

End-point measurement approach to assess quantum coherence in energy fluctuations

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We discuss the role of quantum coherence in the energy fluctuations of open quantum systems. To this aim, we introduce a protocol, to which we refer to as the end-point-measurement scheme, allowing to define the statistics of energy changes as a function of energy measurements performed only after the evolution of the initial state. At the price of an additional uncertainty on the initial energies, this approach prevents the loss of initial quantum coherences and enables the estimation of their effects on energy fluctuations. We demonstrate our findings by running an experiment on the IBM Quantum Experience superconducting qubit platform.

When the size of a physical system is scaled down to the micro-/nano-scopic domain, fluctuations of relevant quantities start playing a pivotal role in establishing the energetics of the system. Such fluctuations obey fundamental relations, known as *fluctuation theorems*, that recast the laws of thermodynamics in such a new regime. Should the range of energies involved in a given system bring its dynamics within the domain of quantum theory, the very nature of energy fluctuations become even more interesting as encompassing both classical (i.e. thermal) and quantum contributions. The characterization of the latter, and the understanding of how they conjure with the former to set the dynamics of fundamental energy transformations, are very stimulating open problems.

One of the key achievements of the field of thermodynamics of quantum processes [1–4] is the identification of a strategy for the assessment of the energetics stemming from non-equilibrium quantum dynamics. The so-called two-point measurement (TPM) protocol [5–8], where the energy is measured both at the initial and final time, has been introduced to determine the work statistics of a quantum system driven by a time-dependent protocol. However, in quantum mechanics, measurements condition the evolution of the measured system [9]. In particular, in TPM an energy measurement performed before the dynamics takes place destroys the quantum coherences in the initial state of the system, forcing it into an energy eigenstate [10, 11]. Such a loss of coherence is common to interferometric formulations of the TPM protocol, which have been put forward to ease the inference of the energetics of out-of-equilibrium systems [12–14].

Recently, much effort has been devoted to understand the role of coherence in quantum thermodynamics [15–25]. In particular in Refs. [15, 16, 20, 26] full counting statistics [27, 28] has been used to study work fluctuations in quantum systems initialized in an arbitrary state, pointing out that the quantum interference stemming from considering quantum coherences could lead to negative quasi-probability work distributions [29].

In this paper, we propose an *end-point-measurement* (EPM) protocol to quantify the statistics of energy-change fluctua-

tions in the (possible) presence of quantum coherence in the initial state of a system. The motivation for such protocol is two-fold: *i*) it is directly inspired from the typical quantum mechanical setup in which a state is prepared, then evolved, and only at the end measured; and *ii*) such a protocol removes the need for the first projective measurement required by TPM, thus preventing the collapse of the initial state of the system onto the energy basis. This is in contrast with recent proposals such as Ref. [25], where the system has to be prepared in a mixture of eigenstates of an observable O that does not commute with the Hamiltonian of the system. This is equivalent to an experiment measuring O at the initial time so that in each trajectory the starting point is an eigenstate of O . Our proposal is different from this and other TPM schemes, since we do not use any initial projective measurement and the initial state fully evolves according to its quantum dynamics. This is the typical situation encountered when considering the evolution of quantum systems, where the measurement is performed only at the final time – like during quantum computing algorithms. Thus, analyzing the differences and analogies between our scheme and other existing protocols helps in comparing the typical measurement procedures with those in quantum thermodynamics.

Remarkably, we are able to characterize the fluctuations of energy changes by distinguishing between contributions stemming from quantum coherences and those resulting from initial populations, albeit at the cost of a quantifiable extra uncertainty. These results offer the possibility to set coherence-induced quantum effects apart from those due to thermal fluctuations. Renouncing to the initial energy measurement on the system entails a substantive experimental simplification, thus making such approach an alternative to the TPM scheme when quantum signatures are considered. We demonstrate the effectiveness of EPM in pinpointing the role of initial coherences in the statistics of energy fluctuations by performing a series of experiments using the IBM Quantum Experience (IBMQ) platform. This highlights the applicability of our scheme for the characterization of the energetics of quantum computation, a topic which is receiving growing attention in recent years [30–33].

Coherence in the energy eigenbasis.— Let us consider a d -dimensional quantum system \mathcal{S} evolving according to a one-parameter family of completely-positive and trace-preserving (CPTP) maps $\Phi_t : \rho_i \rightarrow \rho_f = \Phi_t[\rho_i]$ [34] within the time interval $[t_i, t_f]$. Here, ρ_i (ρ_f) is the initial (final) density operator of the system. Our derivation can be specialized to the case of closed systems with time-dependent Hamiltonian, where energy fluctuations identify as work, or to open time-independent ones where only heat-transfer occurs.

Let us thus consider a system \mathcal{S} subject to *no* initial projective measurement and characterize energy fluctuations only through a final-time measurement. The only energy measurement of our protocol is performed at the final time t_f . This generates the trajectories $\mathcal{T}_i^k : \rho_i \rightarrow \Pi_f^k$ with $\Pi_f^k \equiv |E_f^k\rangle\langle E_f^k|$ denoting the projector onto the k -th energy eigenstates $|E_f^k\rangle$ of the Hamiltonian at time t_f , i.e., $H(t_f) = \sum_k E_f^k \Pi_f^k$. The stochasticity of the outcomes provided by the EPM protocol, with respect to the initial energies that \mathcal{S} would have if the energy had been measured, makes $\Delta E \equiv E_f - E_i$ a random variable.

Dynamically, the initial quantum coherence in the state of \mathcal{S} , written in the energy basis, is accounted for by considering the probability distribution of the final energy due to the evolved initial state ρ_i , comprising its coherence. By fixing the energy of \mathcal{S} at t_f , there is a probability law weighting the trajectories \mathcal{T}_i^k , which can be arranged in N groups corresponding to the number of possible energy values at t_i . This is a classical law, interpreted as the uncertainty on the values of E_i , and thus ΔE . By performing energy measurements at the final time t_f , one can embed the effects of initial coherences into single realizations of the evolution. The uncertainty on E_i reflects the fact that its values are obtained as if we were performing a *virtual* projective measurements, thus without any state collapse. This entails independence of the measurements at t_f with respect to the initial virtual one.

Suppose the initial state ρ_i is not diagonal in the energy basis of \mathcal{S} : One can object that there is an observable O on whose basis ρ_i is diagonal. However, there is an expected difference between the cases where *a*) a measurement of O is done at time t_i , then one starts each trajectory from an eigenstate of O and averages a posteriori over all possible results of the first measurement [25], and *b*) no measurement is implemented and the dynamics can show interference in the energy basis. Such difference will be quantified later.

If the energy is not measured at t_i , how can we talk about the initial energies E_i ? Such information, and the related thermodynamic cost, is encoded in ρ_i , which is such that, if we decide to measure the energy, we would find the initial energies E_i . One could prepare ρ_i a large number of times, and in a fraction of them measure energy to verify that the eigenvalues E_i^{ℓ} 's of the Hamiltonian at $t = t_i$, i.e., $H(t_i) = \sum_{\ell} E_i^{\ell} \Pi_i^{\ell}$, are obtained with the probability assigned by ρ_i [cf. Fig. 1]. At the remaining times one uses ρ_i as input for our protocol *without* measuring energy at t_i .

Energy-change distribution and link with fluctuation relations.— Let us assume a time-dependent Hamiltonian

process and define the probability distribution associated to ΔE by analyzing its properties. At the single-trajectory level, the density operator after the end-point energy measurement is one of the eigenstates Π_f^k of the time-dependent Hamiltonian $H(t_f)$. Such state is achieved with probability

$$p_f^k \equiv \text{Tr}(\rho_f \Pi_f^k) = \text{Tr}(\Phi_{t_f}[\rho_i] \Pi_f^k). \quad (1)$$

Thus, given the change $\Delta E^{k,\ell} \equiv E_f^k - E_i^{\ell}$ in terms of the eigenvalues of $H(t)$, the probability distribution of ΔE is

$$P_{\text{coh}}(\Delta E) = \sum_k p_f^k \sum_{\ell} p_i^{\ell} \delta(\Delta E - \Delta E^{k,\ell}), \quad (2)$$

where $p_i^{\ell} \equiv p(E_i^{\ell}) = \text{Tr}(\rho_i \Pi_i^{\ell})$ is the probability of obtaining E_i^{ℓ} if an energy measurement was performed on \mathcal{S} (initial virtual measurement). In Eq. (2), the suffix "coh" stands for "coherence". The joint probability $p(E_i^{\ell}, E_f^k)$ associated to the stochastic variable $\Delta E^{k,\ell}$, such that $P_{\text{coh}}(\Delta E) = \sum_{\ell,k} p(E_i^{\ell}, E_f^k) \delta(\Delta E - \Delta E^{k,\ell})$, can then be written as

$$p(E_i^{\ell}, E_f^k) = p_i^{\ell} p_f^k = \text{Tr}(\rho_i \Pi_i^{\ell}) \text{Tr}(\Phi_{t_f}[\rho_i] \Pi_f^k) \equiv p_{\text{coh}}^{\ell,k}. \quad (3)$$

As already noticed, the assumption behind Eq. (3) is the statistical independence of the final energy projective measurements and initial virtual one. This comes from the fact that the initial measurement is not performed and only the statistics related to the initial state preparation is used. The following properties hold:

Property (i) $P_{\text{coh}}(\Delta E)$ is such that $\sum_{k,\ell} p_{\text{coh}}^{\ell,k} = 1$.

Property (ii) The average energy variation $\langle \Delta E \rangle_{P_{\text{coh}}} \equiv \int d\Delta E P_{\text{coh}}(\Delta E) \Delta E$ reproduces the average energy change induced by the CPTP map Φ_t , that is

$$\langle \Delta E \rangle = \text{Tr}(H(t_f) \rho_f) - \text{Tr}(H(t_i) \rho_i), \quad (4)$$

where we have assumed statistical independence between virtual initial energy measurements and final ones [35].

Property (iii) $P_{\text{coh}}(\Delta E)$ does not reduce to the TPM probability distribution for $[\rho_i, H(0)] = 0$, i.e., it cannot result from a fluctuation theorem (FT) protocol in the sense of Ref. [19].

Even by replacing the initial state ρ_i in Eq. (2) with a state diagonal in the (initial) energy basis, it is not possible to recover the conventional energy-change statistics resulting from the TPM protocol. The latter is recovered only when the initial state is an energy eigenstate (cf. the Supplementary Material (SM) accompanying this paper [36]). For an initial state diagonal in the energy eigenbasis, the discrepancy between the TPM and EPM joint probabilities is due to classical uncertainty on the initial state of \mathcal{S} , which is retained in our scheme but is lost in TPM due to the initial energy measurement. As shown in Ref. [36], this agrees with the no-go theorem in Ref. [37]. For the same reasons, besides a few exceptions, the distribution $P_{\text{coh}}(\Delta E)$ may *not* be convex under a linear mixture of protocols that only differ by the initial density operator ρ_i [36]. Therefore, given $\rho_i = \zeta \rho_{i,1} + (1-\zeta) \rho_{i,2}$ with $\zeta \in [0, 1]$, $P_{\text{coh}}(\Delta E | \rho_i)$ cannot in general be expressed

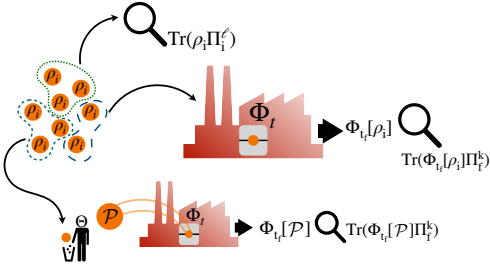


FIG. 1. Protocol for the quantification of energy fluctuations and the extraction of information about coherence. An ensemble of identical systems, prepared in the initial state ρ_i , is divided in three subgroups. One is used to obtain $p_i^\ell = \text{Tr}(\rho_i \Pi_f^\ell)$ via an initial energy measurement. The second goes through a dephasing channel, returning a state \mathcal{P} diagonal in the energy basis. This then undergoes map Φ_{t_f} and is used to determine $p_i^k = \text{Tr}(\Phi_{t_f}[\mathcal{P}] \Pi_f^k)$. The systems in the third subgroup are not initially measured but subjected to the dynamics and used to obtain $p_i^k = \text{Tr}(\Phi_{t_f}[\rho_i] \Pi_f^k)$.

as a linear composition of the distributions $P_{\text{coh}}(\Delta E|\rho_{i,1})$ and $P_{\text{coh}}(\Delta E|\rho_{i,2})$.

In order to pinpoint the effect of coherence in the energy basis of ρ_i and separate it from classical uncertainty, we take $\rho_i = \mathcal{P} + \chi$ with \mathcal{P} diagonal in the energy basis and χ encoding the coherence contributions ($\text{Tr}(\chi) = 0$). Then $p_{\text{coh}}^{\ell,k}$ in Eq. (3) can be split as $p_{\text{coh}}^{\ell,k} = p_i^\ell p_i^k \equiv p_i^\ell p_{\mathcal{P}}^k + p_i^\ell p_\chi^k$ with

$$p_i^k \equiv p_{\mathcal{P}}^k + p_\chi^k = \text{Tr}(\Phi_{t_f}[\mathcal{P}] \Pi_f^k) + \text{Tr}(\Phi_{t_f}[\chi] \Pi_f^k). \quad (5)$$

The term $p_i^\ell p_{\mathcal{P}}^k$ encodes information on classical uncertainty on the initial system populations, while $p_i^\ell p_\chi^k$ takes into account the effects of initial coherence. We introduce $p_{\text{coh}}^{\mathcal{P}} \equiv p_i^\ell p_{\mathcal{P}}^k$ and, owing to the statistical independence of outcomes $\{E_i^\ell\}$ and $\{E_f^k\}$, such terms can be separately analyzed. In particular, the term containing information on the initial coherence can be determined as illustrated in Fig. 1.

Note that the absence of initial coherences makes the EPM distribution equal to the product of the marginals of the TPM distribution [38]. We thus have $\mathcal{H}(p_{\text{TPM}}) \leq \mathcal{H}(p_{\text{coh}}|_{\chi=0})$, where $\mathcal{H}(p)$ is the Shannon entropy of a generic distribution p . This inequality follows from the positivity of mutual information. However, the same result is not true in general if initial coherence is present (cf. the case study of a three-level thermal engine in Ref. [36]).

We now address the differences with the protocol in Ref. [25] – which we label MLL – to study the effects of coherence. In MLL, an initial state decomposed in terms of its eigenstates $\{|s\rangle\}$ as $\rho_i = \sum_s p^s |s\rangle\langle s|$, is associated with the joint probability $p_{\text{MLL}}^{\ell,k} \equiv \sum_s p^s |\langle s|E_i^\ell\rangle|^2 \text{Tr}(\Phi_{t_f}[|s\rangle\langle s|] \Pi_f^k)$. This reduces to the joint probability of the TPM protocol for ρ_i diagonal in the energy basis, and to the distribution $p_{\text{coh}}^{\ell,k}$ of our protocol for initial pure states. However, for a generic initial state, such correspondences are lost and MLL requires ρ_i to be one of its eigenstates, as the construction of $p_{\text{MLL}}^{\ell,k}$ requires to know the evolution of each component of ρ_i . The

EPM protocol thus requires less information on the dynamics at the cost of extra uncertainty on the statistics of ΔE (cf. Ref. [36] for a comparison between EPM, MLL and TPM).

Linear response approximation.– We now further characterize the distribution of energy changes and address its 1st and 2nd statistical moments. As with MLL, Eq. (4) recovers the expected difference of the averaged initial and final Hamiltonian. This is true in the TPM scheme only when the initial state is the mixture resulting from the first energy measurement. From Eq. (2) one gets

$$\begin{aligned} \langle \Delta E^2 \rangle &= \langle \Delta E^2 \rangle_{\mathcal{P}} + \text{Tr}(H^2(t_f) \Phi_{t_f}[\chi]) \\ &\quad - 2 \text{Tr}(\Phi_{t_f}[\chi] H(t_f)) \text{Tr}(\mathcal{P} H(t_i)), \end{aligned} \quad (6)$$

with $\langle \Delta E^2 \rangle_{\mathcal{P}}$ given by assuming $\rho_i \rightarrow \mathcal{P}$. Note that Eq. 6 coincides with the result of MLL (TPM) only if the initial state is pure (an eigenstate of $H(t_i)$). Moreover, if \mathcal{P} is a projector, then $\langle \Delta E^2 \rangle_{\mathcal{P}} = \langle \Delta E^2 \rangle_{\text{TPM}}$ and all the differences in the 2nd moments are due to coherences in ρ_i . The latter are unavoidably destroyed in the TPM protocol.

Characteristic function and physical meaning.– The information about the statistics of the energy-change distribution is encoded in the characteristic function $\mathcal{G}(u) \equiv \langle e^{iu\Delta E} \rangle_{P_{\text{coh}}} = \int d\Delta E e^{iu\Delta E} P_{\text{coh}}(\Delta E)$ corresponding to the distribution $P_{\text{coh}}(\Delta E)$. As the outcomes $\{E_f^{(k)}\}$ of the final energy measurement are statistically independent from the initial virtual ones $\{E_i^{(\ell)}\}$, we have

$$\mathcal{G}(u) = \text{Tr}(e^{-iuH(t_i)} \rho_i) \text{Tr}(e^{iuH(t_f)} \Phi_{t_f}[\rho_i]), \quad (7)$$

showing that the fluctuations of ΔE originate both from the action of map $\Phi_{t_f}[\rho]$ on the initial state of \mathcal{S} and the uncertainty in its energy at $t = t_i$. We now highlight the deviation of the EPM-inferred statistics from a standard FT [6, 7]. We consider $\mathcal{G}(i\beta)$, where β is a *reference* inverse temperature (taken as a free parameter), and introduce the reference equilibrium states $\rho_{i(f)}^{\text{th}} \equiv e^{-\beta H(t_i(f))} / Z_{i(f)}$ with $Z_{i(f)} \equiv \text{Tr}(e^{-\beta H(t_i(f))})$. For $\rho_i = \rho_i^{\text{th}} + \chi$ we get

$$\langle e^{-\beta(\Delta E - \Delta F)} \rangle = d [\text{Tr}(\rho_f^{\text{th}} \Phi_{t_f}[\rho_i^{\text{th}}]) + \text{Tr}(\rho_f^{\text{th}} \Phi_{t_f}[\chi])], \quad (8)$$

with ΔF the free energy difference and d the dimension of the Hilbert space of \mathcal{S} (cf. Ref. [36] for details). Eq. (8) deviates from unity, i.e. from a standard fluctuation theorem, even for unital channels and due to two terms. The first, $d \text{Tr}(\rho_f^{\text{th}} \Phi_{t_f}[\rho_i^{\text{th}}])$, is the additional uncertainty introduced by not performing the initial energy measurement and is present even for $\chi = 0$. The second quantifies the deviation due to initial quantum coherences and bridges stochastic thermodynamics and quantum signatures of open dynamics. Eq. (8) is thus one of the main results of this paper.

Experimental Results.– To illustrate experimentally the power and versatility of EPM, we make use of the IBMQ platform. In particular, we perform a series of experiments based on the use of a two-qubit gate, by following the protocol illustrated in Fig. 1 for the extraction of initial coherence contributions.

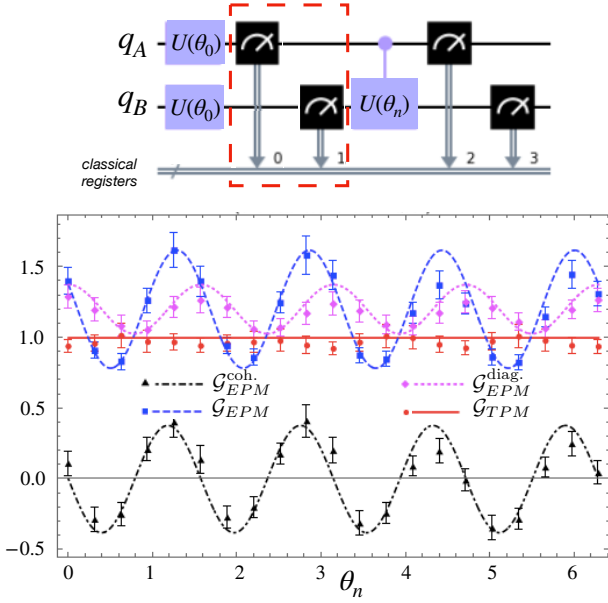


FIG. 2. **Top:** Circuits implemented in IBMQ. The initial state is prepared by applying two identical single-qubit gates $U(\theta_0)$ onto $|00\rangle$ (we use $\theta_0 = 2$ [36]). In TPM, two initial projective measurements destroy any coherence in the computational basis, while in EPM such measurements (enclosed in the dashed red box) are absent. We then implement the controlled gate $U(\theta_n)$, with $\theta_n \equiv n\pi/10$ and $n = 0, \dots, 20$, followed by two projective measurements in the computational basis. The results are stored in four classical registers to allow the analysis of the energy change statistics. **Bottom:** Comparison of the characteristic functions for EPM and TPM. The lines show the theoretical predictions, while the points (with their error bars) the experimental results. Each data point has been obtained from 2048 experimental runs. The solid red line and circles are related to the results obtained by applying TPM. The dashed blue line and squared refer to the EPM characteristic function. Finally, the dotted magenta line and rhombuses (dot-dashed black line and triangles) show the contribution of the diagonal (off-diagonal) parts of the initial state ρ_i in the computational basis. The inverse (physical) temperature of the diagonal part of the initial state is $\beta = 0.443/\epsilon$ where $\epsilon \sim 5$ MHz is the energy gap for the superconducting qubits, as provided by the IBMQ documentation.

On the IBMQ quantum computer, we implement a two-qubit circuit with initial (pure) separable state $\rho_i = \rho_i^{\text{th}} + \chi$, where $\rho_i^{\text{th}} = e^{-\beta(H_A + H_B)}/Z$ (with $Z = \text{tr}[\rho_i^{\text{th}}]$ and inverse temperature β) is a thermal state of the local Hamiltonian $H_A + H_B = \epsilon(\sigma_z^{(A)} + \sigma_z^{(B)})$ of the two qubits ($\epsilon \sim 5$ MHz is the energy gap between the logical states of each superconducting qubit). Here, ρ_i^{th} is diagonal in the computational basis, while χ stands for the initial coherence in this basis. Such initial state can be easily prepared starting from the default configuration of the logical qubit of the IBMQ device by way of properly designed single-qubit gates (cf. Fig. 2 and Ref. [36]).

The top panel of Fig. 2 shows the circuit implemented in the IBMQ. After the initialization, the circuit performs a controlled gate. The difference between EPM and TPM is in the

absence of the first two projective measurements (red box in the figure) for the former. Then, we repeat the experiments by varying one of the parameters of the controlled gate. It is worth noticing that, while an “effective” Hamiltonian of the circuit could be obtained by reverse engineering the implemented unitary evolution, the IBMQ does not enable to directly measure it, as only local measurements of σ_z (and, thus, of the qubits local energies) are allowed. Thus, in analogy with the experiment in Ref. [39], just the statistics of the local energy fluctuations are taken into account.

In the bottom panel of Fig. 2, we consider the deviation of $\langle e^{-\beta(\Delta E - \Delta F)} \rangle$ from unity when using the EPM protocol. In the considered case, the free energy variation vanishes. Thus, we are comparing the characteristic functions, evaluated at $u = i\beta$, of EPM and TPM. The Jarzynski identity $\mathcal{G}_{\text{TPM}}(i\beta) = 1$, stemming from TPM, is nicely recovered from the experimental data. This is compared to the contributions in Eq. (8) linked to the diagonal and off-diagonal parts of the initial state. For the case investigated here, we observe a non-negligible contribution from the initial coherence χ of ρ_i , and a clear discrepancy between the TPM result and the contribution to the EPM characteristic function depending on the (thermal) diagonal part ρ_i^{th} of ρ_i . As stressed above, such a discrepancy originates from the additional uncertainty on the initial energies introduced by our protocol. Moreover, the statistics of energy changes in Fig. 2 can be reproduced to a good approximation by looking at just the firsts two moments of the EPM (or TPM) distribution [36]. Therefore, an analysis in linear approximation is able to capture the main features of the energy fluctuations that pertain to the quantum circuits under scrutiny.

Conclusions.— We have introduced an EPM protocol for the evaluation of the energy-change fluctuations that takes into account the presence of quantum coherence in the initial state of the system. The protocol does not require information on the dynamics nor special preparations, which casts it apart from other schemes [25, 40, 41], and solely relies on the final energy measurement. The EPM approach could be more conducive of experimental validation than the notoriously challenging TPM one, and could thus enlarge the range of systems whose energy fluctuations could be tested. For instance, quantum computing platforms present a natural arena in which the methods developed in this work could find fruitful applications, as showcased by our analysis of the IBMQ two-qubit logic circuit. Indeed, the EPM approach not only allows to account for the effect of the initial coherence but also resemble the way in which quantum computing algorithms are actually performed, where only a final measurement is present. Furthermore, the EPM approach may also come in handy for systems with degenerate energy levels, as in many-body physics. Indeed, for initial states involving only levels within degenerate subspaces and a dynamics that leaves the latter invariant, the TPM scheme would return vanishing energy fluctuations. In contrast, our EPM would allow for the characterization of the energy change statistics resulting from the initial

coherence alone.

Acknowledgments.— The authors gratefully acknowledge L. Buffoni, N. Fabbri, S. Hernández-Gómez, G.T. Landi, M. Lostaglio, S. Martina and F. Poggiali for fruitful discussions and comments. This work was supported by MISTI Global Seed Funds MIT-FVG Collaboration Grant "NV centers for the test of the Quantum Jarzynski Equality (NVQJE)", H2020-FETOPEN-2018-2020 project PATHOS (grant nr. 828946), UNIFI grant Q-CODYCES, the MSCA IF project pERFEcTO (grant nr. 795782), the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) project number BR 5221/4-1, the H2020-FETOPEN-2018-2020 project TEQ (grant nr. 766900), the DfE-SFI Investigator Programme (grant 15/IA/2864), COST Action CA15220, the Royal Society Wolfson Research Fellowship (RSWF\R3\183013), the Royal Society International Exchanges Programme (IEC\R2\192220), the Leverhulme Trust Research Project Grant (grant nr. RGP-2018-266), the UK EPSRC (grant nr. EP/T028106/1), and the CNR/RS (London) project "Testing fundamental theories with ultracold atoms". We acknowledge the use of IBM Quantum services for this work. The views expressed are those of the authors, and do not reflect the official policy or position of IBM or the IBM Quantum team.

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