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PAPER

Diagnostics of quantum-gate coherences deteriorated by unitary errors via end-point-measurement statistics

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Abstract
Quantum coherence is a central ingredient in quantum physics with several theoretical and technological ramifications. We consider a figure of merit encoding the information on how the coherence generated on average by a quantum gate is affected by unitary errors (coherent noise sources) in the form of rotation-angle and rotation-axis errors. We provide numerical evidences that such information is well captured by the statistics of local energy measurements on the output states of the gate. These findings are then corroborated by experimental data taken in a quantum optics setting.

1. Introduction

The characterization of the quality of a given operation is a key step towards the validation of quantum technologies: any information-processing task needs to be assessed against relevant performance-quantifying figures of merit. A relevant instance of such key necessity is the evaluation of the quality of quantum gates to assess fault tolerance [1, 2].

Quantum coherence is a pivotal property of quantum states and operations [3], and embodies the ultimate feature setting quantum and classical mechanics apart. Its presence in resource states or generation through dynamics are paramount to the achievement of quantum advantages [4]. Evidences in this respect have been provided for transport across biomolecular networks [5–10], nano-physics [11, 12] and low-temperature thermodynamics [13–18]. Recently formulated resource-theory approaches [3, 4, 19, 20] have enabled the assessment of the role of quantum coherence in a range of tasks in quantum technologies [21–24]. As quantum coherence is closely related to and can be converted into other powerful quantum resources [25–27], its characterization is growing both in interest and relevance. In [28], a scheme for the direct estimation of quantum coherence through the implementation of entangled measurements on two copies of the state at hand has been experimentally demonstrated in a linear-optics platform. While providing an interesting approach to the quantification of coherences without relying on a tomographic approach based on the reconstruction of the system state and the evaluation of a suitable quantitative measure [3, 4], this approach poses challenges embodied by the need for entangled measurements to be used.

In this paper we combine the need for the characterization of quantum coherence in quantum processes and states with the observation that any information-processing task implies a process of energy exchange between the elements of the computational register. In this regard, we make use of tools specifically designed to address the phenomenology of energetics in non-equilibrium quantum processes to build a diagnostic instrument for the quality of quantum coherence resulting from a quantum gate. In particular, we employ
the recently introduced end-point measurement (EPM) scheme aimed at characterizing the statistic of energy-changes [29, 30] while, crucially, accounting for coherence of the initial state in the energy basis. We unveil a remarkable connection between the statistics of local observables—focusing in particular on energy measurements [31]—and the coherence induced by the action of a quantum gate, in the relevant case of control-unitary two-qubit gates, affected by rotation-angle and rotation-axis errors (coherent noises). In order to provide a figure of merit that accounts for the coherence-inducing capabilities of the gate at hand, irrespectively of the specific input states, we focus on an input-averaged quantity that has no need for the tomographic reconstruction of the computational register states. Our results, albeit limited to unitary errors, are well aligned with a stream of recent works in which non-equilibrium thermodynamic relations have been used as a diagnostic tool for the non-unitarity and dissipation of commercial quantum computing architectures [31–37].

The remained of this paper is organized as follows. In section 2, we describe both the gates being considered to illustrate our approach and the unitary errors (rotation-angle and rotation-axis errors) taken into account in our study. Section 3 introduces the figure of merit, based on local energy fluctuations, that we employ for the diagnostics of the quantum two-qubit gates and coherent noise errors of interest. In section 4, we illustrate the experimental setting employed to validate the connections between energy fluctuations—resulting from the dynamics of the considered noisy gates—and the characterization of the same gates in term of quantum coherences. Finally, section 5 summarises our results and highlights open questions that remain to be addressed.

2. Quantum gates and unitary errors

As benchmarks for our investigation, we will consider one- and two-qubit gates. Then, we compare their capability to generate coherences dynamically, when perfectly implemented and when affected by a specific, yet experimentally relevant, source of imperfections.

When considering the single-qubit operations, we refer to the unitary transformation

\[ R(\theta) = e^{i \frac{\pi}{2} (I - n \cdot \sigma)} = \cos(2\theta)\sigma_z + \sin(2\theta)\sigma_x, \]

where \( \sigma \equiv (\sigma_x, \sigma_y, \sigma_z) \) the vector of Pauli operators \( \sigma_k \) \( (k = x, y, z) \) and \( I \) the \( 2 \times 2 \) identity operator.

Equation (1) embodies a rotation of an angle \( \pi \) about the axis identified by the vector \( n \equiv (\sin(2\theta), 0, \cos(2\theta)) \). Such transformation is also used to construct the conditional two-qubit gate

\[ G(\theta) \equiv \sigma^a_+ \otimes I^b + \sigma^a_- \otimes R^b(\theta) \]

with \( \sigma^a_\pm = (\sigma^i_\pm \pm i\sigma^j_\pm)/2 \) denoting the ladder operators and \( j = a, b \) the label for the qubits being considered. The states of the computational basis for each qubit are \( \{|0\rangle_j, |1\rangle_j\} \) where \( \sigma^j_0 |k\rangle = (-1)^k |k\rangle \) \( (k = 0, 1) \). The conditional gate \( G(\theta) \) applies a rotation of \( \pi \) around axis \( n \) (or the identity matrix) to the state of qubit \( b \) when the control qubit is in the state \( |1\rangle_a \) (or in the state \( |0\rangle_a \), while the logical state of the control qubit is simultaneously flipped.

The implementation of quantum gates is often affected by experimental imperfections that give rise to computational errors [38–40]. In general, if we denote by \( U = \{ R(\theta), G(\theta) \} \) the perfect target gate we want to implement and \( \mathcal{U}(\rho) = U\rho U\dagger \) the corresponding unitary map, its realization prone to errors will be denoted by \( (\mathcal{E} \circ \mathcal{U})(\rho) ) \equiv \mathcal{E}(\mathcal{U}(\rho)) \), where \( \mathcal{E}(\cdot) \) is a completely positive trace preserving (CPTP) channel. The latter represents the error in the gate implementation. Among the most insidious and important errors are unitary ones, i.e. errors that do not affect the purity of the state. They result in

\[ (\mathcal{E} \circ \mathcal{U})(\rho) = V\rho V\dagger, \]

where \( V \) is a unitary operation characterizing the noisy channel. In our study, we will focus our attention on two experimentally relevant classes of unitary errors, namely rotation-angle errors and rotation-axis errors. The latter are described by

\[ V_{\text{axis}}(\theta, \phi) = \sigma^a_+ \otimes I^b + i\sigma^a_- \otimes \tilde{R}^b_{\text{axis}}(\theta, \phi) \]

where we have introduced the rotation \( \tilde{R}_{\text{axis}}(\theta, \phi) \equiv -i (\hat{n} \cdot \sigma) \) with \( \hat{n} \equiv (\sin(2\theta)\cos(\phi), \sin(\phi), \cos(2\theta)\cos(\phi)) \) denoting the rotation axis that differs from \( n \) by an angle \( \phi \). Such error leaves the rotation angle unaffected. On the other hand, when considering rotation-angle errors, we look into

\[ V_{\text{angle}}(\theta, \varphi) = \sigma^a_+ \otimes I^b + \sigma^a_- \otimes \tilde{R}^b_{\text{angle}}(\theta, \varphi) \]
we briefly review the salient

defined as
generated by the gates affected by unitary errors and the noiseless ones respectively. Such estimator is

core of our investigation. We thus consider the estimator of the mismatch between the quantum coherence

dynamics), the EPM’s probability density function (PDF) for a given energy-change is

features of this framework.

interested reader, and in order to make our work self-contained, in appendix

scheme apart from the seminal two-point measurement (TPM) scheme [1], which has been recently formulated with the deliberate mandate of highlighting the role played, in such

3. Figures of merit

The quantification of the errors affecting a quantum gate is paramount to the achievement of fault-tolerant quantum computing. In this regard, without resorting to more expensive techniques as artificial intelligence ones [41, 42], a typical way to estimate errors is through figures of merit such as the average gate fidelity [43, 44]

\[ F(E \circ U, U) \equiv \mathbb{E}[\psi] \operatorname{Tr} \left[ (E \circ U)(\rho_{\psi}) U(\rho_{\psi}) \right], \tag{7} \]

where the symbol \( \mathbb{E}[\psi] \) stands for the ensemble average over all pure initial states \( |\psi\rangle \) such that \( \rho_{\psi} \equiv |\psi\rangle\langle\psi| \). Such quantum states are drawn uniformly, according to the Haar measure, from the state space.

While allowing for a coarse grained characterization of the quality of a quantum gate, equation (7) requires the experimentally demanding tomographic reconstruction of the maps being involved [45–47]. Moreover, quantum states and processes that, according to fidelity-based figures or merit, are deemed to be close to each other might be endowed with significantly different physical properties [48], thus weakening the foundations of any comparison based on quantities akin to equation (7). Finally, \( F(E \circ U, U) \) would not allow to easily single out the quality of the experimental process in regard to the generation of quantum coherence.

In order to bypass such bottlenecks, we put forward a figure of merit that more fits to the purpose at the core of our investigation. We thus consider the estimator of the mismatch between the quantum coherence generated by the gates affected by unitary errors and the noiseless ones respectively. Such estimator is defined as

\[ E(E \circ U, U) \equiv \mathbb{E}[\psi] \left[ \left| C_{\ell_1} \left( (E \circ U)(\rho_{\psi}) \right) \right| - C_{\ell_1} \left( U(\rho_{\psi}) \right) \right], \tag{8} \]

where \( C_{\ell_1}[\rho] \equiv \sum_{n \neq k} |\rho_{nk}| \) denotes the \( \ell_1 \) measure of quantum coherence of the generic state \( \rho \) [4]. The average is again performed over all pure initial states in order to remove any dependence of the quantifier from the specific state that one may consider. We dub equation (8) the average gate coherence fidelity. It quantifies how much the coherence content of the quantum state after the application of the gate changes, on average, due to the presence of errors (figure 1(a) and (c)). While equation (8) has a clear interpretation, determining \( C_{\ell_1} \) is in general not a trivial task. In fact, it would require either the tomographic reconstruction of the states—and thus the evaluation of their degree of coherence—or the use of entangled measurements on two copies of each state, in line with [28].

We now show that a different quantity, with a clear operational meaning and a fundamentally local nature, is closely connected with the average gate coherence fidelity for the gates and errors that we are considering, thus offering a route to its quantification. We focus our attention on the statistics of the energy fluctuations resulting from any physical mechanism of information processing, and thus also those at hand here. We look for the probability that, upon implementing a given dynamical process, the computational register under scrutiny is subjected to a change of its energy. We make use of the so-called EPM scheme [29, 30], which has been recently formulated with the deliberate mandate of highlighting the role played, in such dynamical energy fluctuations, by quantum coherences. It is exactly the latter aspect that casts the EPM scheme apart from the seminal two-point measurement (TPM) scheme [49], which washes away quantum coherences by projective measurements. The possibility to compute fluctuations of random variables at two (or more) time instants while preserving quantum coherence fully motivates the choice of the EPM approach (see also [50–53] and references therein for other alternatives to the TPM). Further, the EPM scheme only requires a single final energy measurement on the system, following a dynamical evolution of the state. This is perfectly in line with quantum computing processes, where initially prepared pure states are manipulated and then measured at the end. In the following, we employ the framework of the EPM scheme. For the interested reader, and in order to make our work self-contained, in appendix A we briefly review the salient features of this framework.

For a quantum system prepared in a state \( \rho_0 \) and subjected to a CPTP map \( \mathcal{M}_t \), (here \( t \) identifies the instant of time in the dynamics), the EPM’s probability density function (PDF) for a given energy-change is
defined as

$$p_{\text{EPM}}(\Delta E_{k,t}) = p(E_{\text{fin}}^k) p(E_{\text{in}}^j) = \text{Tr}[\Pi_{\text{fin}}^k \rho_0] \text{Tr}[\Pi_{\text{in}}^j M_{\text{fin}}(\rho_0)],$$

(9)

where $\Pi_{\text{in}}^j$ and $\Pi_{\text{fin}}^k$ are the projectors on the $j$-th initial (final) energy eigenstate of the system, and $\Delta E_{k,t} = E_{\text{fin}}^k - E_{\text{in}}^j$ is the corresponding energy-change. $E_{\text{fin}}^k$ ($E_{\text{in}}^j$) denotes the eigenvalues of the initial (final) Hamiltonian.

Then, we introduce the characteristic function of the EPM distribution:

$$G(u) = \langle e^{iu\Delta E}\rangle_{\text{EPM}} = \text{Tr}[e^{-iuH_0} \rho_0] \text{Tr}[e^{iuH_0} M_{\text{fin}}(\rho_0)]$$

with $H_0$ the (time-dependent) Hamiltonian of the system and $\rho_0$ the initial state. The EPM characteristic function can be cast as

$$G(u; M_t) = \sum_{Q=\mathbb{P},\chi} G_Q(u; M_t)$$

(10)

and $u \in \mathbb{C}$. In equation (10) we have decomposed the initial state as $\rho_0 = \mathbb{P} + \chi$ with the diagonal part $\mathbb{P}$ (in the basis of the initial Hamiltonian $H_0$) and the traceless component $\chi$ that encodes the quantum coherence in the energy basis. We can thus isolate the contribution $G_Q(u; M_t)$ of the characteristic function stemming from the initial quantum coherence.

In the context of the problem addressed by our study, we consider the statistics of the local energy originated by the Hamiltonian $H = \sigma_x^a \otimes P + P \otimes \sigma_x^b$. This just entails local measurements in the computational basis $\{00,01,10,11\}$, embodying a remarkable simplification of the estimation process. Then, we consider the following figure of merit:

$$\eta_{\chi}(\mathcal{E} \circ \mathcal{U}, \mathcal{U}) \equiv \mathbb{E}_\psi \left[ |G_{\chi}(i; \mathcal{E} \circ \mathcal{U}) - G_{\chi}(i; \mathcal{U})|^2 \right].$$

(11)

Equation (11) is built upon the difference between the coherence-dependent components of the EPM characteristic function that result from the local-energy PDF corresponding to the ideal (target gate) and its error-affected version (figure 1(b) and (d)). In appendix B, we address analytically the figures of merit at the core of our study.

3.1. Required number of measurements

Before proceeding, let us discuss the cost of reconstructing our figure of merit for a two-qubit gate. From equations (10) and (11) we see that, in order to obtain $\eta_{\chi}$, we need $\text{Tr}[e^{-iH_0} \mathcal{E} \circ \mathcal{U}(|\psi_0\rangle\langle\psi_0|)]$ for all pure initial states $|\psi_0\rangle$. This can be accomplished by performing local energy measurements and initializing the two-qubit gate in 16 distinct initial states. In fact, by expanding the generic initial state in the computational basis $\{|i\rangle\} = \{|00\rangle,|01\rangle,|10\rangle,|11\rangle\}$, we have

$$\text{Tr}[e^{-iH_0} \mathcal{E} \circ \mathcal{U}(|\psi_0\rangle\langle\psi_0|)] = \langle \psi_0 | V^\dagger e^{-iH_0} V | \psi_0 \rangle = \sum_{\alpha i j} e^{-E_{\alpha k}} a_i a_j^\dagger \langle j | V^\dagger \Pi_{\text{fin}}^{(\alpha)} V | i \rangle,$$

(12)

where we have used $H_{\text{fin}} = \sum_{\alpha} E_{\alpha} \Pi_{\text{fin}}^{(\alpha)}$ and $|\psi_0\rangle = \sum_i a_i |i\rangle$. This shows that, in order to evaluate (by post-processing) our averaged estimator, all the 64 different matrix elements $\langle j | V^\dagger \Pi_{\text{fin}}^{(\alpha)} V | i \rangle$ will be needed.
Figure 2. Sketch of the experimental setting. The two photons are generated through type I SPDC on a 3 mm BBO crystal pumped with a 405 nm CW laser. The photons are filtered with a FWHM 7.5 nm interference filter and sent to the setup depicted in the figure through single mode fibers. The photons are prepared in the $|0\rangle$, $|1\rangle$, or $|+\rangle$ states using HWPC$_1$ and HWPS$_1$ respectively. The waveplates on the signal arm are used to implement unitary errors in a controllable way, and the preparation and measurement settings are included in the overall transformation; this is not necessary on the control arm, for which the plates control the preparation and the measurement directly. The C-SIGN gate is constituted by a main PPBS transmitting 1/3 and reflecting 2/3 of the vertically polarized light. There are also two additional PPBS—one per arm—that are rotated by 90 degrees, thus operating on the H polarization. The additional PPBS allow to compensate for the intensity unbalance generated by the main PPBS.

shown in appendix C, this set of values can be achieved by initializing the quantum system in the four computational basis states and in twelve additional, separable states, which strongly eases the experimental implementation of this protocol.

By extension, for $n$ qubits ($d = 2^n$) we would need to initialize the system in $2^{3n}$ states and then perform local energy measurements, i.e. we would need $2^{3n}$ projective measurements. These resources scale exponentially with the number of qubits. Despite this, such trend is favorable with respect to the $d^4 = 2^{4n}$ measurements required by quantum process tomography [47]. It is then clear that our scheme offers an advantage with respect to quantum tomography from the point of view of both the number and the nature of the required operations.

4. Experimental results

We will now test our numerical prediction using a quantum optics implementation of the controlled two-qubits gate affected by rotation axis errors.

We encode the logical states $|0\rangle_j$ and $|1\rangle_j$ in the horizontal and vertical polarization states $|H\rangle_j$ and $|V\rangle_j$ of a photon (here, $j = a, b$). The realization of the two-qubit gate is based on the design of a controlled-sign gate illustrated in figure 2. In order to implement the map associated with rotation-axis errors $V_{\text{axis}}(\theta, \phi)$, we perform rotations on the polarization of the signal photon using a set of half (HWP) and quarter (QWP) wave plates before and after the interaction between the signal and control photons. For this purpose, we set the angle of both HWPs to $\alpha = \theta/2 + \phi/4$ and the angle of the QWPs to $\beta_{\text{QWPS}} = \phi/2 + \pi/2$ and $\beta_{\text{QWPS}} = \phi/2$ respectively.

Remarkably, the expected behavior of the gate allows to capture the essential features of the EPM-based diagnostics by focusing on a reduced set of input states: in different experiments, we initialize the two-qubit gate in $|+\rangle \equiv (|0\rangle + |1\rangle) \otimes (|0\rangle + |1\rangle)/2$ as well as in $|00\rangle, |01\rangle, |10\rangle, |11\rangle$. These choices provide enough settings to compare coherent and incoherent cases with figures close to the averaged one. As an illustrative example, we fix the value of $\phi = 20^\circ$ by letting vary $\theta$ between $0^\circ$ and $45^\circ$. Finally, in output of the two-qubit gate, we collect sets of measurement outcomes by projecting on the basis $\{|00\rangle, |01\rangle, |10\rangle, |11\rangle\}$.

In figure 3 we compare our theoretical predictions with the experimental data. In the previous section, we have discussed how the figure of merit $\eta_c$ bears close resemblances to the average gate coherence fidelity $\mathcal{C}$ upon the average over all initial pure states. The experimental determination of the average estimator lays
Figure 3. Analysis of the experimental data. In panels (a)–(e), the dots represent the experimental data, while the solid lines denote the theoretical predictions. Specifically, (a) Red: $p(00|00)$, Blue: $p(01|00)$, Black: $p(11|00)$, Magenta: $p(10|00)$; (b) Red: $p(00|01)$, Blue: $p(01|01)$, Black: $p(10|01)$, Magenta: $p(11|01)$; (c) Red: $p(00|10)$, Blue: $p(01|10)$, Black: $p(10|10)$, Magenta: $p(11|10)$; (d) Red: $p(00|11)$, Blue: $p(01|11)$, Black: $p(10|11)$, Magenta: $p(11|11)$; (e) Red: $p(00|++)$, Blue: $p(01|++)$, Black: $p(10|++)$, Magenta: $p(11|++)$. (f) Red dots: inference of $1.6153 |G_\chi(i;EU) - G_\chi(i;U)|$ with experimental data, Blue x-mark dash-dotted line: theoretical prediction of $2.24774 |G_\chi(i;EU) - G_\chi(i;U)|$, Black dashed line: $3.7404 |C_1(EU) - C_1(U)|$. All the curves in the panels are plotted as a function of $\theta \in [0, \pi/4]$ rad and $\phi = \pi/9$ rad, and by initializing the implemented quantum gate in the single initial state $|++\rangle$. The error bars of the experimental data are smaller than the size of the symbols used to represent each data-point.

beyond the scope of our current work (cf appendix C for an additional analysis). Nonetheless, with our restricted set of initialization states we can faithfully reconstruct the kernel $|G_\chi(i;EU) - G_\chi(i;U)|$ of our estimator for the initial state $\rho_0 = |++\rangle\langle++|$ and compare it with the corresponding gate coherence fidelity $|C_1(EU) - C_1(U)|$ for the same initial state (cf figure 3(f)).

These measurements support our previous observation on how, beyond convenience, the quantities estimated in this way have a qualitatively similar behavior to the averaged figures of merit $\eta_\chi$ and $\mathcal{C}$. The observed discrepancies are not due to the lack of averaging, but flag genuine non-idealities of the gate adding up to the unitary error. Specifically, imperfect non-classical visibility for the vertical polarizations, as well as residual unwanted interference for the horizontal polarizations are responsible for these extra faults [31].
Note that, as the probabilities to measure the $\ell$th local energy of the gate at time $t_{\text{fin}}$ is also equal to

$$p(E_{\text{fin}}^k; Q = \chi) = \text{Tr}[|kq\rangle\langle kq|\mathcal{M}_{t_{\text{fin}}}^{(\chi)}] = p(\langle kq |++) - \frac{1}{4} \sum_{n,m=0}^{1} p(\langle kq |nm)$$

with $k, q = 0, 1$, the contribution $\mathcal{G}_{\chi}$ of the EPM characteristic function is reconstructed experimentally from measuring the conditional probabilities $p(00|kq), p(01|kq), p(10|kq), p(11|kq), p(\langle kq |++)$ (panels (a)–(e) in figure 3). Conversely, the $\ell_1$ measure of quantum coherence $C_{\ell_1}$ are obtained by numerical simulations as a function of $\theta \in [0, \pi/4]$ rad and $\phi = \pi/9$ rad.

5. Conclusions

In this paper, we introduce and discuss a new tool for the diagnostics of one- and two-qubit gates subjected to unitary errors that are typically cumbersome [38, 39]. We specifically consider unitary errors—which are among the most subtle errors for quantum computational platforms—in the form of rotation-angle and rotation-axis errors. We point out how an estimator ($\eta_{kq}$) based on the recently introduced EPM scheme [29, 30], compares with the average gate coherence fidelity $\mathcal{E}$. The determination of our estimator requires only local energy measurements of the qubits output states, and we show that it qualitatively reproduces the average gate coherence fidelity. We also compare the estimator and the gate coherence fidelity on a single initial state by using an all-optical set-up.

Our results employ thermodynamics tools, i.e. the characteristic function of the EPM energy-change statistics, to investigate the faithfulness of quantum logic gates. This is indeed a growing research field that is attracting the attention of the wider quantum community [31–33, 35, 54]. For our case, beyond requiring only local energy measurements, the EPM approach provides a complementary way to perform diagnostics of quantum-gate coherences, without resorting to tomographic procedures.

It would be interesting to pinpoint, both analytically and numerically, the limitations of the introduced diagnostics tool in the case of general non-unitary noise. Moreover, it would be worth investigating the general properties of $\eta_{kq}$ as an estimator of quantum coherence in quantum technology applications, from quantum communication to quantum batteries [55], quantum transport [56], and clocks [57].

Data availability statement

All data that support the findings of this study are included within the article (and any supplementary files).

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Appendix A. End-point measurement approach to energy-change fluctuations

The EPM protocol has been recently introduced to take into account the presence of quantum coherence in the statistics of energy changes for a system undergoing open quantum dynamics.

The protocol differs from the usual two-point measurement (TPM) [49] approach, in which initial and final projective measurements (in the energy basis) are used and erase any signature of initial coherence, while it is in line with several recent attempts to go past the TPM’s limitations [50–53].

Let us consider a quantum system initialized in state $\rho_0$ and undergoing a generic process described by a CPTP quantum map ($\mathcal{M}_t$) evolving it from time zero to a generic time $t$. We can then consider the energy-change distribution $P(\Delta E)$
The EPM joint probability distribution is an actual probability distribution, i.e. for the undisturbed average energy-change is recovered:

\[ P(\Delta E) = \sum_{k,\ell} p(\Delta E_{k,\ell}) \delta(\Delta E - \Delta E_{k,\ell}), \quad (A1) \]

where \( \delta(\cdot) \) is the Dirac delta function. Here, \( \Delta E_{k,\ell} \equiv E_{\text{fin}}^{k,\ell} - E_{\text{in}}^{k,\ell} \) is one of the possible realization of the stochastic variable \( \Delta E \) representing the energy-change, with \( E_{\text{in}}^{k,\ell} \) and \( E_{\text{fin}}^{k,\ell} \) denoting the eigenvalues of the Hamiltonian of the system at the initial and final times of the process. In particular, we indicate with the spectral decomposition of the initial and final Hamiltonian.

In this appendix, we examine closely the quantities of interest in the main text of the paper. Let us thus take the initial pure states into account the expressions of the considered figures of merit before performing the averaging over the initial state and the actual effect of the quantum coherence in

\[ H_{\text{in}} = \sum_{k} E_{\text{in}}^{k} \Pi_{\text{in}}^{k} \quad \text{and} \quad H_{\text{fin}} = \sum_{\ell} E_{\text{fin}}^{\ell} \Pi_{\text{fin}}^{\ell} \quad (A2) \]

the relations obtained by means of the TPM scheme. Such deviations are due to both the non-linearity of the scheme with respect to the initial state and the actual effect of the quantum coherence in the initial state. It should be noted that, the set of probabilities \( \{p(E_{\text{in}}^{k})\} \) and \( \{p(E_{\text{fin}}^{\ell})\} \) can be experimentally assessed via two independent protocols: the first aimed at characterizing the initial projective energy measurement is what distinguish the EPM approach from the TPM scheme, allowing to account for initial quantum coherences. It should be noted that, the set of probabilities \( \{p(E_{\text{in}}^{k})\} \) and \( \{p(E_{\text{fin}}^{\ell})\}) \) can be experimentally assessed via two independent protocols: the first aimed at characterizing the quantum system at times \( t_{\text{in}} \) and \( t_{\text{fin}} \). Operationally, this corresponds to considering the probabilities \( p(E_{\text{in}}^{k}) \) of the outcomes \( E_{\text{in}}^{k} \) resulting from measuring \( H_{\text{fin}} \) at the end of the process without any disturbance to the initial state \( \rho_{0} \). Then, the final probabilities are weighted by the probabilities \( p(E_{\text{fin}}^{\ell}) \) associated to the initial energy statistics. Hence, the joint probability from the EPM scheme combines a single final measurement of the system energies with an a-priori knowledge of the initial state statistics. The absence of an initial projective energy measurement is what distinguish the EPM approach from the TPM scheme, allowing to account for initial quantum coherences. It should be noted that, the set of probabilities \( \{p(E_{\text{in}}^{k})\} \) and \( \{p(E_{\text{fin}}^{\ell})\}) \) can be experimentally assessed via two independent protocols: the first aimed at characterizing the energy of the initial state, and the second aimed at obtaining the statistics of the final energy measurement.

It is useful to briefly state the main properties of the EPM energy-change distribution, which can be listed as follows

(1) The EPM joint probability distribution is an actual probability distribution, i.e. \( p_{\text{EPM}}(\Delta E_{k,\ell}) \geq 0 \forall (k,\ell) \), and

\[ \sum_{k,\ell} p_{\text{EPM}}(\Delta E_{k,\ell}) = 1. \quad (A4) \]

(2) The ‘undisturbed’ average energy-change is recovered:

\[ \langle \Delta E \rangle_{\text{EPM}} = \sum_{k,\ell} p_{\text{EPM}}(\Delta E_{k,\ell}) \Delta E_{k,\ell} = \text{Tr}[H_{\text{fin}} M_{\text{fin}}(\rho_{0})] - \text{Tr}[H_{\text{in}} \rho_{0}]. \quad (A5) \]

(3) For \( [H_{\text{in}}, \rho_{0}] = 0 \), the EPM energy-change distribution reduces to the distribution of the TPM scheme if and only if \( \rho_{0} \) is an eigenstate of \( H_{\text{in}} \). Thus, one cannot recover the TPM results in general even when the initial state \( \rho_{0} \) is diagonal in the eigenbasis of \( H_{\text{fin}} \). This property derives from the non-linearity of the EPM energy-change distribution under convex combination of initial states.

Finally, it should be mentioned that the analogue of the Jarzynski equality and the Crooks detailed fluctuation theorem have been obtained in the context of the EPM scheme [30]. Both results show deviations from the relations obtained by means of the TPM scheme. Such deviations are due to both the non-linearity of the scheme with respect to the initial state and the actual effect of the quantum coherence in \( \rho_{0} \). Such contributions can be experimentally distinguished allowing to pinpoint the contribution of the initial quantum coherence also in the entropy production of the quantum process under scrutiny. We refer the interested reader to [30] for further details.

**Appendix B. Figures of merit: formal analysis**

In this appendix, we examine closely the quantities of interest in the main text of the paper. Let us thus take into account the expressions of the considered figures of merit before performing the averaging over the initial pure states \( \rho_{0} = \sum_{n,m} \langle \rho_{0} \rangle_{nm} |n\rangle \langle m| \) with \( \langle \rho_{0} \rangle_{nm} \equiv a_{n}^{\dagger} a_{m} \) and \( |\psi_{0}\rangle \equiv \sum_{i} a_{i} |i\rangle \).
B.1. Expressions of $\eta_{TPM}$ and $\eta_P$

If one made use of the two-point measurement (TPM) scheme, then a possible figure of merit for the diagnostic of a quantum gate would be

$$\eta_{TPM} = \mathbb{E}_{\langle \psi \rangle} \left[ \text{Tr} \left[ e^{-H_{\text{fin}}} \left( \mathcal{E}(Ue^{i\alpha}\mathcal{P}U^\dagger) - Ue^{i\alpha}\mathcal{P}U^\dagger \right) \right] \right]$$

(B1)

Thus, using the computational basis (over which the observable $H = H_{\text{fin}} = H_{\text{fin}}$ is diagonal such that in this appendix $A_k \equiv \langle k | H | k \rangle$), one then gets

$$N_{TPM} = \left| \sum_{n,\alpha,m} e^{-H_{\text{fin}}} e^{H_{\text{fin}}} (\rho_0)_{mn} (\langle n | K_\alpha U | m \rangle)^2 - \langle n | U | m \rangle^2 \right|.$$  

(B2)

where $(\rho_0)_{mn} = \langle | m \rangle | \psi_0 \rangle^2$, and we have expressed the noise channel affecting the quantum gate in terms of the corresponding Kraus representation: $\mathcal{E}(\cdot) = \sum_{\alpha} K_\alpha (\cdot) K_\alpha^\dagger$. In the case of a unitary error, just a single Kraus operator is different from zero. In the case of $G_P$ one has

$$\eta_P = \mathbb{E}_{\langle \psi \rangle} \left[ \left( \langle e^{H_{\text{fin}}} \rangle \text{Tr} \left[ e^{-H_{\text{fin}}} \left( \mathcal{E}(U\mathcal{P}U^\dagger) - U\mathcal{P}U^\dagger \right) \right] \right) \right]$$

(B3)

with $\langle e^{H_{\text{fin}}} \rangle_0 = \langle \psi_0 | e^{H_{\text{fin}}} | \psi_0 \rangle$. Now, using again the computational basis (over which the observables $H = H_{\text{fin}} = H_{\text{fin}}$ and $\mathcal{P}$ are diagonal), we get

$$N_P \langle e^{H_{\text{fin}}} \rangle = \sum_{n,\alpha} e^{-H_{\text{fin}}} \left( \langle n | K_\alpha U \mathcal{P} U \mathcal{P} U^\dagger K_\alpha^\dagger | n \rangle - \langle n | U \mathcal{P} U^\dagger | n \rangle \right)$$

$$= \sum_{n,\alpha,m} e^{-H_{\text{fin}}} (\rho_0)_{mn} \left( (\langle n | K_\alpha U | m \rangle)^2 - (\langle n | U | m \rangle)^2 \right).$$

From these expressions we can appreciate that $N_{TPM}$ and $N_P$ encode the same information. In fact, they take into account the differences between the same diagonal and off-diagonal elements of the quantum states after the action of the perfect and imperfect/noisy gates (with different weights though).

B.2. Average gate fidelity

The average gate fidelity is defined as

$$\mathcal{F}(\mathcal{E} \circ \mathcal{U}, \mathcal{U}) \equiv \mathbb{E}_{\langle \psi \rangle} \left[ \langle \psi \rangle | U^\dagger \mathcal{E}(U|\psi\rangle \langle \psi | U^\dagger U | \psi \rangle \right]$$

(B4)

where

$$\tilde{\mathcal{F}} = \sum_{n_1,n_2} \sum_{m_1,m_2} \sum_{\ell_1,\ell_2} (\rho_0)_{n_1,n_2} (\rho_0)_{m_1,m_2} m_2 | U | m_1 \langle m_1 | K_\alpha U | \ell_1 \rangle \langle \ell_2 | K_\alpha^\dagger U^\dagger | m_2 \rangle \langle m_2 | U | n_2 \rangle.$$  

(B5)

B.3. Expressions of $\eta_{\text{EPM}}$ and $\eta_X$

The figure of merit, using the (full) EPM energy statistics, for the diagnostics of a quantum gate is

$$\eta_{\text{EPM}} = \mathbb{E}_{\langle \psi \rangle} \left[ \left( \langle e^{H_{\text{fin}}} \rangle_0 \text{Tr} \left[ e^{-H_{\text{fin}}} \left( \mathcal{E}(U|\psi\rangle \langle \psi | U^\dagger) - U|\psi\rangle \langle \psi | U^\dagger \right) \right] \right) \right]$$

(B6)

Thus, resorting to the computational basis (over which the observable $H = H_{\text{fin}} = H_{\text{fin}}$ is diagonal) as before, $N_{\text{EPM}}$ can be written as

$$N_{\text{EPM}} \langle e^{H_{\text{fin}}} \rangle \equiv \sum_{n,\alpha} e^{-H_{\text{fin}}} \left( (\langle n | K_\alpha U | \psi_0 \rangle)^2 - (\langle n | U | \psi_0 \rangle)^2 \right)$$

$$= \sum_{n,\alpha,m_1,m_2} e^{-H_{\text{fin}}} (\rho_0)_{mn} \left( (\langle n | K_\alpha U | m_1 \rangle)^2 (m_1 | U^\dagger K_\alpha^\dagger | n \rangle - (\langle n | U | m_1 \rangle (m_2 | U^\dagger | n \rangle \right).$$


Four real quantities
Six complex quantities

Now, by initializing the state in $\rho_0$, and $\langle \rho \rangle = \langle m | \psi_0 \rangle \langle \psi_0 | m \rangle$ and $\langle \rho \rangle = \sum_m \langle m | \psi_0 \rangle^2 e^{iH \alpha}$. For the coherence part of $\eta_{EPM}$, instead, one has

$$\eta_X = \mathbb{E}_{\psi_0} \left[ \langle \psi_0 | e^{iH \alpha} | \psi_0 \rangle \text{Tr} \left[ e^{-iH_{fin}} \left( \mathcal{E} (U_X U^T) - U_X U^T \right) \right] \right]$$

$$= \mathbb{E}_{\psi_0} \left[ \mathcal{R}_X \right],$$

where

$$\mathcal{R}_X = \sum_{n, \alpha} e^{-iH_n \alpha} \left( \langle n | K_{\alpha} U_X U^T K_{\alpha}^T | n \rangle - \langle n | U_X U^T | n \rangle \right)$$

$$= \sum_{n, \alpha, m \neq m_2} e^{-iH_n (\rho_0)} \langle m | K_{\alpha} U | m_1 \rangle \langle m_2 | U^T K_{\alpha}^T | n \rangle - \langle n | U | m_1 \rangle \langle m_2 | U^T | n \rangle.$$

**B.4. Average gate coherence fidelity**

The average gate coherence fidelity is formally expressed by

$$\mathcal{C} (\mathcal{E} \circ U, U) \equiv \mathbb{E}_{\psi_0} \left[ | C_{\ell_i} (\mathcal{E} \circ U) - C_{\ell_i} (U) | \right] = \mathbb{E}_{\psi_0} \left[ C \right],$$

where

$$C = \sum_{n \neq k, \alpha, m_1, m_2} \left( | \langle \rho_0 | m_1 | K_{\alpha} U | m_1 \rangle \langle m_2 | U^T K_{\alpha}^T | n \rangle | - | \langle \rho_0 | m_1 | K_{\alpha} U | m_1 \rangle \langle m_2 | U^T | n \rangle \right) \right].$$

Accordingly, in general, the similarities between $\eta_X$ and $\mathcal{C}$ described in the main text stem from the averaging over the initial pure states $\rho_0$, though the analytical expressions for $\eta_X$ and $\mathcal{C}$ (after the averaging) are not at our disposal. However, remarkable similarities in the behavior of the two figures of merit can be observed even at the single-state level. Such similarities have been used in the main text, for example, when comparing theoretical predictions with experimental data obtained by initializing the two-qubit gate in the $| + + \rangle$ state.

**Appendix C. Ways to determine experimentally the EPM-based figure of merit**

Let us focus on the case of two-qubit quantum gates and consider only the EPM final probabilities to measure the corresponding local energy terms

$$P_{fin}^{(\alpha)} = \text{Tr} \left[ \Pi_{fin}^0 V | \psi_0 \rangle \langle \psi_0 | V^T \right] = \langle \psi_0 | V^T \Pi_{fin}^0 V | \psi_0 \rangle.$$

We also have

$$G(| \psi_0 \rangle) = \langle \psi_0 | V^T e^{-iH_{fin}} V | \psi_0 \rangle = \sum_{\alpha} e^{-E_{\alpha}} \langle \psi_0 | V^T \Pi_{fin}^0 V | \psi_0 \rangle$$

that, for noisy unitary gates $V$ affected by coherent errors, is what should be determined experimentally. In this regard, let us expand the initial state in the computational basis $\{| i \rangle \} = \{| 00 \rangle, | 01 \rangle, | 10 \rangle, | 11 \rangle \}$. Then,

$$G(| \psi_0 \rangle) = \sum_{\alpha} e^{-E_{\alpha}} \sum_{ij} a_i a_j^* \langle j | V^T \Pi_{fin}^0 V | i \rangle.$$

Thus, we need all the different quantities $\langle j | V^T \Pi_{fin}^0 V | i \rangle$ if we want to be able to determine (by post-processing) the averaged estimator that we are interested in. These are $4 \times (4 + 6 \times 2) = 64$ terms, i.e. for each of the four energy eigenvalues $E_\alpha$ of the local, final Hamiltonian we have

- Four real quantities $\langle i | V^T \Pi_{fin}^0 V | i \rangle$
- Six complex quantities $\langle j | V^T \Pi_{fin}^0 V | i \rangle$ with $i \neq j$.

Now, by initializing the state in $| \psi_0 \rangle = | i \rangle$ we can recover the four real quantities which are just the final EPM probabilities. In order to recover the others we need other initial states, which we are going to discuss below.
C.1. ‘Straightforward’ initialization

A straightforward way is to initialize the two-qubit system in the 12 states $|\psi_0\rangle = (|i\rangle + |j\neq i\rangle)/\sqrt{2}$ and $|\psi_0\rangle = (|i\rangle + |j\neq i\rangle)/\sqrt{2}$. In fact, by doing so, the final EPM probabilities take the following forms

$$p^{(c)}_{fin} = \frac{1}{2} (|i\rangle V^t \Pi^0_{fin} V|i\rangle + |j\rangle V^t \Pi^0_{fin} V{j\rangle} + \Re\left[|i\rangle V^t \Pi^0_{fin} V{j\rangle}\right]$$

$$p^{(c)}_{fin} = \frac{1}{2} (|i\rangle V^t \Pi^0_{fin} V|i\rangle + |j\rangle V^t \Pi^0_{fin} V{j\rangle} + \Im\left[|i\rangle V^t \Pi^0_{fin} V{j\rangle}\right].$$

(C4)

This means that with a total of $4 \times 4 + 4 \times (6 \times 2) = 64$ projective local measurements we can get all the terms we need. However, note that the additional 12 states needed here are, in general, entangled, which could be a complication for an optical set-up like the one considered in the main text.

C.2. Working with separable input states

If instead we want to use separable states, then we could do as follow. Let us start from the 4 states

$$|\psi_0\rangle = \frac{1}{\sqrt{2}} (|aa\rangle + |ab\rangle), \quad \frac{1}{\sqrt{2}} (|aa\rangle + |ba\rangle)$$

(C5)

with $a, b \in \{0, 1\}$ and $a \neq b$, and correspondingly the four states

$$|\psi_0\rangle = \frac{1}{\sqrt{2}} (|aa\rangle - i|ab\rangle), \quad \frac{1}{\sqrt{2}} (|aa\rangle - i|ba\rangle),$$

(C6)

for a total of eight states providing us four complex quantities (among the six $|i\rangle V^t \Pi^0_{fin} V|i\rangle$ with $i \neq j$. With these initializations, the computation of the EPM final probabilities again gives us, apart from diagonal elements, the real and imaginary parts of 4 of the terms $|i\rangle V^t \Pi^0_{fin} V{j\rangle}$. Then, one can consider initializing the quantum system in the state $|++\rangle$ that, apart from the elements that we can extract from the previous states, would give the term

$$\frac{1}{2} \left(\Re\left[|00\rangle V^t \Pi^0_{fin} V|11\rangle\right] + \Re\left[|10\rangle V^t \Pi^0_{fin} V|01\rangle\right]\right).$$

(C7)

Now, to conclude, one could start from an entangled state [like $\frac{1}{2} (|00\rangle - |11\rangle + |10\rangle + |01\rangle)$ or $\frac{1}{2} (-|00\rangle + |11\rangle + |10\rangle + |01\rangle)$] to also get the difference of the real parts in (C7). This whole process would require $8 + 4 = 12$ initial states as before. In this regard, if we want to get rid also of the single Bell state that we need to achieve the difference of the real parts in equation (C7), we could initialize the system for example in the state $\frac{1}{2} (i|0\rangle + |1\rangle) \otimes (e^{i\theta}|0\rangle + |1\rangle)$, which is separable and provides us the difference of real parts for $\theta = \pi/2$.

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