Kirkwood-Dirac quasiprobability approach to quantum fluctuations: Theoretical and experimental perspectives

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Recent work has revealed the central role played by the Kirkwood-Dirac quasiprobability (KDQ) as a tool to encapsulate non-classical features in the context of condensed matter physics (scrambling, dynamical phase transitions) metrology (standard and post-selected), thermodynamics (power output and fluctuation theorems), foundations (contextuality, anomalous weak values) and more. Given the growing relevance of the KDQ across the quantum sciences, the aim of this work is two-fold: first, we clarify the role played by quasiprobabilities in characterising dynamical fluctuations in the presence of measurement incompatibility, and highlight how the KDQ naturally underpins and unifies quantum correlators, quantum currents, Loschmidt echoes and weak values; second, we discuss several schemes to access the KDQ and its non-classicality features, and assess their experimental feasibility in NMR and solid-state platforms. Finally, we analyze the possibility of a ‘thermodynamics with quasiprobabilities’ in the light of recent no-go theorems limiting traditional treatments.

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I. INTRODUCTION

The existence of incompatible physical observables is one of the features that better casts quantum physics apart from classical mechanics. In fact, incompatible observables are at the basis of Heisenberg’s uncertainty relations [1, 2]; they imply information-disturbance trade-offs of quantum measurements [3] and lead to the impossibility of describing quantum processes in purely classical terms.

The incompatibility of physical observables also limits our ability to associate to them joint probability distributions. A well-known example is represented by the formulation of the quantum mechanics of continuous variable systems in phase-space [4–8]. Classically, the state of a physical system can be represented by a joint probability distribution over its phase-space. Instead, a quantum state can be represented in phase-space by means of the Wigner distribution [4, 6]. Due to the complementarity of the position and momentum operators, the Wigner distribution satisfies all but one of Kolmogorov’s axioms of probability theory. It is a real, normalized distribution, but in general it is not positive semi-definite. This is known as a quasiprobability. In fact, because of the ordering ambiguities arising from the non-commutativity of quantum operators, infinitely many alternative quasiprobabilities exist [9].

Less known than the Wigner function(s), whilst as ubiquitous as them, is the quasiprobability introduced independently by Kirkwood [10] and Dirac [11] in the 30’s, which goes under the name of Kirkwood-Dirac quasiprobability (KDQ). Originally formulated as a representation of the quantum state, the KDQ is a joint probability distribution for incompatible observables. As the Wigner function, the KDQ violates one of Kolmogorov axioms, since it can assume negative and complex values. Better suited for discrete quantum systems without a proper analogue of position and momentum operators, the KDQ has been an object of intense investigation together with its real part, the so-called Margenau-Hill quasiprobability (MHQ) [12–20].

It has been shown that negative or non-real values of the KDQ (and of the MHQ) are proofs of strong non-classicality in the form of contextuality [18]. They also provide quantifiable measures of non-classicality beyond non-commutativity [20, 21]. In fact, the mutual non-commutativity of the quantum observables and the state entering the definition of the KDQ is not a sufficient condition for the emergence of non-classicality [20]. Non-real values of the KDQ can be connected to measurement disturbances [22–25] and to the enhanced power output of a quantum engine [26], while negative values herald advantages in quantum metrological setups [27, 28]. The MHQ and its negative values have been investigated in the remits of quantum thermodynamics [14, 15, 19], showing that it is a plausible quasiprobability distribution for extending the fluctuation theorems to the full quantum regime. Moreover, it can also relate violations of certain heat-flow bounds between two baths with locally-thermal states to negativity and thus non-classicality [19].

In this paper, we aim to show that the KDQ provides a salient means of characterizing fluctuations in the quantum realm, ranging from condensed matter to quantum statistical mechanics and thermodynamics. In section II, we set the stage by formulating a no-go theorem on fluctuations in quantum mechanics. The theorem formally shows that quasiprobabilities are essentially forced upon us if we wish to associate a joint distribution with the correct marginals to incompatible observables. Differently from several existing no-go theorems [29, 30] for quantum systems, the theorem does not require any assumption involving the classical limit or the thermodynamics of the systems. The reader mostly interested in the KDQ can skip ahead.

Next, we focus on the KDQ and MHQ distributions. In section III, we introduce a theorem for the non-existence of fully classical coherence and highlight that the KDQ is widespread across the quantum sciences and directly related to quantities of physical interest, albeit till recently often overlooked. We address in turn the role that the KDQ plays in the linear response theory [31–33], quantum currents [34], the Loschmidt echo and dynamical phase transitions [35, 36], weak values and weak measurements [37, 38]. The list does not include applications part of the recent revival of the KDQ: quantum metrology [26–28] out-of-time-ordered correlators and information scrambling in many-body systems [16, 39].

Despite the breadth of the applications, much less focus has been put onto schemes for measuring the KDQ. In section IV we describe several protocols, each with its own advantages and drawbacks. In particular, we describe: (a) a weak-two-point-measurements protocol, drawn from [13], that rests on a combination of projective and non-selective measurements; (b) interferometric schemes, already applied in other contexts [40–43], that can be run without modification to reconstruct the characteristic function of the KDQ distribution; (c) cloning schemes [44] and block-encoding protocols [45] for the inference of the KDQs; and (d) direct reconstruction approaches [46–52]. All such protocols are described in an operational way, to make direct contact with current and future possible experimental implementations. While these schemes all appeared in the literature before, here we stress their role in reconstructing the KDQ distribution.

Section V is devoted to direct tests of the non-classicality entailed by non-real and non-positive values of KDQs, which do not require the full reconstruction of the distribution. We discuss how partial information about the characteristic function can be used as a witness of non-classicality; we introduce a novel interferometric scheme for a test of non-classicality based on the Ham-
bürger problem; and we outline a SWAP test for testing non-classicality.

In section VI we discuss experimental implementations of the schemes discussed in section IV and, in particular, we advance a proposal to realize, with nitrogen-vacancy (NV) centers in diamond at room temperature, the interferometric scheme aimed both at the reconstruction of the KDQ and the test of non-classicality.

Finally, section VII tackles the applications of the KDQ in the remits of quantum thermodynamic fluctuations. In doing this, we specialize some of the results obtained in the previous sections to the case of energy fluctuations in quantum systems and processes, and show how the KDQ can be used for quantum thermodynamics considerations beyond the standard fluctuation theorems and two-point measurement protocol.

We conclude the paper in section VIII with an outlook of our results, and the impact they have on both future theoretical investigations and experimental implementations on current quantum technologies platforms.

II. A NO-GO THEOREM ON THE CHARACTERIZATION OF FLUCTUATIONS IN QUANTUM THEORY

It is general wisdom that one cannot define joint probabilities for the measurement outcomes of non-commuting observables (such as position and momentum) due to measurement disturbance. In fact, this statement is not entirely correct and simple counterexamples can be constructed [53]. However, the obstacle posed by non-commutativity can be presented in the form of a precise no-go theorem. Consider a process represented by a channel $\mathcal{E}$ acting on the quantum state $\rho$. Let $A(0) = \sum_i a_i(0)\Pi_i(0)$ and $B(t) = \sum_f b_f(t)\Xi_f(t)$ be the observables, written in terms of their spectral decomposition, whose fluctuations we are interested in ($\Pi$ and $\Xi$ are projection operators). Then,

**Theorem 1 (No-go).** Whenever $[\Pi_i(0), \mathcal{E}^\dagger(\Xi_f(t))] \neq 0$ for some $i, f$ (non-commutativity), there exists no joint distribution $p_{i,f}(\rho)$ satisfying the following properties:

1. $p_{i,f}$ has the correct marginals:

   $$\sum_f p_{i,f}(\rho) = \text{Tr} (\Pi_i(0)\rho),$$  
   $$\sum_i p_{i,f}(\rho) = \text{Tr} (\Xi_f(t)\mathcal{E}(\rho)).$$

2. $p_{i,f}(\rho)$ is convex-linear in $\rho$. That is, if $\rho = \sum_k p_k \rho_k$, then $p_{i,f}(\rho) = \sum_k p_k p_{i,f}(\rho_k)$.

The proof, which makes use of Proposition 1 in Ref. [54], is presented in Appendix A. In section VII we will discuss the implications of this no-go theorem on out-of-equilibrium quantum thermodynamics. Here, it sets the stage for quasiprobabilities. In fact, the no-go theorem can be circumvented in three ways:

Drop assumption (1). One can define a joint distribution describing the fluctuations of a different (disturbed) process. The first measurement, over some approximation of $A(0)$, will induce a corresponding disturbance to the outcome statistics of $B(t)$. One can thus look for optimal schemes in terms of information-disturbance trade-offs [54–57]. These are trade-offs between how precisely we access $A(0)$ and how much we disturb the subsequent measurement of $B(t)$.

Drop assumption (2). That is, $p_{i,f}(\rho)$ has to be non-linear in $\rho$. Linearity in $\rho$ immediately follows from standard propagation of probabilities. Suppose one prepares either $\rho_H$ or $\rho_T$ depending on the outcome of a fair coin toss. The overall fluctuations $p_{i,f}(\rho_H)$ associated to the $\rho_H$ preparation and the fluctuations $p_{i,f}(\rho_T)$ associated to the preparation of $\rho_T$ – ought to satisfy $p_{i,f}(\rho) = \frac{1}{2}p_{i,f}(\rho_H) + \frac{1}{2}p_{i,f}(\rho_T)$. A violation of this condition occurs due to an nonlinear dependence of $p_{i,f}(\rho)$ on the initial state $\rho$. This can happen because the measurement scheme defining $p_{i,f}(\rho)$ depends on $\rho$ [58, 59] or $p_{i,f}(\rho)$ has an explicit dependence on a given decomposition of the density operator into pure states [60]. It also occurs when the definition implicitly employs (incompatible) measurements on multiple copies of $\rho$ [53, 61], e.g.,

$$p_{i,f}(\rho) = \text{Tr} (\Pi_i(0)\rho) \text{Tr} (\Xi_f(t)\mathcal{E}(\rho)).$$

See Refs. [62–64] for further discussion.

Drop $p_{i,f}(\rho) \in \mathbb{R}^+$ (keeping $\sum_{i,f} p_{i,f}(\rho) = 1$). This leads to the concept of quasiprobability, which has a long history going back to the phase-space representations of quantum mechanics by Wigner, Kirkwood, Dirac [10, 11, 53, 65], and finds modern applications in the context of quantum optics, quantum foundations, quantum information science and quantum computing [66–68].

Our no-go theorem helps classifying different proposals to the definition of fluctuations in the quantum regime. With so many definitions at our disposal, the challenge is to analyse in detail a framework and prove that it bears fruits in the theoretical and experimental study of fluctuations in the quantum regime. Here, we focus on the quasiprobability approach, and specifically on the Kirkwood-Dirac quasiprobabilities. This choice is due to their numerous applications across the quantum sciences and their clear relation to fundamental questions in statistical mechanics and condensed matter physics, as we are going to clarify in the next section.

III. THE PHYSICS BEHIND THE KIRKWOOD-DIRAC QUASIPROBABILITY

The following considerations aim to provide supporting evidence for the use of the Kirkwood-Dirac quasiprobability (KDQ) as a central object in the study of quantum
fluctuations. We do not wish to make here any ‘uniqueness’ argument since, as it is well-known, the existence of alternative quasiprobabilities is directly related to the ordering ambiguities of quantum mechanics [53, 69, 70]. Rather, we will show how the KDQ brings forth a rich structure that is often left implicit in statistical mechanics and condensed matter physics considerations.

Given the two observables \(A(0)\) and \(B(t)\) introduced in section II, the KD quasiprobability encodes the information on their correlations under the process \(\mathcal{E}\), which occurs in the time interval \([0, t]\). It is thus defined as

\[
q_{ij}(\rho) = \text{Tr} \left( \mathcal{E}^\dagger(\Xi_f(t)) \Pi_i(0) \rho \right),
\]

where \(\mathcal{E}\) is the adjoint* of \(\mathcal{E}\), \(\rho\) is the initial quantum state, and the pair \((i, f)\) labels the eigenvalues of the observables at the initial and final time. The KDQ describes the correlation function between an event at one time \(t = 0\), associated to the projector \(\Pi_i(0)\), and an event at time \(t\), associated to the projector \(\Xi_f(t)\). Negative or complex values of the KDQ can be taken to witness non-classicality [20]. The real part of the KDQ is defined as the Margenau-Hill quasiprobability (MHQ). For the non-classicality [20]. The real part of the KDQ is defined as the Margenau-Hill quasiprobability (MHQ). For the non-classicality [20]. The real part of the KDQ is defined as the Margenau-Hill quasiprobability (MHQ). For the non-classicality [20].

The KDQ satisfies properties (a)-(b) of Theorem 1. Effective near-commutativity of \(\rho\), \(\Pi_i\) and \(\mathcal{E}^\dagger(\Xi_f)\) are mutually commuting, then Eq. (4) reduces to

\[
p_{ij}^{\text{TPM}}(\rho) = \text{Tr} \left( \mathcal{E} (\Pi_i(0)\rho\Pi_i(0)) \Xi_f(t) \right).
\]

The right-hand-side of Eq. (5) is the joint probability of outcomes at \((i, f)\) in a sequential projective measurement of \(A(0)\) followed by the dynamics \(\mathcal{E}\) and the final measurement of \(B(t)\). This is the joint statistics of the so-called two-point-measurement (TPM) scheme [71]. Hence, negative/complex values disappear and a stochastic interpretation is possible.

Effective near-commutativity of \(\rho\), \(\Pi_i\) and \(\mathcal{E}^\dagger(\Xi_f)\) can be achieved both by coarse-graining of the measurement operators [19, 72] and by decoherence that makes the initial state approximately commuting with the initial measurement operator. However, note that there are instances for which \(q_{ij} \in [0, 1]\) despite the presence of non-commutativity [20]. This means that non-classicality of the KDQ is stronger than non-commutativity. Nonetheless, there is a close quantifiable relation between non-classicality, as witnessed by the negativity of the MHQ, and non-commutativity, at least for unitary quantum processes. In fact, the following result can be proven:

**Theorem 2** (Non-existence of fully classical coherence).

*Given an arbitrary unitary quantum process with unitary operator \(U\), an initial state \(\rho\) and an observable \(A\) such that \([\rho, A] \neq 0\), it is always possible to find an observable \(B\), with \([B, A] \neq 0\), such that \(\text{Re}(q_{ij}) < 0\) for some \((i, f)\).*

Theorem 2 states that the quantum coherence of an initial state \(\rho\), with respect to a given observable \(A\) at \(t = 0\), can always give rise to negativity of the MHQ distribution, given an appropriate second observable is chosen at the later time \(t\). The proof of this theorem is reported in appendix B and it offers a recipe for constructing a suitable observable \(B\) such that non-classicality is present. More specifically, \(\text{Re}(q_{ij}) < 0\), for some \((i, f)\), whenever \(U^\dagger \Xi_f U\) is equal to a projector onto any eigenstate of the anti-commutator \(\{\rho, \Pi_i\}\) associated with a negative eigenvalue.

We now describe in a self-contained way some of the roles played by the KDQ across the quantum sciences.

A. Correlators and linear response theory

Since the KDQ \(q_{ij}(\rho)\) is naturally interpreted as the correlation function between the event “observable \(A(0)\) takes value \(a_i(0)\)” and “observable \(B(t)\) takes value \(b_f(t)\)”, it is not surprising that it is related to linear response theory via the so-called fluctuation-dissipation theorems.

To show this, consider the unitary dynamics \(^1\) generated by \(H(t) = H(0) - \lambda(t) A\), with \(A\) a perturbation and \(\lambda(t)\) nonzero only for \(t > 0\). Looking at the change in the average value of the observable \(B(t)\) from time 0 to \(t\), in the linear response regime, one gets

\[
\Delta(B(t)) \approx \int_0^t \lambda(t') \Phi_{AB}(t', t) dt',
\]

where \(\Delta(B(t)) \equiv \text{Tr}(B(t)\rho(t)) - \text{Tr}(B(0)\rho)\). In Eq. (6), \(\Phi_{AB}(t', t)\) is the linear response function [74–76]:

\[
\Phi_{AB}(t', t) = i \text{Tr} \left( [A(t'), B(t)] \rho \right)
\]

where here \(\mathcal{O}(t) \equiv e^{iH(0)t} \mathcal{O} e^{-iH(0)t}\) denotes a generic observable \(\mathcal{O}\) (\(A\) and \(B\) in this subsection) evolved according to the unperturbed dynamics. For an initial thermal state, Eq. (6) reduces to the well-known *Kubo’s formula*. More generally, if the initial state is a fixed point of the unperturbed evolution, the linear response function assumes the convolutional form \(\Phi_{AB}(t-t') = i \text{Tr} \left( [A, B(t-t')] \rho \right)\) [31, 32].

By rewriting Eq. (4) as \(q_{ij}(\rho) = \text{Tr} (\rho \Pi_i(t') \Xi_k(t))\) where \(\Pi_j(t')\), \(\Xi_k(t)\) are the projectors associated to the

\(^1\) What follows, and the connection to the KDQ, can be generalized to the case in which the unperturbed dynamics is open and Markovian while the system is subjected to a unitary perturbation. See also the discussion in [32, 73].
observables $A(t')$ and $B(t)$ respectively, from Eq. (7) we get that
\[ \Phi_{AB}(t', t) = 2 \sum_{j,k} a_j(t') b_k(t) \text{Im} \lambda_{jk}(\rho), \] (8)

with $a_j(t')$ and $b_k(t)$ eigenvalues of $A(t')$ and $B(t)$. Hence, the linear response function is directly related to the imaginary part of the KDQ encoding the correlations of the observable of interest $B(t)$ and the perturbation. This is connected to the fact that the so-called weak values [37] are related to the linear response under a unitary perturbation [24] and that, as we will discuss in the following, weak values can be understood as conditional KDQs bridging the results of [24] with the current discussion.

Before moving on, let us draw another important link between the KDQ and the linear response theory. Consider the situation in which the quantum state $\rho_\lambda$ of a physical system depends on the external parameter $\lambda$ and it is affected by a small change of such parameter. In this case, a time-independent observable $A$ in the linear regime changes according to
\[ \Delta \langle A \rangle = \text{Tr} \left( A (\rho_\lambda - \rho) \right) \approx \chi_A^s \lambda, \] (9)

where $\chi_A^s$ is the static susceptibility of $A$.

A set-up in which the quantum state of a system depends on an external parameter is the premise of quantum metrology. In fact, this connection has been investigated in [31], where it was shown that the static susceptibility can be written as
\[ \chi_A^s = \frac{1}{2} \text{Re} \left( \sum_{i,j} \lambda_i \lambda_j \right), \] (10)

In Eq. (9), $A_0$ is an observable known as the symmetric logarithmic derivative (SLD), which is the central object in computing the quantum Fisher information and thus the quantum Cramér-Rao bound [77, 78], pillars of quantum metrology. Expanding $A_0 = \sum_{i,j} \lambda_i \lambda_j$, we obtain
\[ \chi_A^s = \frac{1}{2} \text{Tr} \left( \rho \Pi_j \Pi_i \right) \text{Re} q_{ij}(\rho), \] (11)

Hence, the static susceptibility can be expressed as a function of the real part of a KDQ measuring the correlations between the observable of interest $A$ and the SLD. For an initial thermal state, Eq. (11) yields the standard form of the fluctuation-dissipation theorem while, if $A = A_0$, $\chi_A^s$ coincides with the quantum Fisher information [31].

In short, our discussion shows how the KDQ is behind several results in linear response theory and their ramifications in thermodynamics and metrology.

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1 The static susceptibility can be related to the linear response function since $\chi_A^s$ is obtained by integrating over time the linear response function for $t \to \infty$ when the perturbation is assumed constant in time, i.e., $\lambda(t) = \lambda = \text{constant}$ [31].

### B. Quantum currents

The KDQ, being a way to characterize quantum fluctuations, also enters implicitly in quantum many-body and condensed matter physics.

A first example is represented by quantum currents that are a central concept in quantum transport and non-equilibrium thermodynamics. In this regard, let us take into account a classical stochastic dynamics on a set of discrete states $\{i\}$. These could label distinct sites in a lattice, or distinct energy states. A standard definition of probability current between states $j$ and $i$ is given by [79]
\[ J_{j \to i}(t) = W_{ij}(t) - W_{ji}(t) \] (12)

that corresponds to the difference between the joint probability of being in $i$ and jumping to $j$ ($W_{ij}$) minus the probability of the opposite trajectory. The particle/energy/... current so defined satisfies the continuity equation for the probability $p_i$ of being in state $i$:
\[ \frac{dp_i}{dt} = \sum_{j \neq i} J_{j \to i}(t). \] (13)

Consider now a quantum system evolving unitarily between the states $|i\rangle$. As discussed in [34], for a quantum system subject to unitary dynamics, Eqs. (12) and (13) are valid provided that
\[ W_{ij}(t) = \text{Re} \delta q_{ij}(\rho(t)), \] (14)

where
\[ \delta q_{ij}(\rho(t)) \equiv \text{Tr} \left( (\rho(t) \Pi_j(t) U(t + dt) U(t) \Pi_i(t + dt) U(t, t + dt)) \right), \]

$\Pi_i(t)$ denotes the projectors associated to the event “the state is $|i\rangle$ at time $t$”, and $U(t, t + dt)$ is the unitary evolution from time $t$ to $t + dt$. Therefore, we can conclude that the KDQ is implicit also in the description of quantum currents [34].

### C. Loschmidt echo

Another relevant appearance of the KDQ is in connection with the Loschmidt echo [35, 36]. The Loschmidt echo is a measure of the revival occurring when an imperfect time-reversal procedure is applied to a complex quantum system [36], and it has many applications from field theories to chaos theory and information scrambling in many-body systems [80–88]. In many-body physics the Loschmidt echo is the central object to study the so-called dynamical quantum phase transitions [89–96]. In fact, dynamical quantum phase transitions are defined as non-analytic behaviours in time of the Loschmidt amplitude [89], which we shall now define.

For initial pure states, the Loschmidt amplitude is defined simply as the projection of the time evolved state
onto the initial state, i.e., $\langle \psi_0 | e^{-iH_0 t} | \psi_0 \rangle$. Instead, for initial mixed states, relevant for example to account for thermal states at non-vanishing temperature, various generalizations exist. In [89, 97, 98], the Generalized Loschmidt Echo (GLE) is defined as

$$G_\rho(t) = \text{Tr} (\rho U(t, 0)),$$  \hspace{1cm} (15)

where $\rho$ is again the initial state and $U(t, 0)$ the unitary operator that rules the time evolution of the quantum system in the interval $[0, t]$.

We now introduce a further extension of the GLE, defined over two distinct time instants. For this purpose, let us consider a quantum quench where a parameter of the system Hamiltonian is suddenly changed at time $t = 0$. We indicate with $H_0 = \sum_i E_i \Pi_i$ the initial Hamiltonian (for $t < 0$) and with $H = \sum_f \tilde{E}_f \Xi_f$ the Hamiltonian after the quench. Taking the Fourier transform (FT) of the GLE, one obtains

$$\hat{G}(\omega) = 2\pi \sum_f \delta(\omega - \tilde{E}_f) p_f$$  \hspace{1cm} (16)

where $p_f \equiv \text{Tr}(\rho \Xi_f)$. Eq. (16) is a point distribution over the final energy after the quench. Hence, the Loschmidt echo in Eq. (15) is just the inverse Fourier transform of the final energy distribution. This suggests a natural generalization. We thus consider the point distribution over the energy variation across the quench, i.e.,

$$\hat{G}(\omega, \omega') = 4\pi^2 \sum_{i,f} \delta(\omega' + E_i)\delta(\omega - \tilde{E}_f) q_{if},$$  \hspace{1cm} (17)

where $q_{if}$ is the joint quasiprobability for the random variable $\tilde{E}_f - E_i$. Accordingly, an extended GLE is achieved by applying the inverse Fourier transform to $\hat{G}(\omega, \omega')$. We get

$$G_\rho(t', t) = \text{Tr} (\rho U(t, 0)V(t', 0)),$$  \hspace{1cm} (18)

where $V(t', 0) = e^{-iH_0 t'}$ is the propagator that governs the unquenched dynamics. In analogy to Eq. (15), it is worth observing that the Loschmidt echo in (18) is the characteristic function of the KDQ for the random variable $\tilde{E}_f - E_i$. Clearly, the latter contains more information than Eq. (15), which is recovered as a marginal or by setting $t' = 0$ (see also Table 1). In general our extended GLE also encodes additional information about initial coherence terms of $\rho$ in the basis of $H_0$.

The observation that the extended GLE $G_\rho(t', t)$ is nothing more than the characteristic function of a KDQ implies that there could be techniques to experimentally probe it. As discussed in section IV.B, the characteristic function of the KDQ can be accessed via an interferometric scheme. In section VI we also put forward an experimental proposal involving NV centers in diamond to interferometrically determine the characteristic function of a generic KDQ and thus of $G_\rho(t', t)$.

| | GLE ($t' = 0$) | Extended GLE |
|-----------------|-----------------|-----------------|
| $G_\rho(t', t)$ | $\text{Tr} (\rho U(t, 0))$ | $\text{Tr} (\rho U(t, 0)V(t', 0))$ |
| $\text{FT}(G_\rho)$ | $2\pi \sum_f \delta(\omega - \tilde{E}_f) p_f$ | $4\pi^2 \sum_{i,f} \delta(\omega' + E_i)\delta(\omega - \tilde{E}_f) q_{if}$ |

TABLE I. GLE vs. Extended GLE

D. Weak values are conditional KQD averages

First introduced by Aharonov et. al. [37], weak values have been extensively studied and related to experimental techniques for signal amplification, quantum state reconstruction and non-classicality witness [99]. Recently, they have been related to non-classical advantages in metrology [26, 27] and associated to proofs of contextuality [18, 38]. In fact, some of these results are phrased in terms of weak values and some in terms of the KDQ, but it is important to realize that the KDQ offers a unified perspective [100].

Let us consider the special case of the KDQ in Eq. (4) whereby the input state is pure, $\rho = |\psi\rangle\langle\psi|$, the dynamics is unitary and the final projector is rank-1. Hence, setting $U^\dagger \Xi(t)U \equiv \Xi(t)|\xi_f\rangle\langle\xi_f|$, we get

$$q_{if} = \langle \psi | \xi_f | \Pi_i | \psi \rangle = q_{if} \frac{\langle \xi_f | \Pi_i | \psi \rangle}{\langle \xi_f | \psi \rangle} = q_{if} \langle \Pi_i | W \rangle, \hspace{1cm} (19)$$

where $\langle \Pi_i | W \rangle = \langle \xi_f | \Pi_i | \psi \rangle/\langle \xi_f | \psi \rangle$ is the original definition of the “weak value of $\Pi_i$ with initial state $|\psi\rangle$” and post-selection $|\xi_f\rangle$ and $q_{if} = |\langle \psi | \xi_f \rangle|^2$. Thus, the weak value of a projector is simply the conditional KDQ $q_{if}/q_{if}$, and the weak value $\langle A \rangle_W$ of an observable $A = \sum_i a_i \Pi_i$ is the average under such conditional KDQ [101]:

$$\langle A \rangle_W = \frac{\langle \xi_f | A | \psi \rangle}{\langle \xi_f | \psi \rangle} = \sum_i a_i q_{if}/q_{if} = \sum_i a_i q_{if}. \hspace{1cm} (20)$$

Weak values have an obvious interpretation and a natural generalization when seen through the lenses of the KDQ, which unifies disparate points of views in the literature. For instance, the so-called anomalous weak values of an observable $A$, i.e., instances in which Re$\langle A \rangle_W$ lies outside the boundaries of the spectrum of $A$, have attracted particular attention [38, 99]. These can only occur when Re$\langle \Pi_i | W \rangle < 0$ for some projector $\Pi_i$ [38], meaning that they are associated to non-classicality of the KDQ. Accordingly, the study of the non-classicality of KQDs subsumes considerations about anomalous weak values.

IV. MEASURING THE KIRKWOOD-DIRAC QUASIPROBABILITY

There are several schemes that allow to access the KD quasiprobabilities:
A. Weak two-point-measurement (WTPM) scheme

Let us introduce the state
\[ \rho_{NS,i} = p_i \rho_i + (1 - p_i) \bar{\rho}_i \]  

where NS stands for “non-selective”, \( p_i = \text{Tr}(\rho \Pi_i) \) and
\[ \rho_i = \frac{\Pi_i \rho \Pi_i}{p_i}, \]  
\[ \bar{\rho}_i = \frac{(I - \Pi_i) \rho (I - \Pi_i)}{1 - p_i}. \]

\( \rho_{NS,i} \) can be obtained by performing non-selective projective measurements with projectors \( \{\Pi_i, I - \Pi_i\} \) or, equivalently, by preparation of the states \( \rho_i \) and \( \bar{\rho}_i \) with the corresponding probabilities. From an experimental point of view, the WTPM requires three sets of measurements:

**Scheme 1 (TPM)**
- Prepare the initial state \( \rho \).
- Measure the quantum observable \( A \).
- Evolve under the quantum map \( \mathcal{E} \).
- Measure the quantum observable \( B \).

This is the well-known two-point measurement (TPM) scheme for the initial and final observables \( A \) and \( B \) respectively [103], which grants access to the joint probability distribution of Eq. (5).

**Scheme 2 (weak TPM)**
- Prepare the initial state \( \rho \).
- Perform the projective, non-selecting measurement \( \{\Pi_i, I - \Pi_i\} \) (or skip the first two steps and directly prepare \( \rho_{NS,i} \)).
- Evolve under the quantum map \( \mathcal{E} \).
- Measure the quantum observable \( B \).

This allows to compute the joint probabilities
\[ p_{ij}^{\text{WTPM}} = \text{Tr}(\mathcal{E}(\rho_{NS,i}) \Xi_f(t)). \]

**Scheme 3 (final measurement only)**
- Prepare the initial state \( \rho \).
- Evolve under the open quantum map \( \mathcal{E} \).
- Measure the quantum observable \( B \).

In this way, we get the probability distribution
\[ p_{ij}^{\text{END}} = \text{Tr}(\mathcal{E}(\rho) \Xi_f(t)) \] where END stands for “end-time energy measurement”.

Therefore, by means of projective measurements only, one can reconstruct (cf. Eq. (14) of Ref. [13])
\[ \text{Re } q_{i,f} = p_{ij}^{\text{TTPM}} - \frac{1}{2} \left( p_{ij}^{\text{END}} - p_{ij}^{\text{WTPM}} \right). \]  

It should be noted that, for the particular case of a single qubit system, the TPM and END (appearing in the literature also as end-point measurement scheme – EPM [61]) schemes suffice to completely characterize \( \text{Re } q_{i,f} \). Remarkably, one of the main strengths of the WTPM scheme is its similarity with the usual TPM one; the only new element being the preparation of \( \rho_{NS,i} \) or measurement of \( \{\Pi_i, I - \Pi_i\} \). This leads us to believe that the WTPM scheme could be implemented in most experimental platforms where the energy variation statistics has already been measured with a TPM scheme. A non-exhaustive list for the latter includes NV centers in diamond [104, 105], single ions [106–108], superconducting qubits [109], and entangled photon pairs [110, 111]. For an experimental implementation of the WTPM scheme in a three-level system with NV centers, we refer the reader to a companion paper [112] where the MHQ \( \text{Re } q_{i,f} \) is reconstructed.

Finally, it is worth noting that, in principle, also \( \text{Im } q_{i,f} \) can be inferred, but it requires the ability to perform selective phase-rotations \( \exp(i\pi \Pi_i/2) \) of the state \( \mathcal{E}^t(\Xi_f(t)) \), as argued in Ref. [13].

B. Interferometric measurement of the KD characteristic function

An equivalent way of characterising the KDQ \( q_{i,f} \) is through its characteristic function
\[ \chi(u, v) = \sum_{i,f} q_{i,f} e^{iB(t)u + iA(t)u} = \text{Tr} \left( E^i(e^{iB(t)v}) e^{iA(0)u} \rho \right). \]  

(25)
The KQD can be then recovered by means of the inverse Fourier transform.

Let us see how the characteristic function can be accessed experimentally. Thus, consider a quantum system $S$ characterized by its Hamiltonian $H_S$, and the external environment $E$ initially in a product state $\rho_S \otimes \rho_E$. The composite system $SE$ evolves unitarily under $U_{SE}$, meaning that $U_{SE}$ achieves the dynamics $E$ on the system $S$ upon tracing out the environment. Then, we introduce an ancillary qubit system $A$ and we consider the controlled unitaries

$$C_V = |0\rangle_A \langle 0| \otimes I_{SE} + |1\rangle_A \langle 1| \otimes V_{SE},$$

where $V_{SE}$ is a unitary gate acting on $SE$. The interferometric protocol is thus as follows [40–42]:

- Prepare the system $S$ in the state $\rho_S$ and the ancilla in the state $|+\rangle_A = (|0\rangle_A + |1\rangle_A)/\sqrt{2}$ (e.g., by applying a Hadamard gate to $|0\rangle_A$).
- Apply $C_V$ with $V_{SE,1} \equiv e^{i(B(t) \otimes I_E)u} U_{SE}$.
- Apply a Pauli $X$ gate to the ancilla.
- Apply $C_V$ with $V_{SE,2} \equiv U_{SE} e^{i(A(0) \otimes I_E)u}$.
- Apply a Pauli $X$ and a Hadamard gate on the ancilla.
- Measure either $X$ or $Y$ of the ancilla state.

As shown in [40–42], the average value of the final $X$ and $Y$ measurements provide, respectively, $\text{Re} \chi(u,v)$ and $\text{Im} \chi(u,v)$ given that

$$\text{Tr}_{SE} \left( e^{i(B(t) \otimes I_E)u} U_{SE} e^{i(A(0) \otimes I_E)u} (\rho_S \otimes \rho_E) U_{SE}^\dagger \right) = \text{Tr} \left( e^{i(B(t)v)u} e^{iA(0)u} \rho_S \right) = \chi(u,v).$$

To overcome possible numerical instabilities of the inverse Fourier transform, one can further adopt a reconstruction procedure based on estimation theory, thus taking as input specific values of the KQD characteristic function, as proposed in [113].

Note that the interferometric scheme has been implemented experimentally in [43] to infer the work distribution that arises from the TPM scheme. As we are going to discuss in more detail in section VI, the same experimental set-up in [43] could be used to determine the KQD by preparing initial states $\rho_S$ which are not diagonal in the energy basis of $H(0)$.

\section*{C. Cloning scheme and generalizations}

In [44, 101, 102], a measurement scheme, called cloning scheme, to access correlation functions was proposed and subsequently experimentally realized in [114]. We have already discussed the relation between the KQD and correlations functions, it then comes as no surprise that the cloning scheme can be used to reconstruct the KQD distribution of a quantum system $S$ [101]. We here follow the notation of Buscemi et al., whereby the central relation is

$$\text{Re} q_{if} = \frac{d+1}{2} \text{Tr} \left( (I \otimes E)[R_+ (\rho_S)](\Pi_i \otimes \Xi_f) \right) - \frac{d-1}{2} \text{Tr} \left( (I \otimes E)[R_- (\rho_S)](\Pi_i \otimes \Xi_f) \right),$$

where $d$ is the dimension of the system’s Hilbert space and $R_{\pm(-)}$ are the optimal symmetric (anti-symmetric) cloners of $S$ for any state $\rho_S$. Specifically, $R_{\pm}$ are defined as [115]

$$R_{\pm}(\rho_S) = \frac{2d}{d \pm 1} P^\pm \left( \frac{I}{d} \otimes \rho_S \right) P^\pm,$$

where $P^\pm$ are the symmetric (anti-symmetric) projectors on the Hilbert space of two copies of the system, i.e., $P^\pm \equiv (I \pm S)/2$ with $S$ the swap operator (thus $S$, by definition, is such that $S |a\rangle \otimes |b\rangle = |b\rangle \otimes |a\rangle \forall |a\rangle, |b\rangle$). The scheme to reconstruct the MHQ \text{Re} $q_{if}$ is then as follows:

- Introduce an ancilla $A$ of the same dimension as the system, prepared in the maximally mixed state.
- Perform the projective measurements with projectors $\{P^+, P^-\}$.
- On the post-measurement state, apply the open map $E$ on the quantum system $S$.
- Perform the measurement $\{\Pi_i\}$ on $A$ and $\{\Xi_f\}$ on $S$.

Accordingly, by denoting with $p_{+, if}$ the probability that in the above scheme one records the outcome $+ \text{ followed by the outcomes } (i, f)$ and similarly for $p_{-, if}$, one obtains

$$\text{Re} q_{if} = \frac{d+1}{2} p_{+, if} - \frac{d-1}{2} p_{-, if}.$$

It is worth noting that the scheme can be readily realized adapting simple quantum optical experiments, as it was observed elsewhere [44]. A similar procedure, somewhat more involved, can be used to reconstruct also $\text{Im} q_{if}$ [44].
As a generalisation, we can define an entire family of cloning schemes. For this purpose, let us consider as in Ref. [44] the linear map

$$\mathcal{T}(\rho) \equiv \mathcal{S}(I \otimes \rho),$$  \hspace{1cm} (31)

where $\mathcal{S}$ is, once again, the swap operator. Note that

$$q_{if} = \text{Tr} ((I \otimes \mathcal{E}) \mathcal{T}(\rho)(\Pi_i \otimes \Xi_f)).$$ \hspace{1cm} (32)

Now, $\mathcal{T}$ can be decomposed as $\mathcal{T} = \mathcal{P} - i\mathcal{K}$, where both $\mathcal{P}$ and $\mathcal{K}$ are Hermiticity-preserving. In turn, Hermiticity-preserving maps can be decomposed as a linear combination of CP maps, i.e., $\mathcal{P} = \sum_s \lambda_s \mathcal{Q}_s$ and $\mathcal{K} = \sum_s \eta_s \mathcal{F}_s$. Both $\sum_s \mathcal{Q}_s$ and $\sum_s \mathcal{F}_s$ are trace-preserving, thus meaning that $\mathcal{Q}_s$ and $\mathcal{F}_s$ are quantum instruments [116]. Therefore,

$$\text{Re} \, q_{if} = \sum_s \lambda_s \text{Tr} ((I \otimes \mathcal{E}) \mathcal{Q}_s(\rho)(\Pi_i \otimes \Xi_f)),$$ \hspace{1cm} (33)

$$\text{Im} \, q_{if} = \sum_s \eta_s \text{Tr} ((I \otimes \mathcal{E}) \mathcal{F}_s(\rho)(\Pi_i \otimes \Xi_f)).$$ \hspace{1cm} (34)

In this way, each term of $\text{Re} \, q_{if}$ and $\text{Im} \, q_{if}$ can be evaluated by implementing, respectively, the quantum instrument $\{\mathcal{Q}_s\}$ or $\{\mathcal{F}_s\}$. We have thus a scheme for every different decomposition of $\mathcal{P}$ and $\mathcal{K}$.

D. Direct reconstruction schemes

When considering pair of observables with mutually overlapping sets of eigenstates, the KDQ gives a complete and unique characterization of a quantum state subject to unitary dynamics (see, e.g., Ref. [13]):

$$\rho = \sum_{if} (a_i|\rho|b_f) |a_i\rangle\langle b_f| = \sum_{if} q_{if} |a_i\rangle\langle b_f|,$$ \hspace{1cm} (35)

with $q_{if} = \text{Tr} (\Xi_i \Pi_i \rho)$, $\Xi_f = |b_f\rangle\langle b_f|$ and $\Pi_i = |a_i\rangle\langle a_i|.$

Clearly, full tomography would allow to reconstruct the KQD in these settings, but that is not practical beyond the simplest systems. More promising are methods for the direct reconstruction of the elements of a generic density matrix, since these allow for the direct access to the corresponding KDQ distribution. In [46–52], the authors propose several schemes for a direct measurement of the KD representation of the wave-function/density matrix of a quantum system. The original proposals employed weak measurements [46, 47, 100] – in fact, recall from section III that the KDQ is closely related to weak values, and the latter can be accessed via weak measurements – but direct reconstruction schemes have been extended to strong measurements and experimentally implemented in quantum optics setups [48–52].

Following [47], which generalizes the results in [46] to mixed states, we can further propose two schemes involving weak measurements. These schemes hinge on the fact that, to access a KDQ distribution, the product of non-commuting observables needs to be measured. Let us thus consider the two observables $A$ and $\mathcal{E}^\dagger(B)^\dagger$. As shown in Eq. (4), the KDQ is obtained if we can measure the quantities $\text{Tr} (\Pi_i(0)\rho \mathcal{E}^\dagger(\Xi_f(t)))$ for any pair of indexes $i, f$. Each scheme that follows requires the use of two quantum pointers, representing quantum ancillary degrees of freedom, to which the quantum system has to be weakly coupled. Thanks to this coupling, one can obtain approximate expressions that connect the desired correlations functions arising from the KDQ distribution to the correlations of the two pointers’ observables that are directly measured.

Scheme 1

This first scheme was initially proposed in [117], further analyzed in [118, 119], and experimentally implemented in [120]. It consists in two sequential, independent weak measurements coupling system and a quantum pointer (here a one-dimensional continuous variable system). Each one of the two chosen system’s observables is coupled with the momentum operator of a corresponding pointer. The evolution is thus represented by

$$U_T = \exp \left( \frac{i \tilde{q}_t}{\hbar} \mathcal{E}^\dagger(\Xi_f(t)) \otimes I \otimes P_2 \right) \times \exp \left( \frac{q_t}{\hbar} \Pi_i \otimes P_1 \otimes I \right)$$ \hspace{1cm} (36)

where $P_k$ denotes the momentum operator of the $k$-th pointer (similar expressions are obtained considering 2-level quantum pointers [52]).

Assume the initial states of the pointers to be uncorrelated Gaussians with width $\sigma$ in the position representation. It can be shown that, in the limit $g_{12}t/\sigma \ll 1$, the evolution induces the pointer shifts

$$(g_{12})^{-1}(2\sigma/t)^2 (L_1 L_2)_f \approx \text{Tr} (\mathcal{E}^\dagger(\Xi_f(t))\Pi_i \rho),$$ \hspace{1cm} (37)

where $L_k \equiv X_k/2\sigma + iP_k\sigma/\hbar$ ($X_k$ being the $k$-th pointer’s position operator) and the average $\langle a_1a_2\rangle_f$ is performed over the final state of the pointers.

Scheme 2

The second scheme is based on conditional, sequential weak measurements. The coupling of the quantum system to the pointers is given by

$$U_D = \exp \left( -i \frac{g_t}{\hbar} \mathcal{E}^\dagger(\Xi_f(t)) \otimes X_1 \otimes P_2 \right) \times \exp \left( -i \frac{g_t}{\hbar} \Pi_i \otimes D_1 \otimes I \right)$$ \hspace{1cm} (38)

with $D_k = X_k$ or $P_k$. One gets:

- For $D = P$ and in the limit $g_{12}g_{23}t^2/\sigma \ll 1$, the final position of the pointer 2 is shifted on average by

$$\langle X_2 \rangle_f \approx (g_{12}g_{23}^2) \text{Re} \text{Tr} (\mathcal{E}^\dagger(\Xi_f(t))\Pi_i \rho),$$

Note that the adjoint of a quantum channel, $\mathcal{E}^\dagger$, is Hermiticity-preserving. Hence, $\mathcal{E}^\dagger(B)$ is an observable.
while there is no shift in the expectation value of the moment.

- For \( D = X \) and in the limit \( g_N g_2 \sigma^2 / \hbar \ll 1 \), the final momentum of the pointer 2 is shifted on average by

\[
(P_2)_f \approx (2 g_N g_2 \sigma^2 / \hbar) \text{ImTr} \left( \mathcal{E}^\dagger(\Xi(t)) \Pi_i \rho \right).
\]

From the expressions above, we can conclude that for the estimation of the quantum correlation functions \( \text{Tr} \left( \Pi_i(0) \rho \mathcal{E}^\dagger(\Xi_f(t)) \right) \) one needs to be able to implement the unitary couplings between the system observables \( \Pi_i(0) \), \( \mathcal{E}^\dagger(\Xi_f(t)) \) and the two quantum pointers, and then perform pointer measurements [52]. This is fairly limiting since often \( \mathcal{E}^\dagger \) is not known. However in the case of unitary dynamics the situation is considerably improved: one simply need the ability to implement the dynamics \( U \) as a black-box, without any knowledge of its matrix elements required.

As mentioned before, in the remits of the direct detection of the density matrix of a quantum system, the schemes above have been generalized to the case of strong measurements. Formally, in [52] the authors show that a scheme analogous to Scheme 1 can be used outside the approximation \( g_N g_2 \sigma / \hbar \ll 1 \) (thus entailing strong measurements). This generalization of Scheme 1 has been shown to offer advantages both in reducing statistical errors for the direct detection of density matrices and in terms of resources when compared to quantum state tomography, especially for high-dimensional systems [52]. In fact, Scheme 1 and its generalization involve performing \( d + 1 \) unitary operations, projective measurements of the system on the basis of the observable \( A \), and a small number of pointer measurements (between three and eight can usually suffice, see [52]), in contrast to the \( O(d^2) \) independent projective measurements required for full quantum state tomography.

E. Block-encoding scheme

Block-encoding methods allow to implement non-unitary matrices on quantum computing architectures as blocks of a unitary gate applied to a composite quantum system (i.e., two or more qubits). Specifically, here we resort to block-encoding algorithms for the estimation of \( n \)-time correlation functions [45] to devise yet another scheme for the reconstruction of the full KDQ distribution. Such a scheme works for any quantum system for which we can prepare a purification of \( \rho \) and subject to unitary dynamics.

Let us thus consider that our quantum system of interest \( S \) (with dimension \( d \)) is initially in the pure quantum state \( |\psi\rangle \), and take two ancillary qubits \( A_1 \) and \( A_2 \) in \( |0\rangle \) at \( t = 0 \). The Hilbert space of the composite system is then the \( 4d \)-dimensional space \( \mathcal{H} = \mathcal{H}_{A_2} \otimes \mathcal{H}_{A_1} \otimes \mathcal{H}_S \).

Given our two observables \( A \) and \( B \), we encode their projectors in two unitary operations acting on the system and one of the ancillary qubits as

\[
U_{\Pi_i} = \mathbb{I}_{A_2} \otimes \mathbb{I}_{A_1} \otimes \Pi_i + \mathbb{I}_{A_2} \otimes \sigma^{(A_1)}_x \otimes (\mathbb{I} - \Pi_i),
\]

\[
U_{\Xi_f} = \mathbb{I}_{A_2} \otimes \mathbb{I}_{A_1} \otimes \Xi_f + \sigma^{(A_2)}_x \otimes \mathbb{I}_{A_1} \otimes (\mathbb{I} - \Xi_f).
\]

The block-encoding scheme to reconstruct the KDQ then proceeds as follow:

- Act with the unitary \( U_{\Pi_i} \), on the system and the first ancilla.
- Apply \( U \) to \( S \). At this point, the state of the composite system transformed as

\[
|0\rangle|0\rangle|\psi\rangle \rightarrow |0\rangle|0\rangle U_{\Pi_i} |\psi\rangle + |0\rangle|1\rangle (\mathbb{I} - \Pi_i) |\psi\rangle.
\]
- Apply the unitary \( U_{\Xi_f} \) on the system and the second ancilla.
- Apply the inverse unitary \( U^\dagger \) to \( S \). As a result, we end up with the quantum state

\[
U_{\text{BE}} |0\rangle|0\rangle|\psi\rangle = |0\rangle|0\rangle U_{\Pi_i} \Xi_f U_{\Pi_i} |\psi\rangle + |0\rangle|1\rangle U_{\Pi_i} (1 - \Xi_f) \Xi_f U_{\Pi_i} |\psi\rangle + |1\rangle|0\rangle U_{\Pi_i} (1 - \Xi_f) U_{\Pi_i} |\psi\rangle.
\]

where \( U_{\text{BE}} \equiv U^\dagger U_{\Xi_f} U U_{\Pi_i} \).
- Perform a Hadamard test to estimate the overlap between \( U_{\text{BE}} |0\rangle|0\rangle |\psi\rangle \) and the initial state \( |0\rangle|0\rangle |\psi\rangle \). The corresponding circuit, employing a third qubit ancilla, is presented in Fig. 2.

To see why this works, note that for quantum systems initialized in a pure state and undergoing unitary dynamics, the KDQ equals to

\[
q_{i,f} = \langle \psi | U^\dagger \Xi_f U \Pi_i |\psi\rangle,
\]

which can be immediately seen to equal the estimate overlap.

V. TESTING NON-CLASSICALITY

The KDQ in general can present negative or complex values (non-reality). These represent a signature of non-classicality that is at the basis of several quantum advantages investigated in the existing literature [24, 27, 28, 121, 122]. The non-classicality of the KDQ can be defined via the quantity [17, 20]

\[
\mathcal{N}[\mathbf{q}(\rho)] \equiv -1 + \sum_{i,f} |q_{i,f}(\rho)|,
\]

where \( \mathbf{q}(\rho) \) denotes the vector containing all KD quasiprobabilities. As proved in Appendix C, \( \mathcal{N} \) has good properties to be a measure of non-classicality. Specifically,
FIG. 2. Circuit representation of the block-encoding scheme, including the Hadamard test, for the reconstruction of KDQ distributions. In the Hadamard test, a phase gate \( P(-\pi/2) = \begin{bmatrix} 1 & 0 \\ 0 & -i \end{bmatrix} \) has to be added after the application of the first Hadamard gate, with the aim to also access the imaginary part of the overlap. By removing the phase gate, one can also access the real part of the overlap. The crossing lines denote a SWAP unitary.

A. Characteristic function as a witness of non-classicality

As described in Section IV B, the characteristic function of the KDQ distribution can be measured via an interferometric scheme. Clearly, upon measuring \( \chi(u,v) \) in an open set in \( \mathbb{R}^2 \), one can (approximately) reconstruct the full distribution by way of the inverse Fourier transform – like it was performed for the case of the TPM work distribution in [43].

However, we can also consider a less “expensive” route to witness non-classicality. In fact, Bochner’s theorem [123–125] states that the Fourier transform of a probability measure over \( \mathbb{R}^m \) is necessarily a normalized continuous positive semi-definite function from the \( \mathbb{R}^m \) to the complex numbers. A function \( \chi : \mathbb{R}^m \to \mathbb{C} \) is positive-semi-definite if for any \( x_1, \ldots, x_n \in \mathbb{R}^m \) the matrix \( \alpha_{ij} = \chi(x_i - x_j) \) is positive semi-definite. This means that, if the characteristic function violates the positive-semi-definite condition, then the KDQ distribution necessarily presents non-classicality in the form of negativity and/or complex values.

A first check on the KDQ characteristic function consists in looking for violations of the condition \( \chi(-u,-v) = \chi^*(u,v) \) implied by the positive-semi-definite definition. This condition is violated only when \( \text{Im}(q_{ij}) \neq 0 \). Thus, the violation of the condition \( \chi(-u,-v) = \chi^*(u,v) \) serves as a witness of complex values in the KDQs and, correspondingly, as a witness of non-classicality.

Hence, violations of the positive-semi-definite condition can be observed by performing the following steps: (i) Measuring interferometrically the KDQ characteristic function in \( n \geq 3 \) points \( x_1, \ldots, x_n \) in \( \mathbb{R}^2 \), (ii) constructing the \( n \times n \) matrix with elements \( \alpha_{ij} = \chi(x_i - x_j) \), and (iii) looking for a negative eigenvalue. In this regard, since \( \chi(0,0) = 1 \) by definition, in principle we can always measure the characteristic function in \( n - 1 \) points of \( \mathbb{R}^2 \) in order to perform the \( n \)-th order test of positivity.

In order to look for negativity specifically, one just needs to extract the characteristic function of the MHQ distribution from the one of the KDQs. This is easily done by using the properties of the Fourier transform,

\[ \text{Im}(q_{ij}) \neq 0 \]
i.e.,
\[ \chi_{MH}(u,v) = \frac{1}{2} (\chi_{KD}(u,v) + \chi_{KD}(-u,-v)). \]

### B. Moments as a witness of negativity

Another way to test the negativity of the MHQ distribution is to look at the inequalities that the moments of a proper probability distribution have to obey. Such inequalities, indeed, could be violated if negativity is present.

The moments of the MHQ distribution are defined by
\[ m_k = \sum_{i,j} q_{ij}^{MH} (b_j - a_i)^k. \]

Now, we want to explore what we can learn about the negativity of the MHQ distribution, given a finite number of moments. The problem of determining whether there exists a probability distribution have to obey. Such inequalities, indeed, could be violated if negativity is present.

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the qubit probe are known or can be easily measured experimentally. The main difficulty of the scheme—akin to the one of the interferometric protocol described in section IV—seems to reside in realizing the interaction Hamiltonian $H_{\text{int}}$.

C. A SWAP test quantifying non-classicality

Finally, we propose a method aimed at extracting directly the information about non-classicality by performing only projective measurements on two copies of a quantum system ($d$-dimensional in general) undergoing unitary dynamics.

Let us consider a system initially prepared in a pure state $|\psi\rangle$ and undergoing the unitary dynamics $U$. The KDQ for a couple of observables $A = \sum_i a_i \Pi_i$ and $B = \sum_f b_f \Xi_f$ can be then written as

$$q_{if} = \langle \psi | U^\dagger \Xi_f U \Pi_i | \psi \rangle = \langle \psi_U | \psi_{i,U,f} \rangle \sqrt{p_{ij}^{\text{TPM}}}, \tag{54}$$

where $|\psi_U\rangle = U|\psi\rangle$ and

$$|\psi_{i,U,f}\rangle = \Xi_f U \Pi_i |\psi\rangle / \sqrt{p_{ij}^{\text{TPM}}}.$$ 

Here $p_{ij}^{\text{TPM}}$ is the probability that the projective measurement of $A$ followed by $U$ and the projective measurement of $B$ returns outcomes $(i, f)$, which is the aforementioned TPM scheme.

Now, let us consider the scheme in Fig. 4. This scheme requires an ancillary qubit and two copies of the system initialized in the initial state $|\psi\rangle$. The first part of the scheme amount to letting one copy of the system evolve under the unitary evolution while the other copy is subjected to a TPM scheme which allows to estimate $p_{ij}^{\text{TPM}}$. The part of the circuit in the grey-shaded area then performs a controlled SWAP gate between the two copies of the system.

The final probability for a $\sigma_z$ measurement on the ancillary qubit to have outcome 0 is given by

$$p_A(0) = \frac{1}{2} \left( 1 + |\langle \psi_U | \psi_{i,U,f} \rangle|^2 \right). \tag{55}$$

Thus, one can get that

$$|q_{if}| = \sqrt{p_{ij}^{\text{TPM}}} \sqrt{2p_A(0) - 1}, \tag{56}$$

which then can be directly used in Eq. (44).

VI. EXPERIMENTAL PERSPECTIVES

As we have discussed so far, the KDQ appears in many corners of quantum physics and encodes the correlations between quantum observables. Additionally, the non-classicality of KDQ distributions is also responsible for several quantum advantages [24, 27, 121, 122].

This motivates the proposal of measurement schemes like the ones presented in sections IV and V. Several protocols are connected to the literature on weak values. In particular, since the KDQ distribution encodes the full information on a quantum state [11], schemes based on weak measurements have been implemented for the tomographic reconstruction of quantum state density matrices. The works [46, 48–52] have been implemented in quantum optics set-ups, and then used as a test-bed to investigate the quantum metrological advantages linked with the KDQ non-classicality [127].

Other schemes among the ones discussed in sections IV and V have the potential to be applied in set-ups other than quantum optics. In this regard, in [43] the authors report the first experimental assessment of fluctuation relations for a quantum spin-1/2 system that undergoes a closed quantum non-adiabatic evolution. In such an experiment, the TPM distribution of work is reconstructed through the inverse Fourier transform of a set containing the measured samples of the corresponding work characteristic function. The work characteristic function is measured by means of the interferometric scheme described in section IV B. There we showed that this scheme, when applied to systems initialized in a quantum state with initial coherence in the energy basis, allows to access the full KDQ distribution. Hence, the same experiment as in [43] could be used to directly witnesses the non-classicality of the KDQ distribution.

A word of caution is in order here. When speaking of work distribution, we are identifying a stochastic variable $w_{ij} = b_f(t) - a_i(0)$ that is characterized by the (quasi)probability distribution $P(w) = \sum_{ij} q_{ij} \delta(w - b_f(t) + a_i(0))$. Note that in $P(w)$ the observables $A$ and $B$ are now identified with the Hamiltonian of the system at the initial and final times. This means that the characteristic function of the work distribution is provided by Eq. (25) with $\chi(w) \equiv \chi(-u, u)$. Accordingly, on the one hand the problem of determining the work characteristic function simplifies due to the fact that now $\chi(u)$ is a

** One could extend to mixed states by repeating the scheme below for each eigenstate of the initial density matrix.
function of a single variable $u$. On the other hand, $P(u)$ is a coarse-grained instance of the original quasiprobabilities $q_{ij}$ and thus, in accordance with (P5) in section V, its non-classicality is less or equal to the one of the full KDQ distribution. As a result, the non-observation of non-classicality in the work (quasi)probability distribution $P(w)$ does not rule out that $\Re[q(\rho)] \neq 0$.

Finally, we also refer the reader to the companion paper [112], where we discuss the first –to our knowledge– experimental implementation of the weak-TPM scheme. In such work, the MHQ distribution is experimentally reconstructed for a three-level quantum system encoded in a NV center in diamond, and negativity is observed.

### A. Case study

Since we have argued that the set-up of [43], provided by a NMR system, could be readily used to reconstruct the KDQ characteristic function, we here numerically investigate such a system as a case study.

The quantum system of [43] consists of the liquid-state NMR spectroscopy of the $^1H$ and $^{13}C$ nuclear spins of a chloroform-molecule sample. Specifically, the $^1H$ spin is used as the ancillary system, while the driven system is identified with the $^{13}C$ spin that in [43] is initialized in an effective thermal state of the initial Hamiltonian. The Hamiltonian of the $^{13}C$ spin reads as

$$H(t) = 2\pi \hbar \nu(t) \left( \sigma_x \sin(\pi t/2\tau) + \sigma_y \cos(\pi t/2\tau) \right), \quad (57)$$

where $\nu(t) = \nu_1(1-t/\tau) + \nu_2 t/\tau$, $\tau = 0.1$ ms, $\nu_1 = 2.5$ kHz, and $\nu_2 = 1.0$ kHz. Using these parameters, we can readily simulate the close dynamics of the system and obtain the KDQ. In particular, by initialising the system in the quantum state $|+\rangle = (|0\rangle + |1\rangle)/\sqrt{2}$, where $|0\rangle$, $|1\rangle$ are the eigenstates of the initial Hamiltonian $H(0)$, the KDQ presents both negative and imaginary values.

On the other hand, starting from a thermal state of the initial Hamiltonian leads to a positive KDQ distribution coinciding with the TPM one, as shown in Fig. 5.

As discussed in section V, one can test conditions for nonzero imaginary components of the KDQ (respectively, for negative real components) by measuring interferometrically the characteristic function at 2 (respectively, 3) different times. The appearance of non-classicality in this system is shown in Fig. 6, where we perform these tests in our simulations.

### B. Proposal of solid-state implementation

Interferometric schemes can also be applied to bipartite systems other than the NMR one of Ref. [43]. In particular, we propose to consider a two-qubit system in a solid-state platform: the electronic spin of a NV center in diamond, and the nuclear spin of the nitrogen atom that forms the NV. Both of these are spin-triplets, but can be treated as two qubits by selectively addressing the desired transitions.

In our proposal, the NV electronic qubit works as the ancillary system, while the N nuclear spin is the system qubit. The expectation value of $\sigma_x$ and $\sigma_y$ of the ancilla can be measured with high fidelity, since the electronic spin state can be read out optically, due to the different photoluminescence of the spin projections. Then, the system Hamiltonian is implemented by driving the nuclear spin with a radiofrequency signal (with typical Rabi frequency of the order of tens of kHz), leaving the electronic spin unaltered. A microwave signal is used to drive the electronic spin dynamics, without modifying the nuclear spin. Hence, local gates can be applied to each spin individually thanks to the very different excitation frequency of the nuclear and electronic spins. Local gates can be also applied conditioned on the state of the other spin.
of the real parameter \( u \) with known results in classical thermodynamics, like the fluctuation-dissipation theorem, can be drawn. Here, we thus attempt to provide a comprehensive conceptual setting that contextualizes quasiprobabilities as an appropriate tool to describe thermodynamic and, more in general, out-of-equilibrium quantum processes.

VII. THERMODYNAMICS WITH QP DISTRIBUTIONS

Let us now address the question of adopting quasiprobability distributions to assess the statistics of thermodynamic quantities, such as the work \( w \) and the heat \( q \), in the quantum regime [15, 19]. Specifically, we investigate to which extent quasiprobability distributions are suited to characterize quantum energy fluctuations. This is especially relevant when a strict correspondence with known results in classical thermodynamics, like the fluctuation-dissipation theorem, can be drawn. Here, we thus attempt to provide a comprehensive conceptual setting that contextualizes quasiprobabilities as an appropriate tool to describe thermodynamic and, more in general, out-of-equilibrium quantum processes.

A. An operational underpinning

In the quantum regime, energy fluctuations are subject to specific constraints originating from the postulates of quantum mechanics. This is evident when characterizing the statistics of thermodynamic quantities defined over two times, e.g., work fluctuations, where one has to deal with the unavoidable information-disturbance trade-offs inherent in every measurement scheme. For example, the seminal two-point measurement (TPM) scheme extracts the statistics of energy at two times while destroying quantum coherence and correlation in the energy eigenbasis. This has motivated various recent works [14, 59, 61, 131–135] proposing alternative schemes to the TPM one (see Ref. [136] for a review).

Despite the intense interest raised by these questions, the research line about quantum energy fluctuations mostly developed independently of notions such as Heisenberg’s uncertainty relations, information-disturbance trade-offs and quasiprobability representations, which are the go-to tools employed when dealing with non-commutativity in other contexts. Just to make an example, within quantum mechanics or quantum optics we are completely used to the idea that the non-commutativity between observables such as position \( X \) and momentum \( P \) implies that the more information a scheme extracts about one, the more the statistics of the other will be disturbed [137]. In addition, we are also used to say that the Wigner quasiprobability provides a useful description of the joint distribution of \( (x, p) \), with the negativity being a useful notion of non-classicality.
But in the context of work fluctuations, where the two observables are energy at two different times, the debate has focused on what is the “right” definition of work, and the question of witnessing and quantifying the underlying non-commutativity has not featured prominently.

However, operationally we are dealing with the same phenomenon. For $X$ and $P$, one experimentally observes that the measurement statistics in general depends on the order with which we measure them. In the context of work fluctuations for a closed system, where we want to measure energy at two times, consider the two following protocols:

1. The energy at the initial time $t = 0$ is measured, the system is evolved, and then also the energy at the final time $t = \tau$ is measured. The work $w$ is the difference between the two energy outcomes.

2. The system is evolved and the energy at the final time $t = \tau$ is measured. The reverse dynamics is implemented and the energy at the initial time is measured. The work $w$ is (minus) the difference between the two energy outcomes.

While the second scheme may appear slightly odd, it is clear that classically the two are exactly equivalent. Quantum mechanically, in general, they are not. One is the analogue of measuring $X$ followed by $P$, and the other is the analogue of measuring $P$ followed by $X$. Operationally, it is this non-commutativity that leads to multiple inequivalent definitions of work, and the quasiprobabilities as a tool to quantify non-classicality in thermodynamic work fluctuations.

B. A formal underpinning

Recently, several no-go theorems have attempted to formalize the obstacles that every proposal to define and measure (work) fluctuations in the quantum regime must face. These theorems rely on certain natural thermodynamic assumptions, such as the recovery of results from stochastic thermodynamics for special classes of states [29, 30]. Theorem 1, which we have introduced in section II, instead, gives a purely information-theoretic account of the issue. Specifically, by identifying the time-dependent observables $A$ and $B$ with the Hamiltonian at the initial and final times, $A = H(0)$ and $B = H(t)$ respectively, Theorem 1 forbids the existence of a (linear) joint probability distribution over these two energy measurements whenever incompatibility arises, independently of the specific thermodynamic assumptions at play. The value of this simple observation is that all the tools and insights coming from the study of incompatible measurements in quantum mechanics can be readily applied to the thermodynamic question of defining work fluctuations.

Before moving on, let us discuss the relation between Theorem 1 and recent no-go theorems on the definition of work fluctuations in the quantum regime [29, 30]. The reader that prefers to skip this part can do so, since the rest of the work does not depend on this analysis.

The no-go theorem by Perarnau-Llobet et. al. [29] includes assumption (2) of Theorem 1 and weakens assumption (1) to

\[ \sum_{i \neq j} p_{ij}(\rho)(E_f - E_i) = \text{Tr}(H(t)E(\rho)) - \text{Tr}(H(0)\rho). \quad (58) \]

Moreover, the no-go theorem in [29] requires a third assumption, i.e.,

\[ (3) \text{ Fix the joint distribution } p_{ij}(\rho) \text{ for diagonal states:} \]

\[ \text{Whenever } |\rho, H(0)\rangle = 0, \quad p_{ij}(\rho) = p_{ij}^{\text{TPM}}(\rho), \quad (59) \]

with $p_{ij}^{\text{TPM}}(\rho)$ defined in Eq. (5).

While assumption (3) is reasonable in a classical thermodynamic setting, and it is inspired by stochastic thermodynamic considerations, it may appear overly restrictive to impose a special form to the joint distribution for all diagonal states.

Perhaps for this reason, the no-go theorem by Hovhannisyan et. al. in Ref. [30] replaces (3) with an assumption (3’) that only involves thermal states:

\[ (3') \text{ For any thermal state } \tau_\beta \equiv e^{-\beta H(0)}/\text{Tr} \left( e^{-\beta H(0)} \right), \]

the Jarzynski equality [140] holds

\[ F_\beta(H(t)) - F_\beta(H(0)) = -\beta^{-1} \log \left\langle e^{-\beta(E_f(\tau_\beta) - E_i(\tau_\beta))} \right\rangle, \quad (60) \]

where $\beta > 0$, $F_\beta(X) \equiv -\beta^{-1} \log \text{Tr} \left( e^{-\beta X} \right)$ and $\left\langle e^{-\beta(E_f(\tau_\beta) - E_i(\tau_\beta))} \right\rangle \equiv \sum_{ij} p_{ij}(\tau_\beta) e^{-\beta(E_f(\tau_\beta) - E_i(\tau_\beta))}$.

The Jarzynski equality is a cornerstone result in classical non-equilibrium thermodynamics, where $F_\beta(H(t)) - F_\beta(H(0))$ is naturally interpreted as the equilibrium free-energy difference. (3’) expresses the wish to define fluctuations in a way that the Jarzynski equality still holds for initial thermal states, and the no-go theorem proves its incompatibility in conjunction with (1w) and (2).

Compared to these two results, the strength of our no-go theorem is that it is based on purely information-theoretic arguments. In particular, assumptions (1) and (2) do not involve the specific values of the random variables (measurement outcomes) $E_i(0)$ and $E_f(t)$. Table II summarizes these various results.

C. Circumventing the no-go theorem for energy fluctuations

As we have already seen in section II, we have to drop one among the assumptions (1) and (2) of Theorem 1 in
order to characterize the statistics of energy fluctuations with a joint probability distribution in the presence of non-commutativity between $\rho$, $H(0)$, and $E^\dagger(H(t))$. Alternatively, one has to resort to quasiprobabilities. Let us thus discuss each of these alternatives in the quantum thermodynamics context.

*Drop assumption (1).* That is, we consider disturbing measurement schemes that do not recover the marginals over an initial and final energy measurements. In quantum thermodynamics, the best known protocol dropping assumption (1) is the celebrated TPM scheme [71, 141], whereby one simply measures $H(0)$ at the initial time and sequentially $H(t)$ at the final time. This is an extremal choice among the strategies dropping (1), since the distribution over $H(0)$ is error-free and all the disturbance is pushed onto the second energy measurement. In fact, the marginal energy distributions at times $s = 0$ and $s = t$ in the TPM scheme are, respectively,

$$\sum_i q^\text{TPM}_{if} = \text{Tr}(\Pi_i(0)\rho)$$

$$\sum_i q^\text{TPM}_{if} = \text{Tr}(E^\dagger(\Pi_f(t))D(\rho))$$

with $D(\rho) \equiv \sum_i \text{Tr}(\Pi_i(0)\rho)\Pi_i(0)$ denoting the dephasing channel in the eigenbasis of the initial Hamiltonian $H(0)$. As highlighted in section IV A, the TPM scheme has several experimental implementations, both in closed and open quantum systems, for the test of quantum fluctuation theorems and thermodynamic relations [43, 104–111, 142–144]. Also intermediate possibilities dropping assumption (1) can be considered, where some error on $H(0)$ is tolerated to decrease the disturbance on $H(t)$ according to a given cost function. For a detailed discussion of this approach in a thermodynamic context, we refer the reader to Ref. [57] where the issue of dropping assumption (1) is specifically studied under the perspective of the approximate joint measurability of $H(0)$ and $E^\dagger(H(t))$.

*Drop assumption (2).* Assumption (2) follows immediately if the joint probabilities $p_{if}(\rho)$ for the energy variation $\Delta E = E_f - E_i$ are obtained from a generalized measurement on the final state [29]. So, the first way to induce the breakdown of assumption (2) is to characterize energy fluctuations by means of a protocol that depends on the initial state, thus entailing a non-linearity of $p_{if}(\rho)$ in $\rho$. Along this direction, it is worth mentioning the Bayesian network approach recently introduced in [59, 145], which involves an initial measurement in the eigenbasis of the system density operator. We also refer to [30] for further discussion. As a general comment, any dependence of the measurement protocol on the initial state seems to be in contradiction with the definition of energy in classical thermodynamics that does not depend on the particular phase-space distribution taken as input ensemble. Another measurement strategy that drops assumption (2), without introducing an explicit state-dependence of the protocol, is the end-point measurement (EPM) approach [61]. This definition puts together the energy statistics of two incompatible measurement schemes, performed respectively at times $s = 0$ and $s = t$, and in fact it corresponds to Eq. (3), also reported in Ref. [53]. In practice, one needs to generate multiple copies of $\rho$ and perform a measurement of $H(0)$ on half of the copies, while the other half are evolved under $\mathcal{E}$ and then $H(t)$ is measured on them. As a general comment, a limitation with this definition is that in every scenario one postulates no correlations between initial and final energy, in contrast to what one expects considering the corresponding classical scenario.

*Drop $p_{if}(\rho) \geq 0$.* This is the quasiprobability approach in which one associates to realizations of the stochastic variable $\Delta E = E_f - E_i$ a complex number $q_{if}(\rho)$ satisfying $\sum_{if} b_{i,f}^*(\rho) = 1$, linear in $\rho$ and with the correct marginals.

**D. The KDQ as a work quasi-probability**

Here we explore the study of thermodynamic fluctuations by means of the quasiprobabilities $q_{if}(\rho) = \text{Tr}(\Pi_i(0)\Pi_f(t)\rho)$, where $H(0) = \sum_i E_i(0)\Pi_i(0)$, $H(t) = \sum_f E_f(t)U(t)^\dagger H(t)U(t) = \sum_i E_f(t)\Pi_i(t)$ are the initial and final Hamiltonian in the Heisenberg picture.

Let us start by noting that this object has a satisfactory classical limit. Whenever two among $\rho$, $\Pi_i(0)$ and $E^\dagger(\Pi_f(t))$ commute, the KDQ reduces to Eq. (5), i.e.,

$$q_{if}(\rho) = \text{Tr}(\Pi_i(0)\rho)\text{Tr}(E^\dagger(\Pi_f(t))\Pi_i(0))$$

When this occurs for every $i,f$ the KDQ is an actual probability distribution and a classical stochastic interpretation is possible. Effective commutativity can result from decoherence or coarse-graining of the energy measurements. In this limit the KDQ coincides with the statistics originating from the TPM scheme, which in turn can be associated to the classical definitions of work in the case of unitary dynamics [146].

We now turn our attention to the moments of the work variable $w_{if} \equiv E_f(t) - E_i(0)$ according to the KDQ. Let

| No-go theorem | Correct marginals (1) | Energy conservation (1w) | Convex (2) | Recovers TPM (3) | Recovers Jarzynski (3') |
|---------------|------------------------|--------------------------|------------|------------------|--------------------------|
| Ref. [29]     | ×                      | ×                        | ×          | ×                | ×                        |
| Ref. [30]     | ×                      | ×                        | ×          | ×                | ×                        |

TABLE II. Sets of properties proven to be mutually incompatible in no-go theorems for the description of work fluctuations.
\[\rho(t) = U(t)\rho U^\dagger(t).\] As already anticipated, one has
\[\langle w\rangle_{\text{KD}} = \sum_{ij} q_{ij} w_{ij} = \text{Tr}(\rho(t)H(t)) - \text{Tr}(\rho H(0)),\]
which coincides with the usual notion of average work as the difference between the average energy at the final and initial times. More interesting is the variance
\[\text{Var}[w]_{\text{KD}} = \langle w^2\rangle_{\text{KD}} - \langle w\rangle^2_{\text{KD}}\]
\[= V_R + iV_I,\]
(64)
since it contains both a real and an imaginary part. The real part, which is equivalent to the work variance computed using the MHQ, reads
\[V_R = \text{Var}[H(0)] + \text{Var}[H(t)] - 2\text{Cov}(H(0), H(t)),\]
(65)
where \(\text{Cov}(H(0), H(t))\) is the usual notion of quantum covariance, i.e.,
\[\text{cov}(H(0), \tilde{H}(t)) = \text{Tr}\left(\left\{\left(\langle H(0) - \langle H(0)\rangle, \langle \tilde{H}(t) - \langle \tilde{H}(t)\rangle\right)\right\}\rho\right),\]
(66)
and
\[\text{Var}[H(t)] = \text{Tr}(\rho(t)H(t)^2) - \text{Tr}(\rho(t)H(t))^2.\]
Recall that classically one has that
\[\text{Var}[w]_{\text{clas}} = \text{Var}[E(0)] + \text{Var}[E(t)] - 2\text{Cov}(E(0), E(t))\]
(67)
with the usual definitions for the random variables \(E(0)\) and \(E(t)\). Hence, \(V_R\) is fully analogous to the classical formula for the variance of the difference of the two random variables, with the natural identification of the covariance with the quantum one and \(\text{Var}[H(0)], \text{Var}[H(t)]\) the energy variance of the quantum energy measurements at the initial and final time.

For the imaginary part, instead, we have
\[V_I = i\text{Tr}\left(\rho[H(0), \tilde{H}(t)]\right),\]
(68)
which is a purely quantum component that directly measures the non-commutativity between the measurements at the initial and final times. Eq. (68) also quantifies the inequivalence of the two work protocols 1. and 2., described in section VII A. We thus see that the KDQ encodes relevant information about the quantum energy fluctuations and how non-commutativity affects them.

Comparing the classical and quantum variances of work using Eqs. (67) and (65), we can show that, quantum mechanically, fluctuations of work (or of the energy-variation, \(\Delta E\)), in the general case are restricted by the uncertainty principle encoded in the Heisenberg-Robertson inequality \(\text{Var}[A(0)]\text{Var}[B(t)] \geq \text{Cov}(A(0), B(t))^2 + \text{Tr}\left(\frac{1}{2}\rho\left[A(0), B(t)\right]\right)^2\) (see Appendix D for the formal derivation of this result). Classically, instead, the covariance of two random variables is bounded by their variances, so that for the system energies one has: \(\text{Var}[E(0), E(t)] = \sqrt{\text{Var}[E(0)]\text{Var}[E(t)]}\). Replacing in Eq. (67), we see that \(\text{Var}[w]_{\text{clas}}\) is bounded from above and below by the energy variances at the beginning and at the end of the process. Quantum mechanically, this bound becomes stronger in presence of non-commutativity. In fact, the Heisenberg-Robertson uncertainty inequality implies
\[\left|\text{Cov}(H(0), \tilde{H}(t))\right| \leq \sqrt{\text{Var}[E(0)]\text{Var}[E(t)] - \frac{1}{2}V_I^2}.\]
(69)
The presence of the imaginary part of the variance, which has no classical analogue as it encodes non-commutativity, entails that the real part (that, as we argued, is a natural analogue of the classical variance) is restricted within a smaller interval as a function of \(\text{Var}[E(0)], \text{Var}[E(t)]\) compared to what is possible classically:
\[|V_R - \text{Var}[H(0)] - \text{Var}[E(t)]| \leq \sqrt{\Delta_c^2 - 2V_I^2},\]
(70)
where \(\Delta_c \equiv \sqrt{4\text{Var}[H(0)]\text{Var}[\tilde{H}(t)]}\) denotes the classical bound and \(V_I\) is the quantum correction. This result is illustrated in Fig. 7 for the set-up of Ref. [43] discussed in detail in section VI. In this case, the quantum process is unitary and the work variance for both the KDQ and TPM distributions are plotted as a function of the process duration \(t\), together with the quantum (red) and classical (blue) variance bounds. Thus, the example in Fig. 7 clearly shows a situation in which \(\text{Re Var}[w]_{\text{KD}}\) is strongly restricted with respect to its classical counterpart.

What about higher-order fluctuations? In principle, one can try to build up fluctuation theorems out of the KQD distribution\(^{1}\). In fact, for an initial thermal state one recovers
\[\langle e^{-\beta w}\rangle_{\text{KD}} = e^{\beta\Delta F}.\]
(71)
However, this relation does not hold out-of-equilibrium, neither classically nor quantum-mechanically. Similarly to [14], one can formally write the equality
\[\langle e^{-\alpha E}\rangle_{\text{KD}} = e^{-\alpha \Delta F}\mathcal{N},\]
(72)
where \(\alpha\) denotes an inverse energy scale and \(\mathcal{N} \equiv \text{Tr}(\mathcal{E}^{1}(\rho_{\text{th}}(t))\rho_{\text{th}}(0)^{-1}\rho)\). This KD fluctuation theorem should be compared with
\[\langle e^{-\alpha E}\rangle_{\text{TPM}} = e^{-\alpha \Delta F}\gamma\]
(73)
\(^{1}\) See also the discussion in [147, 148] highlighting the relevance of quasiprobabilities in the derivation of generalized fluctuation theorems.
for the standard TPM probability distribution, where
\[
\gamma \equiv \text{Tr}(\mathcal{D}(\rho)\rho_{th}^{-1}(0)\mathcal{E}_{\text{eff}}(\rho_{th}(t)))
\]
is denoted as efficiency [149–151]. Both \(\gamma = 1\) and \(N = 1\) when \(\rho\) is thermal at inverse temperature \(\alpha\) and the dynamics is unital.

Contrary to Eq. (73), Eq. (72) encodes also the information on the full initial quantum state comprising the coherence in the \(H(0)\) basis, which is erased in the TPM scheme. Both relations, however, share the same problem: their lack of universality, with the right-hand-side depending on the microscopic details of the dynamics. As a possible application, the KD fluctuation theorem tells us that if we measure \(\text{Re}N < 0\) or \(\text{Im}N \neq 0\), then \(\mathcal{R}[q] > 0\). In this sense, the measurement of both \(\text{Re}N < 0\) and \(\text{Im}N \neq 0\) can be used as a witness of non-classicality.

Finally, to further analyse the KD quasiprobability, it can be useful to look at the cumulant generating function

\[
K_{\text{KD}}(\alpha) \equiv \log \langle e^{-\alpha \Delta E} \rangle_{\text{KD}} = \log \text{Tr}(\rho e^{\alpha H(0)} e^{-\alpha R(t)}).
\]

It is worth noting that, since the KDQ can also assume negative and complex values, in Eq. (74) the logarithm is intended in the sense of the principal value, whose imaginary part lies in the interval \([-\pi, \pi]\). By expanding the exponentials in Eq. (74), we can show that the cumulant generating function admits an expansion in terms of the quantum correlation functions

\[
C_{Q}(n, m) \equiv \langle H(0)^{n} \hat{H}(t)^{m} \rangle = \text{Tr}(\rho H(0)^{n} \hat{H}(t)^{m}),
\]
i.e.,

\[
K_{\text{KD}}(\alpha) = \log \sum_{n, m=0}^{+\infty} (-1)^{m} \frac{\alpha^{n+m}}{n!m!} C_{Q}(n, m).
\]

This is a direct generalization of the cumulant generating function given by applying the TPM scheme, where we would have an analogous expansion in terms of the two-point thermal (auto)correlation functions \(C(n, m) \equiv \text{Tr}(\rho_{th}(0) H(0)^{n} \hat{H}(t)^{m})\). Note that the expressions for the TPM scheme coincide with the above if we replace everywhere \(\rho\) with its dephased version \(\mathcal{D}(\rho)\).

VIII. CONCLUSIONS

In this work, we investigate aspects of the Kirkwood-Dirac quasiprobability (KDQ) distribution that allows us to characterize the joint statistics of incompatible observables in a quantum process, focusing in particular on reconstruction protocols and witnessing non-classical behaviour.

It is well-known that quasiprobabilities are a viable approach to the description of the joint statistics of incompatible observables in quantum mechanics. As we show in section II, quasiprobabilities are the only way to define an object reproducing the correct marginals statistics and respecting the linearity of probability theory.

Here we focus on the KDQ due to its numerous recent applications in disparate fields such as thermodynamics, metrology, tomography, chaos theory, measurement-disturbance, foundations of quantum mechanics. In reviewing the conceptual foundations and some of the applications pedagogically, as well as uncovering some previously unnoticed connections to the field of dynamical quantum phase transitions, we hope to provide a useful primer to the growing results in this area.

Given the growing relevance of the KDQ, it is timely to devise strategies to experimentally access it or, at least, its non-classical features encoded in its negative and non-real components. We do this in great detail by reviewing and proposing measurement schemes suitable for the task. Some of the proposed schemes can be implemented in current quantum experiments and are also suitable for quantum simulation on quantum computing platforms. In order to complete the picture, we also give experimental perspectives on the feasibility of some of the schemes discussed, and we propose a possible realization of an interferometric scheme in a solid-state NV center experiment.

Finally, we delve into the implications of using the KDQ in the context of quantum thermodynamics, where it can account for purely quantum features beyond standard projective measurement schemes. In quantum thermodynamics, the task of extracting the statistics of quantum fluctuating variables is the basis of the fluctuation theorems and fluctuation-dissipation relations. In this context, we discuss quasiprobabilities as an appropriate tool for describing thermodynamics. The KDQ, indeed, encodes the contribution of the non-commutativity of state and observables in a quantum work protocol or, more generally, in an open quantum process. This sets it apart from commonly used projective measurement scheme, as the KDQ allows to probe the effects of
observable incompatibility at the level of the moments of the work (energy) distribution. In fact, we observe that the variance of the KDQ work distribution includes, in general, both real and imaginary parts, with the latter encoding the mutual incompatibility of observables $H(0)$ and $\hat{H}(t)$. This gives rise to stronger restrictions on the values of the KDQ variance than those governing classical random variables. Beyond the variance, the KDQ also allows us to reformulate a would-be-fluctuation theorem. As is also the case for system initialized out-of-equilibrium states or non-unital processes, the KDQ fluctuation theorem does not share the same universality as Jarzynski equality but encodes, nonetheless, relevant information oblivious to more invasive schemes.

**Outlook**

Apart from the results discussed in this work, our investigation opens several interesting research lines, both on the theoretical and experimental sides. First and foremost, the varied array of measurement schemes for the reconstruction of the KDQ distribution calls for a detailed analysis of the most suitable scheme, in connection with different physical systems of interest. Moreover, the rephrasing of many of the schemes in a circuit form also makes them amenable to being implemented on current quantum computing architectures.

The given tools probing the KDQ distribution, the investigation of the role of quantum coherence and quantum features in the statistics of energy fluctuations. In general, both real and imaginary parts, with the latter encoding the mutual incompatibility of observables $H(0)$ and $\hat{H}(t)$. This gives rise to stronger restrictions on the values of the KDQ variance than those governing classical random variables. Beyond the variance, the KDQ also allows us to reformulate a would-be-fluctuation theorem. As is also the case for system initialized out-of-equilibrium states or non-unital processes, the KDQ fluctuation theorem does not share the same universality as Jarzynski equality but encodes, nonetheless, relevant information oblivious to more invasive schemes.

Finally, in the context of quantum thermodynamics, the possible thermodynamic implications and the interpretation of the KDQ non-classicality in quantum out-of-equilibrium regimes remain open questions. Nevertheless, fluctuation theorems beyond Jarzynski equality have been recently employed to benchmark the performance of quantum computing architectures [144, 152, 153]. The tools developed in our work have the potential to offer additional insight into this topic, accounting for exquisitely quantum features in the statistics of energy fluctuations.

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[1] W. Heisenberg, Über den anschaulichen inhalt der quantentheoretischen kinematik und mechanik, Z. Physik 43, 172 (1927).
[2] E. Schrödinger, About Heisenberg uncertainty relation, arXiv preprint quant-ph/9903100 (1999).
[3] C. Branciard, Error-tradeoff and error-disturbance relations for incompatible quantum measurements, Proceedings of the National Academy of Sciences 110, 6742 (2013).
[4] E. Wigner, On the quantum correction for thermodynamic equilibrium, Phys. Rev. 40, 749 (1932).
[5] K. Husimi, Some formal properties of the density matrix, Proceedings of the Physico-Mathematical Society of Japan. 3rd Series 22, 264 (1940).
[6] E. P. Wigner, The problem of measurement, American Journal of Physics 31, 6 (1963).
[7] R. J. Glauber, Coherent and incoherent states of the radiation field, Phys. Rev. 131, 2766 (1963).
[8] E. C. G. Sudarshan, Equivalence of semiclassical and quantum mechanical descriptions of statistical light beams, Phys. Rev. Lett. 10, 277 (1963).
[9] C. Zachos, D. Fairlie, and T. Curtright, Quantum mechanics in phase space: an overview with selected papers (World Scientific, 2005).
[10] J. G. Kirkwood, Quantum statistics of almost classical assemblies, Phys. Rev. 44, 31 (1933).
[11] P. A. M. Dirac, On the analogy between classical and quantum mechanics, Rev. Mod. Phys. 17, 195 (1945).
[12] A. O. Barut, Distribution functions for noncommuting operators, Phys. Rev. 108, 565 (1957).
[13] L. M. Johansen, Quantum theory of successive projective measurements, Phys. Rev. A 76, 012119 (2007).
[14] A. Allahverdyan, Nonequilibrium quantum fluctuations of work, Phys. Rev. E 90, 032137 (2014).
[15] M. Lostaglio, Quantum fluctuation theorems, contextuality, and work quasiprobabilities, Phys. Rev. Lett. 120, 040602 (2018).
[16] N. YungersHalpern, B. Swingle, and J. Dressel, Quasiprobability behind the out-of-time-ordered correlator, Phys. Rev. A 97, 042105 (2018).
[17] J. R. González Alonso, N. YungersHalpern, and J. Dressel, Out-of-time-ordered-correlator quasiprobabilities robustly witness scrambling, Phys. Rev. Lett. 122, 040404 (2019).
[18] R. Kunjwal, M. Lostaglio, and M. F. Pusey, Anomalous weak values and contextuality: Robustness, tightness, and imaginary parts, Phys. Rev. A 100, 042116 (2019).
[19] A. Levy and M. Lostaglio, Quasiprobability distribution for heat fluctuations in the quantum regime, PRX Quantum 1, 010309 (2020).
[20] D. R. M. Arvidsson-Shukur, J. Chevalier Drori, and N. Y. Halpern, Conditions tighter than noncommutativity needed for nonclassicality, J. Phys. A: Math. Theor.
[100] H. F. Hofmann, Complete characterization of post-selected quantum statistics using weak measurement tomography, Phys. Rev. A 81, 021013 (2010).

[101] H. F. Hofmann, How weak values emerge in joint measurements on cloned quantum systems, Phys. Rev. Lett. 109, 020408 (2012).

[102] F. Buscemi, M. Dall’Arno, M. Ozawa, and V. Vedral, Universal optimal quantum correlator, International Journal of Quantum Information 12, 1560002 (2014).

[103] M. Campisi, P. Hänggi, and P. Talkner, Colloquium: Quantum fluctuation relations: Foundations and applications, Rev. Mod. Phys. 83, 771 (2011).

[104] S. Hernández-Gómez, S. Gherardini, F. Poggiali, F. S. Cataliotti, A. Tombettoni, P. Cappellaro, and N. Fabbri, Experimental test of exchange fluctuation relations in an open quantum system, Phys. Rev. Research 2, 023327 (2020).

[105] S. Hernández-Gómez, N. Staudenmaier, M. Campisi, and N. Fabbri, Experimental test of fluctuation relations for driven open quantum systems with an NV center, New Journal of Physics 23, 065004 (2021).

[106] S. An, J.-N. Zhang, M. Um, D. Lv, Y. Lu, J. Zhang, Z.-Q. Yin, H. T. Quan, and K. Kim, Experimental test of the quantum Jarzynski equality with a trapped-ion system, Nat. Phys. 11, 193 (2015).

[107] A. Smith, Y. Lu, S. An, X. Zhang, J.-N. Zhang, Z. Gong, H. T. Quan, C. Jarzynski, and K. Kim, Verification of the quantum nonequilibrium work relation in the presence of decoherence, New J. Phys. 20, 013008 (2018).

[108] T. P. Xiong, L. L. Yan, F. Zhou, K. Rehan, D. F. Liang, L. Chen, W. L. Yang, Z. H. Ma, M. Feng, and V. Vedral, Experimental verification of a Jarzynski-related information-theoretic equality by a single trapped ion, Phys. Rev. Lett. 120, 010601 (2018).

[109] Z. Zhang, T. Wang, L. Xiang, Z. Jia, P. Duan, W. Cai, Z. Zhan, Z. Zong, J. Wu, L. Sun, Y. Yin, and G. Guo, Experimental demonstration of work fluctuations along a shortcut to adiabaticity with a superconducting Xmon qubit, New J. Phys. 20, 085001 (2018).

[110] P. H. S. Ribeiro, T. Häffner, G. L. Zanin, N. R. da Silva, R. M. de Araújo, W. C. Soares, R. J. de Assis, L. C. Céleri, and A. Forbes, Experimental study of the generalized Jarzynski fluctuation relation using entangled photons, Phys. Rev. A 101, 052113 (2020).

[111] G. H. Aguilar, T. L. Silva, T. E. Guimarães, R. S. Piera, L. C. Céleri, and G. T. Landi, Two-point measurement of entropy production from the outcomes of a single experiment withcorrelated photon pairs, arXiv preprint arXiv:2108.03289 (2021).

[112] S. Hernández-Gómez, S. Gherardini, A. Belenchia, M. Lostaglio, A. Levy, and N. Fabbri, Experimental assessment of non-classicality in a solid-state spin qutrit, arXiv preprint arXiv:2207.12960 (2022).

[113] S. Gherardini, M. M. Müller, A. Tombettoni, S. Rufio, and F. Caruso, Reconstructing quantum entropy production to probe irreversibility and correlations, Quantum Sci. Technol. 3, 035013 (2018).

[114] G. S. Thekkadath, R. Y. Saalink, L. Giner, and J. S. Lundeen, Determining complementary properties with quantum clones, Phys. Rev. Lett. 119, 050405 (2017).

[115] R. F. Werner, Optimal cloning of pure states, Phys. Rev. A 58, 1827 (1998).

[116] T. Heinosaari and M. Ziman, The Mathematical Language of Quantum Theory (Cambridge University Press, 2012).

[117] K. J. Resch and A. M. Steinberg, Extracting joint weak values with local, single-particle measurements, Phys. Rev. Lett. 92, 130402 (2004).

[118] G. Mitchison, Weak measurement takes a simple form for cumulants, Phys. Rev. A 77, 052102 (2008).

[119] J. Lundeen and K. Resch, Practical measurement of joint weak values and their connection to the annihilation operator, Physics Letters A 334, 337 (2005).

[120] J. S. Lundeen and A. M. Steinberg, Experimental joint weak measurement on a photon pair as a probe of Hardy’s paradox, Phys. Rev. Lett. 102, 020404 (2009).

[121] A. M. Steinberg, Conditional probabilities in quantum theory and the tunneling-time controversy, Phys. Rev. A 52, 32 (1995).

[122] R. Mohseninia, J. R. González-Alonso, and J. Dressel, Optimizing measurement strengths for qubit quasiprobabilities behind out-of-time-ordered correlators, Phys. Rev. A 100, 062336 (2019).

[123] N. Vakhania, V. Tarieladze, and S. Chobanyan, Probability distributions on Banach spaces, Vol. 1 (Springer Science & Business Media, 2012).

[124] W. Rudin, Fourier analysis on groups (Courier Dover Publications, 2017).

[125] E. Porcu and V. Zastavnyi, Characterization theorems for some classes of covariance functions associated to vector valued random fields, Journal of Multivariate Analysis 102, 1293 (2011).

[126] J. Shohat and J. D. Tamarkin, The Problem of Moments, Mathematical Surveys and Monographs, Vol. 1 (American Mathematical Society, 1943).

[127] N. Lupu-Gladstein, Y. B. Yilmaz, D. R. M. Arvidsson-Shakur, A. Brodutch, A. O. T. Pang, A. M. Steinberg, and N. Y. Halpern, Negative quasiprobabilities enhance phase estimation in quantum-optics experiments, Phys. Rev. Lett. 128, 220504 (2022).

[128] T. Rosskopf, J. Zopes, J. M. Boss, and C. L. Degen, A quantum spectrum analyzer enhanced by a nuclear spin memory, npj Quantum Information 3, 33 (2017).

[129] M. Chen, M. Hirose, and P. Cappellaro, Measurement of transverse hyperfine interaction by forbidden transitions, Phys. Rev. B 92, 020101 (2015).

[130] S. Sangtawesin, C. A. McLellan, B. A. Myers, A. C. B. Arno, M. Ozawa, and V. Vedral, Quantum coherences, Phys. Rev. A 96, 012331 (2017).

[131] A. Sone, Y.-X. Liu, and P. Cappellaro, Quantum fluctuations and the tunneling-time controversy, Phys. Rev. E 99, 022135 (2019).

[132] T. Deffner, J. P. Paz, and W. H. Zurek, Quantum work and the thermodynamic cost of quantum measurements, Phys. Rev. E 94, 042115 (2016).

[133] S. K. Sone, Y.-X. Liu, and P. Cappellaro, Quantum Jarzynski equality in open quantum systems from the one-time measurement scheme, Phys. Rev. Lett. 125, 060602 (2020).

[134] A. Sone, Y.-X. Liu, and P. Cappellaro, Quantum Jarzynski equality in open quantum systems from the one-time measurement scheme, Phys. Rev. Lett. 125, 060602 (2020).

[135] P. Solinas, M. Amico, and N. Zanghì, Quasiprobabilities of work and heat in an open quantum system, Phys. Rev. A 105, 032606 (2022).
In this paragraph, let us provide the proof of a no-go theorem about quantum fluctuations of two observables (in general not commuting) measured at different time instants. Our result can be seen as an alternative to the no-go theorems of Refs. [29, 30], since it has the advantage not to make any reference to a particular measurement protocol (as e.g. the TPM scheme) and highlights the constraints provided by joint measurability in quantum mechanics.

Let us thus consider a process described by the quantum map $\mathcal{E}$ acting on the initial quantum state $\rho$. Then, let

$$A(0) = \sum_i a_i(0)\Pi_i(0) \quad \text{and} \quad B(t) = \sum_f b_f(t)\Xi_f(t)$$

be the observables whose fluctuations we are interested in. Our aim is to prove that there exists no joint distribution $p_{ij}(\rho)$ that is (i) a probability distribution linear in $\rho$ and (ii) admits the correct marginals, unless $[\Pi_i(0), \mathcal{E}^t(\Xi_f(t))] = 0$ for any value of the indexes $i, f$. In other terms, we are going to prove that (i) and (ii) hold together if and only if $[\Pi_i(0), \mathcal{E}^t(\Xi_f(t)))] = 0 \ \forall i, f$.

We first prove that if the joint distribution $p_{ij}(\rho)$ that describes the statistics of the observables $A(0)$ and $B(t)$ is both a probability distribution linear in $\rho$ and admits the correct marginals, then $[\Pi_i(0), \mathcal{E}^t(\Xi_f(t))] = 0$ for any $i, f$. Note that the convex linearity of $p_{ij}(\rho)$ means that, by taking $\rho = \sum_k p_k \rho_k$, $p_{ij}(\rho) = \sum_k p_k p_{ij}(\rho_k)$, while the fact that $p_{ij}(\rho)$ is a probability distribution just entails that $p_{ij}(\rho) \geq 0$ and $\sum_i p_{ij}(\rho) = 1$ for any $i, j$ and any $\rho$. Instead, whenever $p_{ij}(\rho)$ returns the correct marginals, then $\sum_f p_{ij}(\rho) = \text{Tr} (\Pi_i(0)\rho)$ and $\sum_i p_{ij}(\rho) = \text{Tr} (\Xi_f(t)\mathcal{E}(\rho))$.

Thus, by exploiting the Riesz representation theorem, the linearity of $p_{ij}(\rho)$ as a function of $\rho$ implies that there exist a linear operator $M_{ij}$, depending on the indexes $i, f$, such that

$$p_{ij}(\rho) = \text{Tr} (M_{ij}\rho) .$$

Then, if we also assume that $p_{ij}(\rho)$ is a probability distribution (in the standard sense), then the linear operator $M_{ij}$ is a positive operator-valued measure (POVM), thus entailing that $M_{ij}$ is semi-definite positive ($M_{ij} \geq 0$) and

$$\sum_i M_{ij} \geq 0 .$$
We can easily observe that one of the marginal observables is projection valued. Hence, from the Proposition 1 of Ref. [54], we can affirm that the product of marginals commutes, i.e.,

\[
\left[ \Pi_i(0), \mathcal{E}(\Xi_f(t)) \right] = 0 \quad \forall i, f
\]

that in turn corresponds to the condition of joint measurability of \( A(0) \) and \( B(t) \).

We now show that the validity of Eq. (A5) entails that \( p_{i,f}(\rho) \) is a probability distribution linear in \( \rho \) and with correct marginals. From Eq. (A5), in accordance with the Proposition 1 of Ref. [54], one can state that the joint distribution \( p_{i,f}(\rho) \) –returned by a sequential quantum measurement scheme– is provided by the following relations:

\[
p_{i,f}(\rho) = \text{Tr} \left( \rho \Pi_i(0) \mathcal{E}(\Xi_f(t)) \right) = \text{Tr} \left( \rho \mathcal{E}(\Xi_f(t)) \Pi_i(0) \right),
\]

thus implying

\[
\text{Tr}\left( |\rho, \Pi_i(0)\rangle \mathcal{E}(\Xi_f(t)) \right) = 0.
\] (A7)

Eq. (A7) has to be fulfilled for any value of \( i, f \). This means that for a generic open quantum map \( \mathcal{E} \), one has to require that \( [\rho, \Pi_i(0)] = 0 \forall i \), namely one has to take \( \rho \) as a mixed state in the basis of \( A(0) \): \( \rho = \sum_k p_k \Pi_k \). As a result,

\[
p_{i,f}(\rho) = \text{Tr} \left( \rho \Pi_i(0) \mathcal{E}(\Xi_f(t)) \right) = p_i \text{Tr} \left( \mathcal{E}(\Xi_f(t)) \right)
\]

that is identically equal to the joint distribution provided by the TPM scheme. This concludes our proof, since for an initial mixed state in the basis of \( A(0) \) the TPM joint distribution \( p_{i,f}(\rho) \) is a probability distribution linear in \( \rho \) and with correct marginals.

\section*{Appendix B: Proof of Theorem 2}

We report here the proof of Theorem 2 in the main text. This proof follows from the derivation in the Appendix of [154], where it is shown that the Hermitian part of the product of two non-commuting projectors has at least a negative eigenvalue.

Let us thus consider the MHQ given by

\[
\text{ReTr} \left( \rho \Pi_i(0) U^\dagger \Xi_f(t) U \right) = \text{Tr} \left( U^\dagger \Xi_f(t) U \{ \rho , \Pi_i(0) \} \right),
\]

where \( \{ \rho , \Pi_i(0) \} \equiv \rho \Pi_i + \Pi_i \rho \). Since here we are considering unitary quantum processes and the unitary transformation corresponds to a change of basis, we can get rid of the unitary process to get to the core of the proof. Accordingly, we just need to demonstrate that, given a generic initial state \( \rho \) and an initial measurement observable \( A \equiv \sum_a a_i \Pi_i \) such that \( [\rho , A] \neq 0 \), then the Hermitian part of the product of the state and one of the projectors \( \Pi_i \) of \( A \) has at least a negative eigenvalue. This conclusion shall be valid for all the projectors \( \Pi_i \) (with rank \( \geq 1 \)) that do not commute with \( \rho \), i.e., \([\rho , A] \neq 0 \). Whenever this conclusion holds, the projector \( U^\dagger \Xi_f(t) U \) for which \( \text{Re} \langle q_{i,f} \rangle < 0 \), can be simply chosen as the rank-1 projector on the eigenstate of \( \{ \rho , \Pi_i \} \) with negative eigenvalue.

The proof follows the main steps of the one in the Appendix of [154] that we sketch here for self-consistence. Let us thus consider \( G \equiv \{ \rho , \Pi_i(0) \} \) and a generic state \( |\psi \rangle = \Pi_i |\psi \rangle + (I - \Pi_i) |\psi \rangle \equiv |\psi_1 \rangle + |\psi_2 \rangle \), meaning that \( |\psi_1 \rangle \) and \( |\psi_2 \rangle \) lie in the subspace of the projectors \( \Pi_i \) and \( I - \Pi_i \), respectively. Few calculations lead us to

\[
\langle \psi | G | \psi \rangle = 2 \left[ \langle \psi_1 | \rho | \psi_1 \rangle - \text{Re} \langle \psi_1 | \rho | \psi_2 \rangle \right].
\]

Note that, for a given \( |\psi_1 \rangle \), if \( \text{Re} \langle \psi_1 | \rho | \psi_2 \rangle \) vanishes for any \( |\psi_2 \rangle \) then \( [\rho , \Pi_i] = 0 \). Since the latter is not the case by assumption, one can always choose \( |\psi_2 \rangle \) such that \( \text{Re} \langle \psi_1 | \rho | \psi_2 \rangle \neq 0 \). Now, if \( \text{Re} \langle \psi_1 | \rho | \psi_2 \rangle \) is positive, we can just take \(-|\psi_2 \rangle \) and then make \( |\psi_2 \rangle \) big enough so that \( \langle \psi | G | \psi \rangle < 0 \). This concludes the proof since we can now choose \( U^\dagger \Xi_f(t) U \) as the rank-1 projector on the negative eigenvalue eigenstate of \( G \), or just as \( |\psi \rangle \langle \psi | \) for the state \( |\psi \rangle = |\psi_1 \rangle + |\psi_2 \rangle \) built as before. Therefore, in conclusion, one needs a measurement observable \( B \) of the quantum system and/or a unitary quantum
Appendix C: Non-classicality’s properties

As discussed in the main text, the non-classicality of the KDQ is estimated via \([17, 20]\) \(\mathbb{N}(q(\rho)) = 1 + \sum_{i,f} |q_{i,f}(\rho)|\), with \(q(\rho)\) denoting the vector containing all KD quasiprobabilities. Let us summarize here the properties of this measure of non-classicality and for completeness briefly prove them:

**[P1] Faithfulness:** \(\mathbb{N}(q) = 0\) if and only if \(q\) is a probability distribution.

*Proof.* \(q_{i,f}\) satisfies \(\sum_{i,f} q_{i,f} = 1\). If any element \(q_{i,f}\) is negative or not real, it follows that \(|q_{i,f}| > q_{i,f}\) and so \(\mathbb{N}(q) > 0\). The converse holds too. \(\square\)

**[P2] Convexity:** \(\mathbb{N}[p q_1(\rho) + (1-p)q_2(\rho)] \leq p \mathbb{N}[q_1(\rho)] + (1-p)\mathbb{N}[q_2(\rho)]\), with \(p \in [0,1]\)

*Proof.* Setting \(q = pq_1 + (1-p)q_2\), the result follows immediately from the convexity of the absolute value function. \(\square\)

**[P3] Non-commutativity witness:** If \(\mathbb{N}(q(\rho)) > 0\), then there is a choice of \(i,f\) for which \((\rho, \Pi_i(0), \mathcal{E}^\dagger(\Xi_f(t)))\) are all mutually non-commuting.

*Proof.* Let us prove the counterpositive. So for every \(i, f\) we have at least a commuting pair. Note that for each fixed \(i, f, q_{i,f}\) has the general form \(\text{Tr}(ABC)\), where one pair among \(A, B\) and \(C\) is commuting and \(A, B\) and \(C\) are all positive semidefinite operators. Using the cyclic property of the trace, without loss of generality we can assume \([A, B] = 0\).

\[
\text{Tr}(ABC) = \text{Tr}\left(\sqrt{A} \sqrt{B} \sqrt{C}\right) = \text{Tr}\left(\sqrt{A} \sqrt{B} \sqrt{C}\right) = \text{Tr}\left(\left(D^\dagger D\right)C\right). \tag{C1}
\]

Note that we used \([\sqrt{A}, B] = 0\) and we defined \(D = \sqrt{B} \sqrt{A}\). With the above we rewrote \(\text{Tr}(ABC)\) as the trace of the product of two positive semidefinite operators, which is non-negative. Hence, \(\text{Tr}(ABC) \geq 0\). \(\square\)

**[P4] Monotone under decoherence:** Consider the decoherence dynamics \(D_s = (1-s)I + s\mathcal{D}\), where \(s \in [0,1]\) and \(\mathcal{D}\) is a transformation that removes off-diagonal elements either in the basis \(\{\Pi_i\}\) or in any basis obtained by orthogonalizing and completing \(\mathcal{E}^\dagger(\Xi_f)\) to a basis. Then, \(\mathbb{N}[q(D_s(\rho))] \leq \mathbb{N}[q(\rho)]\).

*Proof.* \(\mathbb{N}(q(D_s(\rho))) \leq (1-s)\mathbb{N}(q(\rho)) + s\mathbb{N}(q(D(\rho)))\) by convexity (P2). Furthermore, by construction \(D(\rho)\) commutes either with \(\Pi_i\) for every \(i\) or with \(\mathcal{E}^\dagger(\Xi_f)\) for every \(f\). From (P3), it follows that \(\mathbb{N}(q(D(\rho)) = 0\) and so \(\mathbb{N}(q(D_s(\rho))) \leq (1-s)\mathbb{N}(q(\rho))\). \(\square\)

**[P5] Monotone under coarse-graining:** Suppose \(q_{i,F} \equiv \sum_{i \in I, f \in F} q_{i,f}\), where \(I, F\) are disjoint subsets partitioning the indices \(\{i\}, \{f\}\). Then \(\mathbb{N}(q') \leq \mathbb{N}(q)\).

*Proof.* \(\mathbb{N}(q') = \sum_{i,j} |q_{i,j}| = \sum_{i,j} |\sum_{i \in I, j \in j} q_{i,j}| \leq \sum_{i,j} \sum_{i \in I, j \in j} |q_{i,j}| = \mathbb{N}(q)\). \(\square\)

Appendix D: Restrictions to energy-variation variance due to uncertainty principle: Formal derivation

Let us start from the computation of the energy-variation variance in term of the KD distribution, i.e., \(\text{Var}[\Delta E]_{\text{KD}}\). The latter is formally defined by

\[
\text{Var}[\Delta E]_{\text{KD}} \equiv \langle \Delta E^2 \rangle_{\text{KD}} - \langle \Delta E \rangle_{\text{KD}}^2 = \sum_{i,f} p_{i,f} \left(\hat{E}_f - E_i\right)^2 - \left(\sum_{i,f} p_{i,f}(\hat{E}_f - E_i)\right)^2 \tag{D1}
\]

that simplifies as

\[
\text{Var}[\Delta E]_{\text{KD}} = \text{Var}[H(0)] + \text{Var}[\hat{H}(t)] - 2 \sum_{i,f} p_{i,f} E_i \hat{E}_f + 2 \langle H(0) \rangle \langle \hat{H}(t) \rangle, \tag{D2}
\]

where \(\text{Var}[H(0)] \equiv \sum_{i,f} p_{i,f} E_i^2 - \langle H(0) \rangle^2 \in \mathbb{R}\), \(\text{Var}[\hat{H}(t)] \equiv \sum_{i,f} p_{i,f} \hat{E}_f^2 - \langle \hat{H}(t) \rangle^2 \in \mathbb{R}\), \(\langle H(0) \rangle \equiv \sum_{i,f} p_{i,f} E_i\), \(\langle \hat{H}(t) \rangle \equiv \sum_{i,f} p_{i,f} \hat{E}_f\), and

\[
\sum_{i,f} p_{i,f} E_i \hat{E}_f = \text{Tr} \left(\rho H(0) \hat{H}(t)\right). \tag{D3}
\]
The Hamiltonians $H(0)$ and $\tilde{H}(t)$ are Hermitian operators. Then, by observing that
\begin{equation}
\text{Tr} \left( \rho \left( H(0) - \langle H(0) \rangle \right) \left( \tilde{H}(t) - \langle \tilde{H}(t) \rangle \right) \right) = \text{Tr} \left( \rho H(0) \tilde{H}(t) - \langle H(0) \rangle \langle \tilde{H}(t) \rangle \right),
\end{equation}
we get
\begin{equation}
\text{Var}[\Delta E]_{KD} = \text{Var}[H(0)] + \text{Var}[\tilde{H}(t)] - 2\text{Tr} \left( \rho \left( H(0) - \langle H(0) \rangle \right) \left( \tilde{H}(t) - \langle \tilde{H}(t) \rangle \right) \right).
\end{equation}
In general, \(\text{Tr} \left( \rho \left( H(0) - \langle H(0) \rangle \right) \left( \tilde{H}(t) - \langle \tilde{H}(t) \rangle \right) \right)\) from now on denoted as \(\text{Tr} \left( \rho \Delta H(0) \Delta \tilde{H}(t) \right)\) with \(\Delta H(0) \equiv H(0) - \langle H(0) \rangle\) and \(\Delta \tilde{H}(t) = \tilde{H}(t) - \langle \tilde{H}(t) \rangle\) is a complex number whose real and imaginary parts can be determined through the following relation:
\begin{equation}
\text{Tr} \left( \rho \Delta H(0) \Delta \tilde{H}(t) \right) = \frac{1}{2} \text{Tr} \left( \rho \Delta H(0), \Delta \tilde{H}(t) \right) - \frac{1}{2} i \text{Tr} \left( i\rho \Delta H(0), \Delta \tilde{H}(t) \right),
\end{equation}
with \(\{\cdot, \cdot\}\) and \([\cdot, \cdot]\) denoting the anti-commutator and commutator, respectively. By definition, the quantity \(\frac{1}{2} \text{Tr} \left( \rho \left( \Delta H(0), \Delta \tilde{H}(t) \right) \right)\) is the quantum covariance of the operators \(H(0)\) and \(\tilde{H}(t)\):
\begin{equation}
\text{Cov}(H(0), \tilde{H}(t)) \equiv \frac{1}{2} \text{Tr} \left( \rho \left( \langle H(0) \rangle, (\tilde{H}(t) - \langle \tilde{H}(t) \rangle) \right) \right).
\end{equation}
Accordingly, by noting that
\begin{equation}
\text{Tr} \left( i\rho \left[ \Delta H(0), \Delta \tilde{H}(t) \right] \right) = \text{Tr} \left( i\rho \left[ H(0), \tilde{H}(t) \right] \right),
\end{equation}
one can finally conclude that
\begin{equation}
\text{Var}[\Delta E]_{KD} = \text{Var}[H(0)] + \text{Var}[\tilde{H}(t)] - 2 \text{Cov}(H(0), \tilde{H}(t)) - \text{Tr} \left( \rho \left[ H(0), \tilde{H}(t) \right] \right).
\end{equation}
According to the KD distribution, \(\text{Var}[\Delta E]_{KD}\) is in general a complex number and its imaginary part equals to \(\text{Tr}(i\rho[H(0), \tilde{H}(t)])\), i.e.,
\begin{equation}
\text{Im Var}[\Delta E]_{KD} = \text{Tr} \left( i\rho \left[ H(0), \tilde{H}(t) \right] \right).
\end{equation}
Secondly, let us define the correlation matrix
\begin{equation}
C = \begin{pmatrix}
\text{Tr} \left( \rho \Delta H(0)^2 \right) & \text{Tr} \left( \rho \Delta H(0) \Delta \tilde{H}(t) \right) \\
\text{Tr} \left( \rho \Delta \tilde{H}(t) \Delta H(0) \right) & \text{Tr} \left( \rho \Delta \tilde{H}(t)^2 \right)
\end{pmatrix} = \begin{pmatrix}
\text{Var}[H(0)] & \text{Tr} \left( \rho \Delta H(0) \Delta \tilde{H}(t) \right) \\
\text{Tr} \left( \rho \Delta H(0) \Delta \tilde{H}(t) \right)^* & \text{Var}[\tilde{H}(t)]
\end{pmatrix},
\end{equation}
where the complex number \(\text{Tr} \left( \rho \Delta \tilde{H}(t) \Delta H(0) \right)\) is the conjugate of \(\text{Tr} \left( \rho \Delta H(0) \Delta \tilde{H}(t) \right)\) = \(\text{Cov}(H(0), \tilde{H}(t)) + \frac{1}{4} \text{Tr} \left( \rho \left[ H(0), \tilde{H}(t) \right] \right)\), being \(H(0)\) and \(\tilde{H}(t)\) Hermitian operators. Therefore, also \(C\) is an Hermitian operator \((C^\dagger = C)\).

Now, let us impose that \(C\) is semi-definite positive \((C \succeq 0)\), so as to ensure that the correlation matrix is physical. The positivity of \(C\) is thus guaranteed when
\begin{equation}
\text{Var}[H(0)] \text{Var}[\tilde{H}(t)] \geq \text{Cov}(H(0), \tilde{H}(t))^2 + \frac{1}{4} \text{Tr} \left( i\rho \left[ H(0), \tilde{H}(t) \right] \right)^2,
\end{equation}
namely
\begin{equation}
\left| \text{Cov}(H(0), \tilde{H}(t)) \right| \leq \sqrt{\text{Var}[H(0)] \text{Var}[\tilde{H}(t)] - \frac{1}{2} \text{Tr} \left( i\rho \left[ H(0), \tilde{H}(t) \right] \right)^2}.
\end{equation}
In this way, by recalling that
\begin{equation}
\text{Re} \text{Var}[\Delta E]_{KD} = \text{Var}[H(0)] + \text{Var}[\tilde{H}(t)] - 2 \text{Cov}(H(0), \tilde{H}(t))
\end{equation}
and \(\text{Im} \text{Var}[\Delta E]_{KD} = \text{Tr}(i\rho[H(0), \tilde{H}(t)])\), we obtain the result
\begin{equation}
\left| \text{Re} \text{Var}[\Delta E]_{KD} - \text{Var}[H(0)] - \text{Var}[\tilde{H}(t)] \right| \leq \sqrt{\text{Var}[H(0)] \text{Var}[\tilde{H}(t)] - \text{Im} \text{Var}[\Delta E]_{KD}^2}
\end{equation}
that concludes our derivation.