparing this distribution to an ideal (reference) distribution $\{p_k^{\text{ideal}}\}$. The most widely used characteristics [9] are the Kolmogorov distance $\sum_k \frac{1}{2}|p_k - p_k^{\text{ideal}}|$ (this is the maximum difference between probabilities of an event combining several outcomes) and the *Bhattacharyya coefficient*,

$$F_1\big(\{p_k\},\{p_k^{\text{ideal}}\}\big) = \sum_k \sqrt{p_k\, p_k^{\text{ideal}}}, \tag{A1}$$

which is the characteristic that is most relevant to our approach for defining fidelities. The Bhattacharyya coefficient has the intuitive geometric meaning of the cosine of the angle θ between the two "probability amplitude" vectors $(\sqrt{p_1},\sqrt{p_2},...)$ and $(\sqrt{p_1^{\text{ideal}}},\sqrt{p_2^{\text{ideal}}},...)$. The separation angle θ is also the angle between quantum state vectors $|\psi\rangle$ and $|\psi^{\text{ideal}}\rangle$ that reproduce these classical probability amplitudes [84], which is a useful connection.

In spite of nice mathematical properties of the definition (A1), it has become fashionable in some quantum computing communities to use this definition *squared* as the fidelity between two probability distributions,

$$F_2\big(\{p_k\},\{p_k^{\text{ideal}}\}\big) = \left[\sum_k \sqrt{p_k\, p_k^{\text{ideal}}}\right]^2. \tag{A2}$$

This change in definition is primarily because the squared definition has a direct connection to the standard overlap $|\langle\psi|\psi^{\text{ideal}}\rangle|^2$ between two wave functions, which in turn is related to the probability of a quantum measurement result when $|\psi\rangle$ is measured "along" $|\psi^{\text{ideal}}\rangle$.

The choice between the two definitions (A1) and (A2) has essentially doubled the number of fidelity definitions that are used in quantum computing, which has created some confusion. As discussed later, our proposed fidelity definitions (24) and (27) follow the logic of the definition (A2) [while using (A1) for the weight factors]. In contrast, our definitions (25) and (28) follow the logic of Eq. (A1), but at the end are converted (by squaring) into the more standard "dimension" of the definition (A2).

Now suppose that one experimentally determines a quantum state ρ with $\text{Tr}(\rho) = 1$ using quantum-state tomography. The Uhlmann fidelity [9,85] of this state compared to a reference (ideal) state ρ^{ideal} is usually defined as

$$F_3(\rho,\rho^{\text{ideal}}) = \text{Tr}\Big(\sqrt{\sqrt{\rho^{\text{ideal}}}\,\rho\,\sqrt{\rho^{\text{ideal}}}}\Big), \tag{A3}$$

but it can also be defined [75,86] as its square,

$$F_4(\rho,\rho^{\text{ideal}}) = [F_3(\rho,\rho^{\text{ideal}})]^2. \tag{A4}$$

Importantly, the Uhlmann fidelity (A3) can be found by minimizing the Bhattacharyya coefficient (A1) over all possible generalized measurements that can be made on the two states to produce probability distributions to be compared [87],

$$F_3(\rho,\rho^{\text{ideal}}) = \min_{\{\mathcal{P}_k\}} F_1[\{\text{Tr}(\mathcal{P}_k\rho)\},\{\text{Tr}(\mathcal{P}_k\rho^{\text{ideal}})\}], \tag{A5}$$

where $\{\mathcal{P}_k\}$ are varied over all possible sets of positive probability operators such that $\sum_k \mathcal{P}_k = \mathbb{1}$. Squaring this equation produces the same relation between definitions (A4) and (A2). In most cases the reference state $\rho^{\text{ideal}} = |\psi^{\text{ideal}}\rangle\langle\psi^{\text{ideal}}|$ is a pure state, in which case the definition (A4) reduces to the simpler state overlap,

$$F_4 \to F_5(\rho,\rho^{\text{ideal}}) = \text{Tr}(\rho\,\rho^{\text{ideal}}) = \langle\psi^{\text{ideal}}|\rho|\psi^{\text{ideal}}\rangle. \tag{A6}$$

As mentioned above, the simplicity of this overlap motivates the choice of the squared definitions (A4) and (A2), which we have adopted here and in the main text. (Note that the full Uhlmann formula for F_4 does not permit any simple interpretation.)

Now suppose that one experimentally determines a quantum process matrix χ with quantum process tomography (QPT). This matrix is mathematically equivalent to a (generally un-normalized) density operator, so the definition of its fidelity compared to an ideal process matrix χ^{ideal} can be based on the fidelity definition (A4) for density matrices. To see this, recall that for N qubits such a matrix χ is found by first choosing a matrix basis $\{E_i\}$ that usually consists of all

4^N tensor products of the four Pauli operators $\{I,\sigma_x,\sigma_y,\sigma_z\}$, and then writing the process as a state-transformation function of the form

$$\rho \mapsto \sum_{i,j} \chi_{i,j}\, E_i\, \rho\, E_j^\dagger, \tag{A7}$$

where $\chi_{i,j}$ are the complex components of the $4^N \times 4^N$ Hermitian process matrix χ. Typically, the reference (ideal) process is assumed to be purity preserving, and thus characterized by a single Kraus operator M: $\rho \mapsto M\rho M^\dagger$. This operator can be expanded in terms of the Pauli matrix basis as $M = \sum_i \alpha_i\, E_i$, where $\alpha_i = \mathrm{Tr}(E_i^\dagger M)/2^N$ are its complex components. Hence, the reference process matrix components have the form

$$\chi_{i,j}^{\mathrm{ideal}} = \alpha_i \alpha_j^*. \tag{A8}$$

This expression can be related to a density matrix by formally defining a complex vector $|M\rangle$ of the components α_i of M and then expressing the reference process matrix χ^{ideal} as a dyadic (outer) product

$$|M\rangle = (\alpha_1, \ldots, \alpha_{4^N})^T, \tag{A9}$$

$$\chi^{\mathrm{ideal}} = |M\rangle\langle M|. \tag{A10}$$

If M is unitary then the reference process is trace preserving and $\mathrm{Tr}(\chi^{\mathrm{ideal}}) = 1$, so χ^{ideal} is completely equivalent to a pure-state density operator. If the experimental process χ is also trace preserving, then it is also equivalent to a density operator acting in the Hilbert space with dimension 2^{2N}, corresponding to a generally mixed state (the Jamiołkowski-Choi "channel-state duality" [88–90]). Therefore, the fidelity definition (A6) can be used directly, leading to the standard definition [75,91]

$$F_6(\chi, \chi^{\mathrm{ideal}}) = \mathrm{Tr}(\chi\, \chi^{\mathrm{ideal}}) \tag{A11}$$

for the fidelity of a quantum process χ. If the reference process χ^{ideal} is not unitary (but is still trace preserving), then this definition is naturally replaced with the definition based on Eq. (A4),

$$F_7(\chi, \chi^{\mathrm{ideal}}) = \left[\mathrm{Tr}\left(\sqrt{\sqrt{\chi^{\mathrm{ideal}}}\,\chi\sqrt{\chi^{\mathrm{ideal}}}}\right)\right]^2. \tag{A12}$$

Choosing the nonsquared fidelity definition (A3) instead will produce the equally valid process fidelity definition $\sqrt{F_7}$ (and correspondingly $\sqrt{F_6}$); however, this variation is not typically used in QPT experiments, so we do not consider it here.

If the process χ is not trace-preserving, it necessarily involves a selection; in other words, we consider the process as happening only in some "successful" cases (e.g., when a detector clicks). There are several meaningful ways to generalize the definitions (A11) and (A12) to this case. For example, if the ideal process is still unitary, we can continue using the standard definition F_6 (A11) without any change. This will mean that we take into account all realizations of the process, including "unsuccessful" ones, for which we assign zero fidelity. Alternatively, we can consider only "successful" realizations. In this case there are also several ways to generalize the standard fidelity definition (e.g., [92]); here we consider the way that is based on the Jamiołkowski-Choi channel-state duality.

For nonunitary M in Eq. (A10) (e.g., a partial projection), dividing χ^{ideal} by its trace $\mathrm{Tr}(\chi^{\mathrm{ideal}}) = \langle M|M\rangle = \sum_i |\alpha_i|^2$ still produces a positive matrix with unit trace that is formally equivalent to a pure-state density operator. Similarly, $\chi/\mathrm{Tr}(\chi)$ is a positive matrix with unit trace, and therefore it is also formally equivalent to a (generally mixed) density operator. As a result, the definition [55,78,81,82]

$$F_8(\chi, \chi^{\mathrm{ideal}}) = \frac{\mathrm{Tr}(\chi\, \chi^{\mathrm{ideal}})}{\mathrm{Tr}(\chi)\,\mathrm{Tr}(\chi^{\mathrm{ideal}})} = \frac{\langle M|\chi|M\rangle}{\mathrm{Tr}(\chi)\,\langle M|M\rangle} \tag{A13}$$

satisfies the condition $0 \leqslant F_8 \leqslant 1$, with $F_8 = 1$ only if $\chi = \mathrm{const} \times \chi^{\mathrm{ideal}}$. In the case when both χ and χ^{ideal} are not purity preserving (for example, when decoherence is considered even for the "ideal" process), both equivalent density operators will be mixed, so it will be necessary to use the full Uhlmann form of the state fidelity definition (A4) instead of its simplified form (A6) for the corresponding density matrices; this trivially generalizes Eq. (A13) to

$$F_9(\chi, \chi^{\mathrm{ideal}}) = \frac{\left[\mathrm{Tr}\left(\sqrt{\sqrt{\chi^{\mathrm{ideal}}}\,\chi\sqrt{\chi^{\mathrm{ideal}}}}\right)\right]^2}{\mathrm{Tr}(\chi)\,\mathrm{Tr}(\chi^{\mathrm{ideal}})}. \tag{A14}$$

We emphasize that the definitions (A13) and (A14) compare the two operations only when they are successfully realized (selected).

Given the fidelity definitions reviewed above, we now consider a generalized measurement that has several outcomes k. Each distinguishable outcome corresponds to a separate quantum process,

$$\rho \mapsto \sum_{i,j} \chi_{i,j}^{(k)}\, E_i\, \rho\, E_j^\dagger, \tag{A15}$$

characterized by a process matrix $\chi^{(k)}$ that can be determined experimentally with QPT. The sum of these process matrices produces the total *nonselective* process matrix that sums over all possible outcomes: $\sum_k \chi^{(k)} = \chi^{\mathrm{ns}}$. The nonselective process χ^{ns} will be trace-preserving (assuming no loss) so the trace of this matrix is unity. In contrast, the trace of each outcome matrix is the probability $p_k = \mathrm{Tr}(\chi^{(k)})$ of obtaining the outcome k if one prepares a maximally mixed state (or, equivalently, if one averages over all possible preparations). All the outcome matrices $\chi^{(k)}$ and their associated probabilities p_k should be involved in the definition of the total fidelity of the generalized measurement.

The reference measurement will typically have purity-preserving processes $\chi^{(k),\mathrm{ideal}}$ for all outcomes k that are completely characterized by single Kraus operators $M^{(k)}$, as discussed above, along with their associated component vectors $|M^{(k)}\rangle$, process matrices $\chi^{(k),\mathrm{ideal}} = |M^{(k)}\rangle\langle M^{(k)}|$, and outcome probabilities $p_k^{\mathrm{ideal}} = \mathrm{Tr}(\chi^{(k),\mathrm{ideal}}) = \langle M^{(k)}|M^{(k)}\rangle$. The total nonselective process matrix $\chi^{\mathrm{ns,ideal}}$ will also typically be trace-preserving (and thus have unit trace).

Defining a sensible overall fidelity F^{tot} that properly includes information about all outcomes k involves the following basic conceptual constraints.

(a) F^{tot} should be a symmetric function of all the matrices $\chi^{(k)}$, so the outcomes are interchangeable.

(b) The definition F^{tot} should be in the range $[0,1]$.

(c) $F^{\text{tot}} = 0$ only when $F_9(\chi^{(k)}, \chi^{(k),\text{ideal}}) = 0$ for all k. (Note that F_9 reduces to F_8 for purity-preserving ideal processes. This applies to all discussions below.)

(d) $F^{\text{tot}} = 1$ only when $F_9(\chi^{(k)}, \chi^{(k),\text{ideal}}) = 1$ for all k and $F_2(\{p_k\}, \{p_k^{\text{ideal}}\}) = 1$. (This implies $p_k = p_k^{\text{ideal}}$ for all k, and therefore $\chi^{(k)} = \chi^{(k),\text{ideal}}$).

(e) The definition should be symmetric under the exchange of $\chi^{(k)} \leftrightarrow \chi^{(k),\text{ideal}}$.

To satisfy these constraints, candidate definitions should be constructed from other meaningful quantities in the range [0,1], such as the symmetric classical fidelities $F_2(\{p_k\}, \{p_k^{\text{ideal}}\})$ (or alternatively F_1), the outcome process fidelities $F_9(\chi^{(k)}, \chi^{(k),\text{ideal}})$, and the outcome probabilities p_k, p_k^{ideal}, which are all functions of the matrices $\chi^{(k)}$.

A simple choice for a candidate definition that satisfies all the above constraints and includes each outcome probability and fidelity explicitly is

$$F^{\text{tot}} = C \times \left[\sum_k \sqrt{p_k p_k^{\text{ideal}}}\, F_9(\chi^{(k)}, \chi^{(k),\text{ideal}})^{\alpha} \right]^{\beta}, \quad \text{(A16)}$$

where α, β are real numbers and the factor C is discussed below. The symmetric weighting factors $\sqrt{p_k p_k^{\text{ideal}}}$ automatically penalize for unequal outcome probability distributions p_k and p_k^{ideal}, while the symmetric fidelities F_9^{α} penalize for the differences between each outcome separately. The power α determines the relative importance of these penalties, while β is the overall power. The optional prefactor C can contain any number of additional penalization factors that independently satisfy the above constraints. Examples of factors that can be included in C are

(1) $C_1 = [\sum_k \sqrt{p_k p_k^{\text{ideal}}}]^{\beta_1}$,
(2) $C_2 = [\frac{1}{n} \sum_k F_9(\chi^{(k)}, \chi^{(k),\text{ideal}})^{\alpha_2}]^{\beta_2}$,
(3) $C_3 = [\sum_k p_k F_9(\chi^{(k)}, \chi^{(k),\text{ideal}})^{\alpha_3}]^{\beta_3}$,
(4) $C_4 = [\sum_k p_k^{\text{ideal}} F_9(\chi^{(k)}, \chi^{(k),\text{ideal}})^{\alpha_4}]^{\beta_4}$,
(5) $C_5 = \prod_k F_9(\chi^{(k)}, \chi^{(k),\text{ideal}})^{\alpha_5^{(k)}}$,

where n is the number of outcomes, each $\alpha_{2,3,4}$ and $\beta_{1,2,3,4}$ is a real number, and the outcome-dependent weights $\alpha_5^{(k)}$ can be chosen as $\alpha_5^{(k)} = p_k$, or p_k^{ideal}. Note that the examples C_3, C_4, and C_5 break the symmetry constraint unless they are properly combined. Also note that C_2, C_3, C_4, and C_5 do not penalize for $p_k \neq p_k^{\text{ideal}}$, so they can replace the main term in Eq. (A16) only if additionally multiplied by C_1. While each of these factors can penalize the total fidelity in interesting ways, we choose the simplest functional form with $C = 1$ as the most practical definition.

The remaining parameters α, β in Eq. (A16) can be constrained by requiring F^{tot} to consistently reduce to the existing definitions of fidelity as limiting cases. To match the form of the single-outcome fidelity F_7 and/or F_6 when only one $p_k = p_k^{\text{ideal}} = 1$ with the rest zero, we need to choose $\beta = 1/\alpha$, so we are left with only one free parameter α. This parameter can be chosen by matching with the classical probability fidelities F_1 or F_2 when $F_9(\chi^{(k)}, \chi^{(k),\text{ideal}}) = 1$ for all k; this gives $\alpha = 1$ ($\beta = 1$) or $\alpha = 1/2$ ($\beta = 2$), correspondingly.

The choice of $\alpha = 1$ identifies F_1 as the preferred classical fidelity for the sum over k, yielding the definition

$$F_1^{\text{tot}} = \sum_k \sqrt{p_k p_k^{\text{ideal}}}\, F_9(\chi^{(k)}, \chi^{(k),\text{ideal}}), \quad \text{(A17)}$$

which reduces to Eq. (24) in the main text when the simplified form F_8 is used for the individual outcome fidelities,

$$F_1^{\text{tot}} \to \sum_k \frac{\text{Tr}(\chi^{(k)}\, \chi^{(k),\text{ideal}})}{\sqrt{\text{Tr}(\chi^{(k)})\, \text{Tr}(\chi^{(k),\text{ideal}})}}. \quad \text{(A18)}$$

The alternative choice of $\alpha = 1/2$ consistently identifies F_2 as the preferred classical fidelity for both the sum over k and each individual outcome fidelities F_9. This choice produces the definition

$$F_2^{\text{tot}} = \left[\sum_k (p_k p_k^{\text{ideal}})^{1/2}\, F_9(\chi^{(k)}, \chi^{(k),\text{ideal}})^{1/2} \right]^2, \quad \text{(A19)}$$

which reduces to the definition (25) in the main text when the simplified form F_8 is used,

$$F_2^{\text{tot}} \to \left[\sum_k \sqrt{\text{Tr}(\chi^{(k)} \chi^{(k),\text{ideal}})} \right]^2. \quad \text{(A20)}$$

The advantage of the definition (A18) is that it is a linear combination of the outcome fidelities F_8. However, because of the denominator, it is a complicated function of the process matrices. This complication is related to a subtle inconsistency in the definition: While F_1 is chosen as the preferred classical fidelity for the sum over k, F_2 has been chosen as the preferred classical fidelity that matches the squared form of the fidelity F_8. Thus, the compromise between the two choices of classical fidelity preserves the linearity of F_1^{tot} in the outcome fidelities F_8, but makes the final expression in terms of process matrices complicated.

Since this definition (A20) is logically consistent in choosing F_2 for both cases, its form in terms of process matrices is simpler. In fact, the only difference between this definition and the classical fidelity in (A2) is that the factor inside the square root is an overlap of noncommutative χ_k matrices, rather than the product of classical probabilities. Furthermore, removing the outer square from this definition consistently chooses F_1 as the preferred classical fidelity for both the sum over k and each (nonsquared) outcome fidelity $\sqrt{F_9}$. As a result, the total fidelity $\sqrt{F_2^{\text{tot}}}$ becomes a linear function of the nonsquared outcome fidelities $\sqrt{F_9}$ automatically.

As noted earlier, more complicated definitions of F^{tot} can also be considered. However, we feel that the two simplest definitions (A17) and (A19) will be the most useful in practice. The "probability-only" definitions (27) and (28) in the main text are also essentially the definitions (A17) and (A19), but applied to the POVM elements $\mathcal{P}_k$ instead of the process matrices $\chi^{(k)}$ [the extra factor d^{-1} comes from different normalizations: $\text{Tr}(\mathcal{P}_k) = \text{Tr}(\chi^{(k)})\, d$].

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