Certifying quantum signatures in thermodynamics and metrology via contextuality of quantum linear response

Matteo Lostaglio\textsuperscript{1,2}

\textsuperscript{1}ICFO-Institut de Ciencies Fotoniques, The Barcelona Institute of Science and Technology, Castelldefels (Barcelona), 08860, Spain
\textsuperscript{2}QuTech, Delft University of Technology, P.O. Box 5046, 2600 GA Delft, The Netherlands\textsuperscript{*}

We give a general test to certify that the quantum phenomenology in the linear response regime cannot be described by any noncontextual emulator. This allows us to provide the first proof of a quantum signature in the operation of a quantum engine certified against generic classical emulations. Furthermore, we describe contextual advantages for local metrology. Given the ubiquity of linear response theory, we anticipate that our tools will allow to certify the absence of classical emulators for a wide array of quantum phenomena.

Linear response theory describes the reaction of a quantum system to a small perturbation. The theory finds countless applications in many fields of quantum physics, including molecular, atomic and nuclear physics, quantum optics and statistical mechanics. In this paper we present a general test to certify when the linear response of a quantum system cannot be reproduced by any noncontextual ontological model.

As an application, we identify quantum signatures in the power of a heat engine. In the context of quantum thermodynamics, the issue of identifying truly quantum advantages has been a long-standing open problem in the field. Several theoretical claims have been made that quantum coherence can offer improvements over certain incoherent thermodynamic engines and refrigerators (e.g., [1–9] and references therein), backed by recent experimental effort [10]. Many effects can however be reproduced within classical models, so it is disputed if quantum phenomena are instrumental to the improved performance of these machines [11, 12]. Differently from previous treatments we show that, in the presence of certain experimental features, one can certify quantum signatures against any classical emulator. Using these tools we show that the phenomenology of the two-stroke quantum engine model in the weak coupling regime [4] does not admit classical emulators. To our knowledge, this is the first example of such certificate.

As a second application, we turn to local metrology and consider the archetypal example of phase estimation using a qubit system. We show that, given the phenomenology of the phase estimation experiment, a nonzero Fisher information is incompatible with all classical (noncontextual) models. This complements a recent result showing that certain features of post-selected metrology are non-ontical) models. This complements a recent result showing that certain features of post-selected metrology are non-contextual. This complements a recent result showing that certain features of post-selected metrology are non-contextual. This complements a recent result showing that certain features of post-selected metrology are non-contextual.

We believe that the tools developed here, applicable as they are to any quantum system in the linear response regime, can find applications in the identification of genuine quantum signatures in a wide range of different platforms.

Non-contextual ontological models. When constructing classical emulators, it is natural to imagine them as ultimately reducible to a collection of classical systems (particles, oscillators) undergoing Hamiltonian dynamics with some generic interactions. For example, Ref. [11] uses such models to reproduce the short-time cooling enhancement which in quantum theory is attributed to the presence of quantum coherence. Here we want to certify any ‘genuine quantum signature’ against all these classical emulators; in fact, we will allow an even larger class of emulators: any noncontextual ontological model (OM).

We may start from the operational/experimental description of preparations, transformations and measurements, understood as sets of laboratory instructions according to which these operations are performed. To each, we associate the corresponding physical description in the OM, as summarized in the table below:

1. To every preparation procedure \( P \) one assigns a probability distribution \( \mu_P(\lambda) \) over some (measureable) set of physical states \( \lambda \). For example, if \( P \) involves leaving the system alone for a long time and \( \lambda = (x_1, \ldots, x_N, p_1, \ldots, p_N) \) are phase space points, \( \mu_P(\lambda) \) may be a thermal distribution.

2. A transformation procedure \( T \) is described by an update rule giving the probability that any final state \( \lambda' \) is reached, given that the initial state was \( \lambda \). We denote this transition probability by \( T_T(\lambda'|\lambda) \). For example, \( T_T(\lambda'|\lambda) \) may be generated by a rate equation among a discrete set of \( \lambda \), as in the classical emulators described in Ref. [12]. Or, if \( \lambda = (x, p) \), then \( T_T(x'=x(t), p'=x(0), p(0)) = \delta(x' - x(t))\delta(p' - p(t)) \), where \( (x(t), p(t)) \) is the solution of Hamilton’s equations with initial conditions \( (x(0), p(0)) \).

3. A measurement procedure \( M \) with outcomes \( k \) is associated to a response function \( \xi_M(k|\lambda') \), giving the probability that an outcome \( k \) is returned by \( M \) if the physical state is \( \lambda' \). For example, in classical mechanics, if \( M \) is a measurement of...
Consider the subclass of OM that are noncontextual as naturally follows from the propagation of probabilities. The same has to hold for operationally equivalent measurements, as Speckers notion \([14, \text{Appendix C})\]. One can easily see that Hamiltonian dynamics is an example of a noncontextual OM (see Appendix \(A\)). Other examples include Spekkens’ toy model \([17]\) or Hamiltonian mechanics with an uncertainty principle (the latter is equivalent to Gaussian quantum mechanics \([18]\)). These examples show that noncontextual OM allow to emulate measurement disturbance and even protocols involving superposition and entanglement. The fact that a quantum machine displays these quantum features is a necessary but not sufficient condition to certify an advantage.

In this paper we will hence adopt a stringent notion of quantum signature adopted to analyse several quantum information primitives \([13, 19–22]\): a set of operational features that cannot be reproduced within any noncontextual emulator. Noncontextual models include as special cases the classical emulators previously considered in the literature: e.g., discrete models with jump probabilities generated by rate equations \([12]\); Hamiltonian dynamics obtained via classical limit \([11]\); quantum mechanics in a fixed basis obtained via dephasing in the energy basis \([4]\). Our aim is to exclude all of them at once.

Given this setup, we now develop a test to certify quantum signatures in the phenomenology of the quantum linear response.

**Quantum linear response.** Consider a quantum state \(|\psi(t)\rangle\) in a finite-dimensional Hilbert space evolving according to Schrödinger equation under a time-dependent perturbation \(V(t)\):

\[
\frac{i\hbar}{dt} |\psi(t)\rangle = [H_0 + gV(t)] |\psi(t)\rangle.
\]

We develop our considerations here for pure states, but the extension to mixed states is straightforward. We are interested in the change of expectation values of an observable \(O\) due to the perturbation. By means of a shift, we will assume \(O = \sum_k o_k |o_k\rangle \langle o_k|\) with \(o_k \geq 0\). It is convenient to work in the interaction picture, \(O_I(t) = e^{iH_0 t/\hbar}O e^{-iH_0 t/\hbar}|\psi_I(t)\rangle = e^{iH_0 t/\hbar} |\psi(t)\rangle := U_I(t) |\psi(0)\rangle\) and study

\[
\langle \Delta O_I \rangle_t^Q := \langle \psi_I(t) | O_I(t) | \psi_I(t) \rangle - \langle \psi(0) | O_I(t) | \psi(0) \rangle.
\]

Operationally this corresponds to

\[
\langle \Delta O_I \rangle_t^Q := \sum_k o_k p(k | T_I(P), M_I) - \sum_k o_k p(k | P, M_I).\tag{7}
\]

where \(P, T_i\) and \(M_i\) are the preparation, transformation and measurement procedures described in quantum mechanics by \(|\psi(0)\rangle\), \(U_I(t)\) and \(O_I(t)\), respectively. From Dyson’s series

\[
U_I(t) = 1 - \frac{ig}{\hbar} \int_0^t dt' V_I(t') + O(g^2),\tag{8}
\]

where \(V_I(t) = e^{iH_0 t/\hbar} V(t) e^{-iH_0 t/\hbar}\). Quantum linear response gives

\[
\langle \Delta O_I \rangle_t^Q = \frac{ig}{\hbar} \int_0^t dt' \langle \psi(0) | V_I(t') O_I(t) | \psi(0) \rangle + O(g^2).\tag{9}
\]

The most important aspect of this formula is that generally the response is of \(O(g)\), unless there are any pairwise commutations among \(|\psi(0)\rangle \langle \psi(0)|\), \(O_I(t)\) and \(\int dt' V_I(t')\).
Another crucial experimental fact is encoded in the following channel equality [23]. Suppose that for $g$ small enough

$$
\frac{1}{2}U_t + \frac{1}{2}U_t^\dagger = (1 - p_d)I + p_dC_t,
$$

(10)

where $U_t(\cdot) := U_t(t)(\cdot)U_t(t)$, $I$ is the identity channel, $C_t$ is some other channel and $p_d = O(g^2)$ as $g \to 0$. We will later give tools to verify if a quantum experiment under consideration admits this decomposition in linear response. For now it suffices to say that in the case of a single qubit this decomposition holds in generality.

Experimentally, Eq. (10) underlines the fact that the transformation $T_t$ (represented by $U_t$ in quantum mechanics) can be reversed, to first order in $g$, by convex combination with another transformation $T_t^*$ (represented by $U_t^\dagger(t)$ in quantum mechanics). In particular, tossing a fair coin and performing either $T_t$ or $T_t^*$ is operationally indistinguishable from doing nothing with probability $1 - p_d = 1 - O(g^2)$. These experimental facts can be summarised as:

$$
\frac{1}{2}T_t + \frac{1}{2}T_t^* \approx_{op} (1 - p_d)T_{id} + p_dT_t^*,
$$

(11)

where $T_{id}$ denotes the ‘do nothing’ operation and $T_t^*$ denotes some other transformation (represented by the channel $C_t$ in quantum mechanics). As we will see, this approximate ‘reversibility by mixing’ or ‘stochastic reversibility’ tells us that the perturbation $T_t$ cannot be ‘too far’ from the do-nothing operation in any noncontextual emulation. We now prove this weakness, encoded operationally in Eq. (11), together with the observation of a $O(g)$ response of a quantum system, admits no classical emulation.

Main theorem. From Eq. (7) and Eq. (1) an OM predicts

$$
\langle \Delta O_t \rangle_i = \sum_k a_k \left[ \sum_{\lambda, \lambda'} \mu_{P}(\lambda)T_{t,\lambda}(\lambda')\lambda\xi_M(k|\lambda') - \sum_{\lambda} \mu_{P}(\lambda)\xi_M(k|\lambda) \right].
$$

(12)

In other words, when the initial state $|\psi(0)\rangle$ is prepared a $\lambda$ is sampled with probability $\mu_{P}(\lambda)$; when the unitary $U_{t}(t)$ is performed the state is updated to $\lambda'$ with probability $T_{t,\lambda}(\lambda')\lambda$; and finally a measurement of the observable $O_{t}(t)$ returns outcome $a_k$ with probability $\xi_M(k|\lambda')$. Then

Theorem 1 (Noncontextual bound on linear response), Suppose the operational equivalence in Eq. (11) is observed. Then in any noncontextual OM

$$
|\langle \Delta O \rangle_i^{NC}| \leq 2p_d a_{\text{max}},
$$

(13)

where $a_{\text{max}}$ is the largest eigenvalue of $O$.

For the proof, see Appendix B. A clarification is now in order. Of course in general one can have a classical linear response of $O(g)$. What the main theorem proves is that a $O(g)$ response, together with the phenomenology described in Eq. (11), cannot be reproduced by any classical emulator. This is because Eq. (11) forces noncontextual models to have a response at most of $O(g^2)$. The central question is then when Eq. (11) will be observed in a quantum experiment for $g$ small enough. The next lemma gives a sufficient condition:

Lemma 2 (Operational condition test). Fix $t > 0$ and suppose there exists $C > 0$ such that the following matrix is positive definite

$$
\tilde{J}_{kj} = 1 - \frac{c_{kj}}{C}, \quad c_{kj} = (\alpha_k - \alpha_j)^2,
$$

(14)

where $\alpha_k$ are the eigenvalues of $\int_0^t V_t(t')dt'$. Then Eq. (10) holds for $g$ small enough.

For the proof see Appendix C. Note that to construct $\tilde{J}$ we only need to use linear response operators. For example, in the case of a single qubit

$$
\tilde{J} = \begin{bmatrix} 1 & \frac{c_{01}}{C} & \frac{c_{02}}{C} \\ \frac{c_{01}}{C} & 1 & \frac{c_{02}}{C} \\ \frac{c_{02}}{C} & \frac{c_{02}}{C} & 1 \end{bmatrix}
$$

which has eigenvalues $x_1 = c_{01}/C$ and $x_2 = 2 - c_{01}/C$. Hence for $C$ large enough one has $\tilde{J} > 0$ for any nondegenerate perturbation ($\alpha_0 \neq \alpha_1$). For a qutrit there are nontrivial counterexamples to $\tilde{J} > 0$, so one needs to perform the test for the specific scheme under consideration.

The above gives a general method to identify quantum signatures (certified against arbitrary noncontextual emulators) in arbitrary quantum systems in the linear regime:

1. Check $\tilde{J} > 0$. This implies that the response of any noncontextual emulator will be at most of $O(g^2)$.

2. Check that there is no pairwise commutation among $|\psi(0)\rangle\langle \psi(0)|$, $O_{t}(t)$ and $\int dt V_{t}(t')$. This implies that the quantum response will be of $O(g)$.

When the two conditions above are satisfied, Theorem 1 returns a proof of contextuality for $g$ small enough. This algorithm provides a powerful tool to identify quantum signatures. Here we apply these considerations to quantum thermodynamics and metrology.

A contextual advantage in a quantum engine. Despite a renewed interest in nonequilibrium thermodynamics of small quantum systems, spurred by recent theoretical and experimental advances, and a large number of proposals for quantum mechanical heat engines, a central outstanding question remains: Are there thermodynamic machines for which quantum mechanics provides an advantage over any classical emulator [1–9]? The thorny issue here, especially in the light of recent experimental effort [10], is to exclude the existence of classical emulators [11, 12]. The standard comparison with a “stochastic engine” – obtained by simple dephasing of the quantum
protocol – is insufficient to rule out alternative classical emulators [11]. We now show how to leverage the results just introduced to overcome these long-standing difficulties.

A heat engine is a machine that works between two baths at different temperatures and whose aim is to extract work from the heat flow between the two baths. It is useful to study the functioning of an engine as a sequence of ‘strokes’, in which only some of the elements are involved. We will focus here on the two-stroke engine:

1. The first stroke couples subsets of energy levels of the system to a hot and a cold bath to generate a non-equilibrium steady state \( \rho(0) \).
2. The second stroke is a unitary driving to implement work extraction.

We will assume that \( \rho(0) \) is a two-level system, as in [10]. Consider the work extraction process over a cycle lasting an amount of time \( \tau \):

\[
H(t) = H_0 + gV(t), \quad V(0) = V(\tau) = 0.
\]

If \( U(t) \) is the unitary process generated by \( H(t) \) from time 0 to \( \tau \), the work \( W \) extracted over the cycle is

\[
W = \text{Tr} (\rho(0)H_0) - \text{Tr} (U(\tau)\rho(0)U^\dagger(\tau)H_0) = \text{Tr} (\rho(0)H_0) - \text{Tr} (U(\tau)\rho(0)U^\dagger(\tau)H_0). \tag{16}
\]

Eq. (9) returns

\[
W^Q = \frac{2g\tau}{\hbar} \text{Im} \text{Tr} (\rho(0)XH_0) + O(g^2). \tag{18}
\]

where we set \( X := \frac{1}{\tau} \int_0^\tau V(t)dt \) (For an interesting relation to the so-called anomalous weak values, see Appendix D). Division by \( \tau \) gives the power, which is \( O(g) \) in the coupling strength unless there is some pairwise commutation between \( X \), \( \rho(0) \) and \( H_0 \). Furthermore, as already noted, the operational equivalence of Eq. (11) is satisfied generically by the unitary driving, since \( \rho(0) \) is a qubit system. Hence, setting \( E_{\text{max}} = \max_i E_i \), Theorem 1 applies. In every noncontextual emulator

\[
W \leq W_{\text{NC}} := 2E_{\text{max}}p_d. \tag{19}
\]

Hence \( W \leq O(g^2) \) as \( g \to 0 \) in any classical emulator, and the same holds for power. Since \( W^Q > W_{\text{NC}} \) for \( g \) small enough, a quantum advantage emerges in the weak coupling limit. The quantum advantage is exhibited in the difference between the \( O(g) \) scaling possible in quantum mechanics as compared with the \( O(g^2) \) bound of any classical emulator. This is consistent with previous results [4, 9, 10, 24], where it was noted that the addition of dephasing transforms a \( O(g) \) scaling into a \( O(g^2) \) scaling (as one can easily check from Eq. (18) above). As discussed, adding dephasing is just one way of obtaining a classical model and tells us nothing about the existence of alternative classical emulators [11, 12].

Theorem 1 ensures is that the quantum \( O(q) \) power scaling is incompatible with every noncontextual emulator when the operational facts encoded in Eq. (11) are satisfied, as they are in the case of the single qubit two-stroke engine. This answers the question “Are there thermodynamic machines whose performance displays quantum signatures certified against any classical emulation?” in the positive.

A contextual advantage in local metrology. Local metrology is a paradigm to study the ultimate limits of parameter estimation. We look here at the archetypal case of phase estimation, where the relevant parameter is the phase \( \eta \) in the dynamics \( U_\eta = e^{-iH\eta} \) for some observable \( H \).

An initial qubit state \( |\psi(0)\rangle \) is prepared, undergoes the dynamics \( U_\eta \) and is measured according to some arbitrary POVM \( M_\eta \). After \( N \) trials, there exists a measurement such that the error (variance) \( \text{Var}(\eta) \) in the estimated phase scales as \( O(1/(4N\Delta H^2)) \), where \( \Delta H^2 := \langle \psi(0)|H^2|\psi(0)\rangle - \langle \psi(0)|H|\psi(0)\rangle^2 \). This is finite only if the state is (a nontrivial) superposition of eigenstates of \( H \), otherwise \( \text{Var}(\eta) = +\infty \). Hence dephasing trivially prevents sensing in this scheme. But what about other noncontextual emulators, which as already discussed can be much more complex than quantum mechanics plus dephasing? Here we show \( \text{Var}(\eta) = +\infty \) in every noncontextual model reproducing the operational phenomenology of quantum sensing.

Let \( p(x|\eta) \) be the probability of getting outcome \( x \) from a measurement \( M \) when the true value of the parameter is \( \eta \). So \( p(x|\eta) = p(x|T_\eta(P),M) \) if \( P, T_\eta \) and \( M \) are the operational descriptions of preparation, transformation and measurement procedures, represented in quantum theory by \( |\psi(0)\rangle \), \( U_\eta \) and \( \{M_\eta\} \). Recall that an estimator \( \hat{\eta}(x_1,x_2,...) \) maps the measurement outcomes \((x_1,x_2,...)\) to a guess \( \eta \) for the unknown parameter. For independent observations, the variance of any unbiased estimator is lower bounded by \( 1/(NF_{\eta}^{P,M}) \), with \( F_{\eta}^{P,M} \) the Fisher information

\[
F_{\eta}^{P,M} = \sum_x p(x|\eta) \left( \frac{\partial}{\partial \eta} \ln p(x|\eta) \right)^2. \tag{20}
\]

The best strategy involves optimising over all allowed preparations \( P \) and measurements \( M \), where for simplicity we will assume \( x \) runs over a bounded, while possibly extremely large, set of indexes. In any OM, from Eq. (1)

\[
p(x|\eta) = \int d\lambda d\lambda' \mu_P(\lambda) \mathcal{T}_\eta(\lambda' |\lambda) \xi_M(x |\lambda'), \tag{21}
\]

where \( \mu_P(\lambda), \mathcal{T}_\eta(\lambda' |\lambda), \xi_M(x |\lambda') \) are the OM descriptions of \( P, T_\eta \) and \( M \). Using the relation \( p(x|\eta + \delta) = p(x|T_\eta(T_{\delta}(P),M)) \), where \( F_{\eta} = F_{\eta}(P) \), and the fact that Eq. (11) is satisfied with \( p_d = O(\delta^2) \), we can prove

\[
F_{\eta}^{P,M} = 0 \tag{22}
\]

for any \( P \) and any measurement \( M \) with a finite number of outcomes (see Appendix E). Hence \( \text{Var}(\eta) = +\infty \) as
anticipated. This again is a consequence of the weakness of linear response in noncontextual models.

**Outlook.** We proved that experiments where a quantum systems is driven by a small external perturbation cannot in general be reproduced by noncontextual emulators. While the quantum response can scale linearly in the strength of the perturbation parameter $g$, noncontextual emulators reproducing the operational phenomenology in Eq. (11) only respond quadratically.

(Curiously, one can note that since classical emulators display a quadratic response in the presence of the operational equivalence in Eq. (11), a phenomenon such as the quantum Zeno effect is naturally expected on the basis of the assumption of noncontextuality – see Appendix F).

The $O(g)$ vs $O(g^2)$ gap is a certifiable quantum signature. We gave readily applicable tools to analyze arbitrary linear response experiments. As an application, we answered in the affirmative a long-standing open question in quantum thermodynamics: we proved the existence of certifiable (i.e., provably not classically emulatable) quantum signatures in the operation of quantum engines. A similar signature can be found in local metrology.

Building up on this work, it will be desirable to use the tools introduced here to reanalyse in depth the experimental heat engine signature of Ref. [10], as well as to develop flexible certification tools applicable to larger scale systems. Furthermore, to settle the question of the potential technological relevance of quantum engines, one has to find certificates that rely on physically or technologically more compelling operational constraints than ‘stochastic reversibility’. We can finally certify that the behaviour of quantum engines admits no classical emulation. But the question of their superiority as practical devices is far from settled.

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APPENDIX

A. Classical mechanics is noncontextual

Let’s work this out explicitly in the case of preparation noncontextuality and \( \lambda = (x, p) \), since the generalisation is straightforward. Suppose \( P \simeq_{op} P' \), which implies \( p(k|P, M) = p(k|P', M) \) for all \( M \) and all outcomes \( k \). By definition of OM this implies

\[
\int dxdp \mu_P(x, p) \xi_M(k|x, p) = \int dxdp \mu_{P'}(x, p) \xi_M(k|x, p) \quad \forall M.
\]

Now, the response functions \( \{ \xi_M(k|x, p) \}_M \), for varying \( M \), span all indicator functions over phase space. Hence the previous equation implies \( \mu_P(x, p) = \mu_{P'}(x, p) \), as required by Eq. (2) (strictly, modulo sets of zero measure – but likewise one should strictly define noncontextuality modulo sets of zero measure). Similarly, one can show that Eqs. (3)-(4) also hold. Hamiltonian dynamics is hence a particular member of a family of potential noncontextual emulators.

B. Proof of Theorem 1

Due to its simplicity we first give a proof under the assumption that the number of allowed \( \lambda \) is finite. We then present a second proof that works in generality. The proofs follow the technique used to prove Lemma 5 in Ref. [25].

1. Proof for OM with bounded state space

Split the sum in Eq. (12) into all \( \lambda, \lambda' \) with \( \lambda = \lambda' \) and with \( \lambda \neq \lambda' \). Using \( \mathcal{T}_T'(\lambda|\lambda) \leq 1 \) we get

\[
\langle \Delta O_I \rangle_t \leq \sum_k o_k \sum_{\lambda \neq \lambda'} \mu_P(\lambda) \mathcal{T}_{T'_T}(\lambda'|\lambda) \xi_M(k|\lambda').
\]

Now use the noncontextuality assumption of Eq. (4). Eq. (11) requires

\[
\frac{1}{2} \mathcal{T}_{T'_T}(\lambda'|\lambda) + \frac{1}{2} \mathcal{T}_{T'_T}(\lambda'|\lambda) = (1 - p_d) \delta_{\lambda\lambda'} + p_d \mathcal{T}_{T'_T}(\lambda'|\lambda).
\]

Note that the transition probability associated to \( T_{id} \) in noncontextual models is a Kronecker delta, since one way to realize \( T_{id} \) is to let no time pass. Hence, for \( \lambda \neq \lambda' \), \( \mathcal{T}_{T'_T}(\lambda'|\lambda) \leq 2p_d \mathcal{T}_{T'_T}(\lambda'|\lambda) \), which shows that the transition probabilities between distinct \( \lambda \)s must be of \( O(p_d) \). Then,

\[
\langle \Delta O_I \rangle_t \leq 2p_d \sum_k o_k \sum_{\lambda \neq \lambda'} \mu_P(\lambda) \mathcal{T}_{T'_T}(\lambda'|\lambda) \xi_M(k|\lambda') \leq 2p_d \omega_{\text{max}},
\]

where in the last inequality we extended the sum to all \( \lambda, \lambda' \) and used that

\[
\sum_{\lambda, \lambda'} \mu_P(\lambda) \mathcal{T}_{T'_T}(\lambda'|\lambda) \xi_M(k|\lambda') = p(k|T'_T(P), M_t), \quad \sum_k p(k|T'_T(P), M_t) = 1.
\]

Finally note from Eq. (6)

\[
-\langle \Delta O_I \rangle_t = \sum_k o_k p(k|T'_T(P^*), M_t) - \sum_k o_k p(k|P^*, M_t),
\]

where \( P^* = T_t(P) \). Since the operational equivalence (11) is symmetric in \( T_t, T'_T \) and the bound does not depend on the initial preparation, the same reasoning yields \(-\langle \Delta O_I \rangle_t \leq 2p_d \omega_{\text{max}}\).
2. Proof OM with unbounded state space

Combining Eqs. (1) and (7) in the case of a potentially continuous number of states in the OM we get

$$\langle \Delta O_1 \rangle_t = \sum_k o_k \left[ \int d\lambda \int d\lambda' \mu_\lambda' T_{\lambda T}(\lambda' | \lambda) \xi_{M_\lambda}(k | \lambda') - \int d\lambda \mu_\lambda(\lambda) \xi_{M_\lambda}(k | \lambda) \right].$$

(24)

For each outcome $k$ and $\lambda$ we can partition the space of ontological states $\Lambda$ as

$$\Lambda^k_\lambda = \{ \lambda' \xi_{M_\lambda}(k | \lambda') > \xi_{M_\lambda}(k | \lambda) \}, \quad \Lambda^k = \Lambda \setminus \Lambda^k_\lambda.\quad (25)$$

Then

$$\langle \Delta O_1 \rangle_t = \sum_k o_k \left[ \int d\lambda \int_{\Lambda^k_\lambda} d\lambda' \mu_\lambda'(\lambda') T_{\lambda T}(\lambda' | \lambda) \xi_{M_{\lambda'}}(k | \lambda') + \int d\lambda \int_{\Lambda^k_\lambda} d\lambda' \mu_\lambda'(\lambda') T_{\lambda T}(\lambda' | \lambda) \xi_{M_{\lambda'}}(k | \lambda') - \int d\lambda \mu_\lambda(\lambda) \xi_{M_{\lambda'}}(k | \lambda') \right]$$

$$\leq \sum_k o_k \left[ \int d\lambda \int_{\Lambda^k_\lambda} d\lambda' \mu_\lambda'(\lambda') T_{\lambda T}(\lambda' | \lambda) \xi_{M_{\lambda'}}(k | \lambda') + \int d\lambda \int_{\Lambda^k_\lambda} d\lambda' \mu_\lambda'(\lambda') T_{\lambda T}(\lambda' | \lambda) \xi_{M_{\lambda'}}(k | \lambda') - \int d\lambda \mu_\lambda(\lambda) \xi_{M_{\lambda'}}(k | \lambda') \right]$$

$$= \sum_k o_k \int d\lambda \int_{\Lambda^k_\lambda} d\lambda' \mu_\lambda'(\lambda') T_{\lambda T}(\lambda' | \lambda) \xi_{M_{\lambda'}}(k | \lambda') - \xi_{M_{\lambda}}(k | \lambda)$$

$$\leq \sum_k o_k \int d\lambda \int T_{\lambda T}(\lambda' | \lambda) [\xi_{M_{\lambda'}}(k | \lambda') + T_{\lambda T}(\lambda' | \lambda)] [\xi_{M_{\lambda'}}(k | \lambda') - \xi_{M_{\lambda}}(k | \lambda)]$$

$$= 2p_d \sum_k o_k \int d\lambda \int d\lambda' \mu_\lambda' T_{\lambda T}(\lambda' | \lambda) \xi_{M_{\lambda'}}(k | \lambda') - \xi_{M_{\lambda}}(k | \lambda)]$$

$$\leq 2p_d \sum_k o_k \int d\lambda \int d\lambda' \mu_\lambda' T_{\lambda T}(\lambda' | \lambda) \xi_{M_{\lambda'}}(k | \lambda') \leq 2p_d \sigma_{\text{max}}.\quad (26)$$

where we used: $\xi_{M_{\lambda}}(k | \lambda') \leq \xi_{M_{\lambda'}}(k | \lambda)$ in $\Lambda^k_\lambda$ to get the second line; $\int d\lambda' T_{\lambda T}(\lambda' | \lambda) = 1$ to get the fourth line; and to get the sixth line we used noncontextuality applied to the operational equivalence of Eq. (11) in the main text, i.e.

$$T_{\lambda T}(\lambda' | \lambda) + T_{\lambda' T}(\lambda' | \lambda) = 2(1 - p_d)\delta(\lambda - \lambda') + 2p_d T_{\lambda T}(\lambda' | \lambda). \quad (27)$$

For the last inequality we used

$$\int d\lambda \int d\lambda' \mu_\lambda'(\lambda') T_{\lambda T}(\lambda' | \lambda) \xi_{M_{\lambda'}}(k | \lambda') = p(k | T^*_T(P), M_t), \quad \sum_k p(k | T^*_T(P), M_t) = 1.$$

The proof of $-\langle \Delta O_1 \rangle_t \leq 2p_d \sigma_{\text{max}}$ proceeds symmetrically, noting that

$$-\langle \Delta O_1 \rangle_t = \sum_k o_k \left[ \int d\lambda \int d\lambda' \mu_\lambda'(\lambda') T_{\lambda T}(\lambda' | \lambda) \xi_{M_{\lambda'}}(k | \lambda') - \int d\lambda \mu_\lambda(\lambda) \xi_{M_{\lambda'}}(k | \lambda') \right].$$

(28)

with $P^*$ the preparation procedure $P^* = T^*_T(P)$.

C. Proof of Lemma 2

Fix $t > 0$ and let $U_g = U_g(\cdot) U_g^*$ with $U_g = I - \frac{i}{\hbar} \int_0^t \int_0^t V_2(t') dt' + O(g^2)$. We have $U_g = e^{-iH_g}$ for some Hermitian operator $H_g$. By Hadamard lemma $U_g = e^{-iH_g}$, with $\mathcal{H}_g(X) = [H_g, X]$. Then

$$\frac{1}{2} U_g + \frac{1}{2} U_g^* = \frac{1}{2} e^{-iH_g} + \frac{1}{2} e^{iH_g} = I + \sum_{n=1}^{\infty} \frac{2^n}{(2n)!} H_g^{2n} = (1 - p_d)I + p_d \left( I + \frac{1}{p_d} \sum_{n=1}^{\infty} \frac{(-1)^n}{(2n)!} H_g^{2n} \right). \quad (29)$$

Set $C_g = I + \sum_{n=1}^{\infty} \frac{(-1)^n}{(2n)!} H_g^{2n}$. We want to prove that for $g$ small enough $C_g$ is a quantum channel, i.e. a Completely Positive Trace Preserving (CPTP) map, for some choice of $p_d = O(g^2)$. 

• Trace-preserving condition:

\[ \text{Tr}[C_g(\rho)] = 1 + \frac{1}{p_d} \sum_{n=1}^{\infty} \frac{(-1)^n}{(2n)!} \text{Tr}[H_g^{2n}(\rho)]. \]

(30)

However

\[ \text{Tr}[H_g(\rho)] = \text{Tr}[H_g \rho - \rho H_g] = 0, \quad \text{Tr}[H_g^k(\rho)] = \text{Tr}[H_g^{k-1}(H_g \rho - \rho H_g)], \]

(31)

so proceeding by induction one has \( \text{Tr}[H^n(\rho)] = 0 \) for all \( n \). Hence \( \text{Tr}[C_g(\rho)] = 1 \), so \( C_g \) is trace-preserving.

• Complete Positivity:

Let \( |\phi^+\rangle = \frac{1}{\sqrt{d}} \sum_k |kk\rangle \), with \( H_g |k\rangle = E_k(g) |k\rangle \) (with an implicit dependence of \( |k\rangle \) on \( g \)). By the Choi-Jamiołkowski isomorphism the condition of complete positivity is equivalent to \( J_g := C_g \otimes I(|\phi^+\rangle \langle \phi^+|)/d \geq 0 \) for \( g \) small enough.

\[
J_g = \frac{1}{d} \sum_{k,j} C_g(|k\rangle \langle j|) \otimes |k\rangle \langle j| = \frac{1}{d} \sum_{k,j} [|k\rangle \langle j| \otimes |k\rangle \langle j| + \frac{1}{p_d} \sum_{n=1}^{\infty} \frac{(-1)^n}{(2n)!} H_g^{2n}(|k\rangle \langle j|) \otimes |k\rangle \langle j|]
\]

(32)

\[
= \frac{1}{d} \sum_{k,j} [|k\rangle \langle j| \otimes |k\rangle \langle j| + \frac{1}{p_d} \sum_{n=1}^{\infty} \frac{(-1)^n}{(2n)!} (E_k(g) - E_j(g))^{2n}(|k\rangle \langle j|) \otimes |k\rangle \langle j|],
\]

(33)

where in the last equation we used \( H_g(|k\rangle \langle j|) = H_g |k\rangle \langle j| - |k\rangle \langle j| H_g = (E_k(g) - E_j(g)) |k\rangle \langle j|. \) Now, using \( \cos x = \sum_{n=0}^{\infty} \frac{(-1)^n}{(2n)!} x^{2n} \),

\[
J_g = \frac{1}{d} \sum_{k,j} \left[ \left( 1 - \frac{1}{p_d} \right) + \frac{1}{p_d} \cos(E_k(g) - E_j(g)) \right] |k\rangle \langle j| \otimes |k\rangle \langle j|.
\]

(34)

Note that \( H_g = i \log[I - i \frac{g}{\hbar} \int_0^t V(t') dt'] + O(g^2) = \frac{g}{\hbar} \int_0^t \int_0^t V(t') dt' + O(g^2) \). Hence, if we denote by \( \alpha_k \) the eigenvalues of \( \int_0^t V(t') dt' \) (which do not depend on \( g \), the eigenvalues of \( H_g \) will be \( \frac{g}{\hbar} \alpha_k + O(g^2) \). This follows from the fact that the eigenvalues of \( H_g \) can only differ from those of \( \frac{g}{\hbar} \int_0^t V(t') dt' \) by \( O(g^2) \) [26, 27].

Hence \( E_k(g) - E_j(g) = \frac{g}{\hbar} (\alpha_k - \alpha_j) + O(g^2) \). We have

\[
\cos(E_k(g) - E_j(g)) = \cos \left[ \frac{g}{\hbar} (\alpha_k - \alpha_j) + O(g^2) \right] = 1 - \frac{g^2}{2\hbar^2} (\alpha_k - \alpha_j)^2 + O(g^4).
\]

(35)

This gives

\[
J_g = \frac{1}{d} \sum_{k,j} \left[ 1 - \frac{g^2}{2\hbar^2 p_d} (\alpha_k - \alpha_j)^2 + \frac{O(g^4)}{p_d} \right] |k\rangle \langle j|.
\]

(36)

Set \( p_d = C g^2/(2\hbar^2) \) for some constant \( C > 0 \). Hence, denoting \( c_{kj} = (\alpha_k - \alpha_j)^2 \),

\[
J_g = \frac{1}{d} \sum_{k,j} \left[ 1 - \frac{c_{kj}}{C} + O(g^2) \right] |k\rangle \langle j| = \frac{1}{d} \tilde{J} + O(g^2).
\]

(37)

We study the matrix

\[
\tilde{J} = \sum_{k,j} \left[ 1 - \frac{c_{kj}}{C} \right] |k\rangle \langle j|.
\]

(38)

The eigenvalues of \( J_g \) can only differ from those of \( \tilde{J} \) by \( O(g^2) \) [26, 27]. Hence, if we can find a constant \( C > 0 \) such that \( \tilde{J} > 0 \), then \( J_g > 0 \) for \( g \) small enough.
D. Relation to weak values.

We proved that the quantum mechanical operation of the two-stroke engine cannot be emulated by classical means. Here we gather some more intuition as to why this is the case. It is useful to recast Eq. (18) in two alternative ways. On the one hand, setting $H_f(t) := e^{iH_0 t/\hbar} (H_0 + gV(t)) e^{-iH_0 t/\hbar} = H_0 + gV_f(t)$ one has

$$W^Q = \frac{g}{i\hbar} \int_0^T \text{Tr} \left( [H_f(0), H_f(t)] \rho(0) \right), \quad (39)$$

i.e. $W^Q$ in the weak coupling regime is related to two-points correlations functions, as expected from linear response theory. On the other hand such correlation function can also be rewritten as $(X := \frac{1}{T} \int_0^T V_f(t) dt, H_0 = \sum_i E_i \Pi_{E_i})$

$$W = \frac{2gT}{\hbar} \sum_i \text{Tr} \left( \Pi_{E_i} \rho(0) \right) E_i \text{Im} \left[ E_i \langle X \rangle_{\rho(0)} \right] + O(g^2), \quad (40)$$

where $E_i \langle X \rangle_{\rho(0)} := \frac{\text{Tr}(\Pi_{E_i} X \rho(0))}{\text{Tr}(\Pi_{E_i} \rho(0))}$, i.e. a weighted sum of imaginary parts of so-called generalized weak values [28] (the quantities $E_i \langle X \rangle_{\rho(0)}$). It was previously noticed that the latter characterise the first order response of the probability of obtaining outcome $E_i$ due to a unitary driving [29]. As we can see, that is due to their relation to correlation functions. Furthermore, Ref. [25] has shown that, in finite-dimensional quantum systems, the weak measurement protocols that are used to estimate the quantities $E_i \langle X \rangle_{\rho(0)}$ do not admit a classical, i.e. noncontextual emulation, due to their specific information-disturbance tradeoff. One is then lead to conjecture that the work and power in Eq. (40) may themselves be – in some sense to be made precise – nonclassical. We have proved that this is indeed the case.

E. Proof of Eq. (22): $F^{P,M}_\eta = 0$.

By definition,

$$F_\eta = \lim_{\delta \to 0} \sum_x p(x|\eta) \left[ \frac{\ln p(x|\eta + \delta) - \ln p(x|\eta)}{\delta} \right]^2, \quad (41)$$

$p(x|\eta) = p(x|P_\eta, M) = \int d\lambda \mu_{P_\eta}(\lambda) \xi_M(x|\lambda)$, $p(x|\eta + \delta) = p(x|T_\eta(P_\eta), M)$.

It follows that the difference $p(x|\eta + \delta) - p(x|\eta)$ has the same form as Eq. (24) with a single $\omega_k = 1$ and all others equal to zero. We can connect to the unitary driving scenario of Eq. (5) by setting $H_0 = 0, t = \eta$ and $V(\eta) = H$. Since $V_f(\eta) = H$ and we are considering a qubit system, for any $H$ Lemma 2 ensures that the operational equivalence in Eq. (11) is satisfied with $T_\eta$ described in quantum mechanics by the unitary $U_\eta = e^{-iH\eta}$ and $T^{*}_\eta$ by $U_\eta^\dagger$.

Hence the derivation in Appendix B gives

$$|p(x|\eta + \delta) - p(x|\eta)| \leq 2p_d = O(\delta^2). \quad (43)$$

For the terms with $p(x|\eta) \neq 0$ consider the expression $\ln^2[p(x|\eta + \delta)/p(x|\eta)]$. Since $\ln^2 y$ is monotonically decreasing for $y \leq 1$ and increasing for $y \geq 1$, we distinguish two cases.

If $p(x|\eta + \delta) \geq p(x|\eta)$,

$$\ln^2 \frac{p(x|\eta + \delta)}{p(x|\eta)} \leq \ln^2 \frac{|p(x|\eta + \delta) - p(x|\eta)| + p(x|\eta)}{p(x|\eta)} \leq \ln^2 \left[ 1 + \frac{2p_d}{p(x|\eta)} \right]$$

If $p(x|\eta + \delta) \leq p(x|\eta)$,

$$\ln^2 \frac{p(x|\eta + \delta)}{p(x|\eta)} \leq \ln^2 \frac{|p(x|\eta + \delta) - p(x|\eta)| + p(x|\eta)}{p(x|\eta)} \leq \ln^2 \left[ 1 - \frac{2p_d}{p(x|\eta)} \right]$$

Since $\ln^2[1 - y] \geq \ln^2[1 + y]$ for $y \in [0,1]$, we conclude that in both cases, assuming $p_d$ is small enough,

$$\frac{p(x|\eta)}{\delta^2} \ln^2 \frac{p(x|\eta + \delta)}{p(x|\eta)} \leq \frac{p(x|\eta)}{\delta^2} \ln^2 \left[ 1 - \frac{2p_d}{p(x|\eta)} \right] = \frac{4p_d^2}{\delta^2 p(x|\eta)} + O(p_d^3). \quad (44)$$
Denoting by $\sum'_x$ a sum over all $x$ with $p(x|\eta) \neq 0$ and using $p_d = O(\delta^2)$,

$$F_\eta = \lim_{\delta \to 0} \sum'_x \frac{4}{p(x|\eta)} \times O(\delta^2) = 0$$

(45)

Note that we assumed the number of outcomes to be finite.

F. Zeno effect from noncontextuality

One can also reverse the discussion and analyse phenomena which, while potentially surprising, are nonetheless naturally expected in noncontextual models. This is the case of the quantum Zeno effect. Consider a qubit system undergoing Rabi oscillations under a unitary $U_t$. It is well-known that, if the system is prepared in the initial state $|0\rangle$ and continuously measured in the computational basis, it has vanishing probability of being found in the state $|1\rangle$, so that monitoring “freezes” the evolution.

In a generic OM the experiment is described as follows. A $\lambda$ is sampled according to some probability distribution $\mu_{P_0}(\lambda)$, where $P_0$ is the preparation described in quantum mechanics by $|0\rangle$. Then the state is updated according to matrix of transition probabilities $T_{T_t}(\lambda'|\lambda)$, where $T_t$ is the transformation described in quantum mechanics by $U_t$. Finally the system is measured according to the procedure $M$ (in quantum mechanics, the projective measurement in the $\{|0\rangle, |1\rangle\}$ basis). In the OM the measurement is associated to a response function $\xi_M(k|\lambda)$, which gives the probability outcome $k = 0, 1$ is returned if the state is $\lambda$. We are interested in what happens when we measure many times $M$ in a given time interval.

From our analysis a generic feature of noncontextual OM respecting the operational feature in Eq. (11) is that the stochastic processes associated to quantum unitary dynamics induce a change $\lambda \rightarrow \lambda'$ ($\lambda \neq \lambda'$) with a probability which is quadratic (rather than linear) in the interaction time $t$ when $t$ is small (see proof of Theorem 1 in Appendix B).

Given that, consider the following simple noncontextual model of the quantum Zeno experiment. Take

$$T_{T_t}(\lambda'|\lambda) = (1 - p_d(t))\delta_{\lambda\lambda'} + p_d(t)T_{T_t'}(\lambda'|\lambda)$$

(46)

for some $T_{T_t'}$. Similarly take the matrix of transition probabilities associated to the transformation $T_t'$ (in quantum mechanics $U_t'$) to be

$$T_{T_t'}(\lambda'|\lambda) = (1 - p_d(t))\delta_{\lambda\lambda'} + p_d(t)T_{T_t''}(\lambda'|\lambda)$$

(47)

for some $T_{T_t''}$ . Since Eq. (11) is fulfilled, the assumption of noncontextuality requires $p_d(t) = O(t^2)$ when $t \to 0$.

Given this, let’s see how one can naturally completes the model so that it displays a Zeno effect.

Let $\mu_{P_0}(\lambda) x = 0, 1$ be the (disjoint) probability distributions associated to $|0\rangle$, $|1\rangle$. We will take $\xi_M(x|\lambda) = 1$ on the support of $\mu_{P_0}$ and zero otherwise. Furthermore, the post-measurement state is simply given by $\mu_{P_0}(\lambda)$ if the outcome is $x$. Since the state is initialized in $|0\rangle$, the survival probability $p(x = 0|T_t(P_0), M)$ is bounded by

$$p(x = 0|T_t(P_0), M) = \sum_{\lambda', \lambda} \mu_{P_0}(\lambda) T_{T_t}(\lambda'|\lambda) \xi_M(0|\lambda') \geq 1 - p_d(t) = 1 - ct^2$$

(48)

where we took $p_d(t) = ct^2$ for some constant $c \geq 0$. The post-measurement state is $\mu_{P_0}$ if the measurement returns $x = 0$, and $\mu_{P_1}$ in case of outcome $x = 1$. If we divide the total evolution time $t$ into $N$ steps and perform a measurement after each, the overall survival probability will scale as $(1 - ct^2/N^2)^N = 1 - ct^2/N + O(1/N^2)$, which goes to 1 as the number of measurements $N \to \infty$. The underlying reason is the quadratic scaling of $T_{T_t}(\lambda'|\lambda)$ for $\lambda' \neq \lambda$, itself a consequence of noncontextuality. A Zeno effect emerges from the assumption of noncontextuality of the underlying OM.

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