Non-Abelian Transport Distinguishes Three Usually Equivalent Notions of Entropy Production

Twesh Upadhyaya,[1,2,*,¶] William F. Braasch Jr.,[1,†,¶] Gabriel T. Landi,[3,‡] and Nicole Yunger Halpern[1,4,§]

[1] *Joint Center for Quantum Information and Computer Science, National Institute of Standards and Technology (NIST) and University of Maryland, College Park, Maryland 20742, USA*
[2] *Department of Physics, University of Maryland, College Park, Maryland 20742, USA*
[3] *Department of Physics and Astronomy, University of Rochester, Rochester, New York 14627, USA*
[4] *Institute for Physical Science and Technology, University of Maryland, College Park, Maryland 20742, USA*

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We extend entropy production to a deeply quantum regime involving noncommuting conserved quantities. Consider a unitary transporting conserved quantities ("charges") between two systems initialized in thermal states. Three common formulas model the entropy produced. They respectively cast entropy as an extensive thermodynamic variable, as an information-theoretic uncertainty measure, and as a quantifier of irreversibility. Often, the charges are assumed to commute with each other (e.g., energy and particle number). Yet quantum charges can fail to commute. Noncommutation invites generalizations, which we posit and justify, of the three formulas. The noncommutation of charges, we find, breaks the equivalence of the formulas. Furthermore, different formulas quantify different physical effects of the noncommutation of charges on entropy production. For instance, entropy production can signal contextuality—true nonclassicality—by becoming nonreal. This work opens up stochastic thermodynamics to noncommuting—and so particularly quantum—charges.

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I. INTRODUCTION

Thermodynamics describes the transport of energy and other quantities between systems that have equilibrated individually but not with each other. These quantities are conserved according to principles such as the first law of thermodynamics. The second law decrees which transport can and cannot occur spontaneously. Over the past three decades, researchers have revolutionized the study of transport within microscopic systems, where fluctuations dominate [1–7].

More-recent results have prompted questions about how such exchanges occur in quantum systems, which can have coherences and nonclassical correlations [8–15]. To infer about quantum currents, one must measure quantum systems. But measurement back action can destroy coherences. Thermodynamic processes therefore depend on our measurements of them. This conundrum has inspired considerable research but no resolution is universally agreed upon.

Quantum coherences result from the noncommutation of operators. In classical thermodynamics, the energy and particle number of a system are commuting quantities; they can be measured simultaneously. What if the globally conserved thermodynamic quantities (*charges*) fail to commute?

This recently posed question has upended intuitions and engendered a burgeoning subfield of quantum thermodynamics [16–49]; for a recent perspective, see Ref. [50]. For example, the noncommutation of charges hinders arguments for the form of the thermal state [20,23] and alters the eigenstate thermalization hypothesis, which explains how quantum many-body systems thermalize internally [35]. Other results span resource theories [20–23,39–41, 43–45], heat engines [38], metrology [51], and a trapped-ion experiment [27,48]. In the linear-response regime, noncommuting charges reduce entropy production [28].

We analyze the entropy produced by arbitrarily far-from-equilibrium exchanges of noncommuting charges.

*Contact author: tweshu@umd.edu
†Contact author: wbraasch@umd.edu
‡Contact author: glandi@ur.rochester.edu
§Contact author: nicoleyh@umd.edu
¶These authors contributed equally to this work.

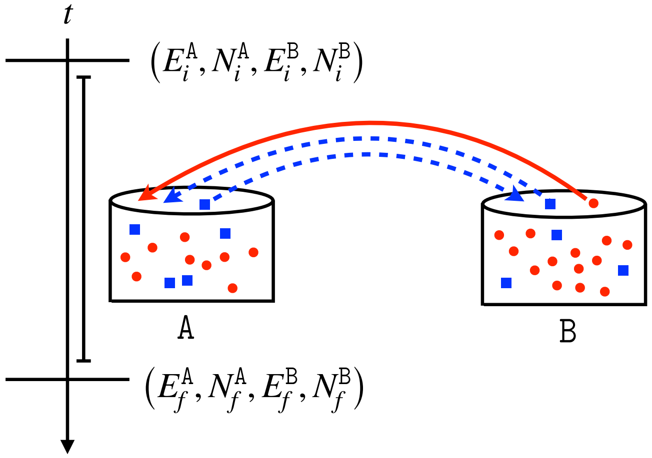

FIG. 1. Two thermal systems exchanging charges. In a paradigm ubiquitous across thermodynamics, two systems locally exchange charges that are conserved globally. The charge flow produces entropy. During each realization of the process, each system begins with some amount of every charge (e.g., energy and particle number) and ends with some amount. These amounts define a stochastic trajectory.

Three formulas for entropy production, which equal each other when all charges commute, have been used widely [52]. We show that these formulas fail to equal each other when charges fail to commute. This incommensurability stems from measurement disturbance: the currents of noncommuting charges cannot be measured simultaneously.

An example illustrates the key idea. Consider two classical thermodynamic observables, such as energy and particle number. Let classical systems $\mathtt{A}$ and $\mathtt{B}$ begin in thermal (grand canonical) ensembles: system $\mathtt{X} = \mathtt{A}, \mathtt{B}$ has energy $E^{\mathtt{X}}$ and particle number $N^{\mathtt{X}}$ with a probability $\propto e^{-\beta^{\mathtt{X}}(E^{\mathtt{X}}-\mu^{\mathtt{X}}N^{\mathtt{X}})}$, where $\beta^{\mathtt{X}}$ denotes an inverse temperature and $\mu^{\mathtt{X}}$ a chemical potential. An interaction can shuttle energy and particles between the systems. If conserved globally, the quantities are called *charges*. Any charge (e.g., particle) entering or leaving a system produces entropy. The entropy produced in a trial—the *stochastic entropy production* (SEP)—is a random variable. Its average over trials is non-negative, according to the second law of thermodynamics. The SEP obeys constraints called *exchange fluctuation theorems*—tightenings of the second law of thermodynamics [6]. Classical fluctuation theorems stem from a probabilistic model: system $\mathtt{A}$ begins with energy $E_i^{\mathtt{A}}$ and with $N_i^{\mathtt{A}}$ particles, $\mathtt{A}$ ends with energy $E_f^{\mathtt{A}}$ and with $N_f^{\mathtt{A}}$ particles, and $\mathtt{B}$ satisfies analogous conditions, with a joint probability $p(E_i^{\mathtt{A}}, N_i^{\mathtt{A}}, E_i^{\mathtt{B}}, N_i^{\mathtt{B}}\,;\, E_f^{\mathtt{A}}, N_f^{\mathtt{A}}, E_f^{\mathtt{B}}, N_f^{\mathtt{B}})$. We view the progression $(E_i^{\mathtt{A}}, N_i^{\mathtt{A}}, E_i^{\mathtt{B}}, N_i^{\mathtt{B}}) \mapsto (E_f^{\mathtt{A}}, N_f^{\mathtt{A}}, E_f^{\mathtt{B}}, N_f^{\mathtt{B}})$ as a two-step *stochastic trajectory* between microstates (Fig. 1).

In the commonest quantum analogue, quantum systems $\mathtt{X} = \mathtt{A}, \mathtt{B}$ begin in reduced grand canonical states $\propto e^{-\beta^{\mathtt{X}}(\hat{H}^{\mathtt{X}}-\mu^{\mathtt{X}}\hat{N}^{\mathtt{X}})}$, where $\hat{H}^{\mathtt{X}}$ denotes a Hamiltonian and $\hat{N}^{\mathtt{X}}$ a particle-number operator. In the *two-point measurement scheme* [4,5], one strongly measures the Hamiltonian and particle number of each system. Then, a unitary couples the systems, conserving $\hat{H}^{\mathtt{A}} + \hat{H}^{\mathtt{B}}$ and $\hat{N}^{\mathtt{A}} + \hat{N}^{\mathtt{B}}$. Finally, one measures $\hat{H}^{\mathtt{A}}$, $\hat{H}^{\mathtt{B}}$, $\hat{N}^{\mathtt{A}}$, and $\hat{N}^{\mathtt{B}}$ again [53]. A joint probability distribution governs the four measurement outcomes. Using the outcomes and distribution, one can similarly define the SEP, prove fluctuation theorems, and define stochastic trajectories [6]. Each measurement may, however, disturb the quantum system [12,54,55].

Noncommutation introduces a twist into this story. Let the above quantum systems exchange charges that fail to commute with each other. For example, consider qubits $\mathtt{X} = \mathtt{A}, \mathtt{B}$ exchanging spin components $\hat{\sigma}^{\mathtt{X}}_{x,y,z}$. The corresponding thermal states are $\propto \exp\left(-\sum_{\alpha=x,y,z} \beta^{\mathtt{X}}_{\alpha}\hat{\sigma}^{\mathtt{X}}_{\alpha}\right)$, wherein $\beta^{\mathtt{X}}_{\alpha}$ denotes a generalized inverse temperature [23,27,35,48]. One cannot implement the two-point measurement scheme straightforwardly, as no system's $\hat{\sigma}^{\mathtt{X}}_{x,y,z}$ operators can be measured simultaneously. One can measure the three spin components of each qubit sequentially, couple the systems with a charge-conserving unitary, and measure the $\hat{\sigma}_{x,y,z}$ of each qubit sequentially again. Yet these measurements wreak havoc worse than if the charges commute: they disturb not only the states, but also the subsequent noncommuting measurements [56].

Weak measurements would disturb the systems less [57,58], at the price of extracting less information [59]. As probabilities describe strong-measurement experiments, *quasiprobabilities* describe weak-measurement experiments (Appendix A). Quasiprobabilities resemble probabilities—being normalized to 1, for example. They violate axioms of probability theory, however, such as by becoming negative. Consider, then, replacing the strong measurements of the above protocol with weak measurements. We may loosely regard $\mathtt{AB}$ as undergoing stochastic trajectories weighted by quasiprobabilities, rather than probabilities. Levy and Lostaglio have applied quasiprobabilities in deriving a fluctuation theorem for energy exchanges [12]. Their fluctuation theorem contains the real part of a *Kirkwood-Dirac quasiprobability* (KDQ) [58,60–63].

KDQs have recently proven useful across quantum thermodynamics [12,57,58,64–67], information scrambling [64,68–71], tomography [72–78], metrology [79–81], and foundations [82–87].

When employed as work or heat distributions, KDQs have multiple desirable properties not achieved by joint probability distributions [57,58,88,89]

Negative and nonreal KDQs can reflect nonclassicality [82,90] and measurement disturbance [74,91–95]. In Ref. [12], negative real KDQs signal anomalous heat currents, which flow spontaneously from a colder to a hotter system. Generalizing from energy to potentially noncommuting charges, our results cover a more fully quantum setting. They also leverage the ability of the KDQ to become nonreal.

To accommodate noncommuting charges, we generalize the SEP. In conventional quantum thermodynamics, three common SEP formulas equal each other [52]. Entropy is cast as an extensive thermodynamic variable by a "charge formula," as quantifying missing information by a "surprisal formula," and as quantifying irreversibility by a "trajectory formula." We generalize all three formulas using KDQs. If the charges commute, the generalizations reduce to the usual formulas. The generalizations satisfy four sanity checks, including by equaling each other when the charges commute. Yet we find deductively that noncommuting charges break the equivalence, generating three species of SEP.

The different SEPs, we find, highlight different ways in which the noncommutation of charges impacts transport:

(1) *Charge SEP.* The noncommutation of charges enables individual stochastic trajectories to violate charge conservation. These violations underlie commutator-dependent corrections to a fluctuation theorem.
(2) *Surprisal SEP.* Initial coherences, relative to eigenbases of the charges, enable the average surprisal entropy production to become negative. Such negativity simulates a reversal of time's arrow. Across thermodynamics, a ubiquitous initial state is a product of thermal states. Only if the charges fail to commute can such a state have the necessary coherences. Hence the noncommutation of charges enables a resource, similar to work, for effectively reversing time's arrow in a common setup.
(3) *Trajectory SEP.* The generalized trajectory SEP can become nonreal, due to the KDQ. Such nonreality signals contextuality—a strong form of nonclassicality [96–98]—in a noncommuting-current experiment.

This work opens up the field of stochastic thermodynamics [99] to noncommuting charges. Furthermore, our work advances the widespread research program of critically comparing thermodynamic with information-theoretic entropies and leveraging information theory for thermodynamics [100–103].

The paper is organized as follows. In Sec. II, we detail the setup and review background material. In Sec. III, we present the three SEP formulas, the physical insights that they imply, and their fluctuation theorems and averages. In Sec. IV, we numerically illustrate our main results with a two-qubit example. In Sec. V, we sketch a trapped-ion experiment based on our results. Finally, in Sec. VI, we conclude with avenues for future work.

As a semantic disclaimer and to provide broader context, note that studies of the second law have engendered debates about what should be called *the* entropy production. We provide an alternative perspective: we show that three SEP formulas, despite being equivalent in the commuting case, become inequivalent if charges cease to commute. Each of these formulas encapsulates a different aspect of entropy production. This perspective harmonizes with demonstrations that, for small systems, the conventional second law splits into multiple second "laws" [20,23,104–108].

II. PRELIMINARIES

We specify the physical setup in Sec. II A. Section II B reviews KDQs; Sec. II C, information-theoretic entropies; and Sec. II D, fluctuation theorems.

A. Setup

Consider two identical quantum systems, $\mathtt{A}$ and $\mathtt{B}$. (From now on, we omit hats from operators.) Each system corresponds to a copy of a Hilbert space $\mathcal{H}$. The bipartite initial state ρ leads to the reduced states $\rho^{\mathtt{A}} := \mathrm{Tr}_{\mathtt{B}}(\rho)$ and $\rho^{\mathtt{B}} := \mathrm{Tr}_{\mathtt{A}}(\rho)$.

On $\mathcal{H}$ are defined single-system observables $Q_{\alpha=1,2,\ldots,c}$, assumed to be linearly independent [47]. For $\mathtt{X} = \mathtt{A}, \mathtt{B}$, we denote $\mathtt{X}$'s copy of Q_α by $Q_\alpha^{\mathtt{X}}$. The dynamics will conserve the global observables $Q_\alpha^{\text{tot}} := Q_\alpha^{\mathtt{A}} \otimes \mathbb{1}^{\mathtt{B}} + \mathbb{1}^{\mathtt{A}} \otimes Q_\alpha^{\mathtt{B}}$, so we refer to the Q_α as charges. In the *commuting case*, all the charges commute: $[Q_\alpha, Q_{\alpha'}] = 0 \ \forall \alpha, \alpha'$. At least two charges do not in the *noncommuting case*: $[Q_\alpha, Q_{\alpha'}] \neq 0$ for some α, α'. Each charge eigendecomposes as $Q_\alpha = \sum_j \lambda_{\alpha,j} \Pi_{\alpha,j}$. We denote tensor-product projectors by $\Pi_{\alpha,k} = \Pi^{\mathtt{A}}_{\alpha,k^{\mathtt{A}}} \otimes \Pi^{\mathtt{B}}_{\alpha,k^{\mathtt{B}}}$, invoking the composite index $k = (k^{\mathtt{A}}, k^{\mathtt{B}})$. To simplify the formalism, we assume that the Q_α are nondegenerate, as in Refs. [6,12,109,110]. Appendix B concerns extensions to degenerate charges. The nondegeneracy renders every projector rank-1: $\Pi_{\alpha,k} = |\alpha_k\rangle\langle\alpha_k|$. We call the Q_α^{tot} eigenbasis $\{|\alpha_k\rangle\}_k$ the αth *product basis*.

Having introduced the charges, we can expound upon the initial state. The reduced states $\rho^{\mathtt{X}}$ are *generalized Gibbs ensembles* (GGEs) [111–115]

$$\rho^{\mathtt{X}}_{\text{GGE}} := \frac{1}{Z^{\mathtt{X}}} \exp\left(-\sum_{\alpha=1}^{c} \beta_\alpha^{\mathtt{X}} Q_\alpha^{\mathtt{X}}\right). \tag{1}$$

$\beta_\alpha^{\mathtt{X}}$ denotes a generalized inverse temperature. The partition function $Z^{\mathtt{X}}$ normalizes the state. If the $Q_\alpha^{\mathtt{X}}$ fail to commute, the GGE is often called the *non-Abelian thermal state* [23,27,35,48]. Across most of this paper, ρ equals the tensor product

$$\rho^{\mathtt{A}}_{\text{GGE}} \otimes \rho^{\mathtt{B}}_{\text{GGE}}. \tag{2}$$

Such a product of thermal states, being a simple nonequilibrium state, surfaces across thermodynamics [Sec. 3.6] [116]. (In Secs. III B 2 and III C 3, we consider initial states ρ that deviate from this form but retain GGE reduced states.)

Our results stem from the following protocol. Prepare AB in ρ. Evolve ρ under a unitary U that conserves every global charge:

$$[U, Q_\alpha^{\text{tot}}] = 0 \ \forall \alpha. \tag{3}$$

U can bring the state arbitrarily far from equilibrium. The final state, $\rho_f = U\rho U^\dagger$, induces the reduced states $\rho_f^{\mathtt{A}} := \text{Tr}_{\mathtt{B}}(\rho_f)$ and $\rho_f^{\mathtt{B}} := \text{Tr}_{\mathtt{A}}(\rho_f)$. The average amount of α-type charge in A changes by $\Delta\langle Q_\alpha\rangle := \text{Tr}(Q_\alpha^{\mathtt{A}}[\rho_{\text{f}}^{\mathtt{A}} - \rho^{\mathtt{A}}])$; and the average amount in B, by $\text{Tr}(Q_\alpha^{\mathtt{B}}[\rho_{\text{f}}^{\mathtt{B}} - \rho^{\mathtt{B}}]) = -\Delta\langle Q_\alpha\rangle$. The generalized inverse temperatures differ by $\Delta\beta_\alpha := \beta_\alpha^{\mathtt{A}} - \beta_\alpha^{\mathtt{B}}$.

B. Kirkwood-Dirac quasiprobability

The relevance of the KDQ stems from the desire to reason about charges flowing between A and B. One can ascribe to A some amount of α-type charge only upon measuring $Q_\alpha^{\mathtt{A}}$. Measuring $Q_\alpha^{\mathtt{A}}$ strongly would disturb A and subsequent measurements of noncommuting $Q_{\alpha'}^{\mathtt{A}}$ [56]. Therefore, we consider sequentially measuring charges weakly. We define the *forward protocol* by combining the preparation procedure and unitary with weak measurements (Sec. III C introduces a reverse protocol):

(1) Prepare AB in ρ.
(2) Weakly measure the product basis of $Q_1^{\mathtt{A}}$ and $Q_1^{\mathtt{B}}$, then the product basis of $Q_2^{\mathtt{A}}$ and $Q_2^{\mathtt{B}}$, and so on until $Q_c^{\mathtt{A}}$ and $Q_c^{\mathtt{B}}$. (One can implement these measurements using the detector-coupling technique in Ref. [footnote 9] [68].)
(3) Evolve AB under U.
(4) Weakly measure the product bases of the charges in the reverse order, from c to 1. (This measurement ordering ensures that our SEP definitions satisfy sanity checks described in Sec. III.)

Lacking strong measurements, this protocol differs qualitatively from two-point-measurement schemes. The forward protocol leads naturally to a KDQ, as shown in Appendix A:

$$\text{Tr}\left(U^\dagger\left[\Pi_{1,f_1}\Pi_{2,f_2}\ldots\Pi_{c,f_c}\right]U\left[\Pi_{c,i_c}\ldots\Pi_{2,i_2}\Pi_{1,i_1}\right]\rho\right) =: \tilde{p}_F(i_1, i_2, \ldots, i_c\,; f_c, f_{c-1}, \ldots, f_1). \tag{4}$$

The list $(i_1, i_2, \ldots, i_c\,; f_c, f_{c-1}, \ldots, f_1)$ defines a stochastic trajectory, as in Sec. I. (Recall the definition, in Sec. II A, of composite-system indices.) Loosely speaking, we might view the trajectory as occurring with a joint quasiprobability $\tilde{p}_F(i_1, i_2, \ldots, i_c\,; f_c, f_{c-1}, \ldots, f_1)$.

$\tilde{p}_F$ can assume negative and nonreal values. One can infer $\tilde{p}_F$ experimentally by performing the forward protocol many times, performing strong-measurement experiments, and processing the outcome statistics [64]. The angle brackets $\langle.\rangle$ denote averages with respect to $\tilde{p}_F$, unless we specify otherwise.

Two cases further elucidate $\tilde{p}_F$ and the forward protocol: the commuting case and the weak-measurement limit. In the commuting case, if ρ is diagonal with respect to the shared eigenbasis of the charges, $\tilde{p}_F$ is a joint probability.

C. Information-theoretic entropies

We invoke four entropic quantities from information theory [117]. Let $X = x_1, x_2, \ldots, x_n$ denote a discrete random variable; $P = \{p_1, p_2, \ldots, p_n\}$ and $R = \{r_1, r_2, \ldots, r_n\}$, probability distributions over X; and ω_1 and ω_2, quantum states. Suppose that X evaluates to x_j. The *surprisal* $-\log(p_j)$ quantifies the information that we learn. (The logarithms in this paper are base-e.) Averaging the surprisal yields the *Shannon entropy*, $S_{\text{Sh}}(P) := -\sum_j p_j \log(p_j)$. The quantum analogue is the *von Neumann entropy*, $S_{\text{vN}}(\omega_1) := -\text{Tr}(\omega_1 \log(\omega_1))$.

The *quantum relative entropy* quantifies the distance between states: $D(\omega_1||\omega_2) = \text{Tr}(\omega_1[\log(\omega_1) - \log(\omega_2)])$. D measures how effectively one can distinguish between ω_1 and ω_2, on average, in an asymmetric hypothesis test. $D(\omega_1||\omega_2) \geq 0$ vanishes if and only if $\omega_1 = \omega_2$.

Analogously, the *classical relative entropy* distinguishes probability distributions: $D(P||R) = \sum_j p_j \left[\log(p_j) - \log(r_j)\right]$. We will substitute KDQ distributions for P and R in Sec. III C 1. The logarithms will be of complex numbers. We address the branch-cut conventions and the multivalued nature of the complex logarithm there.

D. Exchange fluctuation theorems

An exchange fluctuation theorem governs two systems trading charges. (We will drop the *exchange* from the name.) Consider two quantum systems initialized and exchanging energy as in Sec. I, though without the complication of particles. Each trial has a probability $p(\sigma)$ of producing entropy σ. We denote by $\langle\cdot\rangle_P$ averages with respect to the probability distribution. The fluctuation theorem $\langle e^{-\sigma}\rangle_P = 1$ implies the second-law-like inequality $\langle\sigma\rangle_P \geq 0$ [6]. Unlike the second law, fluctuation theorems are equalities arbitrarily far from equilibrium. More-general (e.g., correlated) initial states engender corrections: $\langle e^{-\sigma}\rangle_P = 1 + \ldots$ [12,110].

III. THREE GENERALIZED SEP FORMULAS

We now present and analyze the generalized SEP formulas: the charge SEP σ_{chrg} (Sec. III A), the surprisal SEP σ_{surp} (Sec. III B), and the trajectory SEP σ_{traj} (Sec. III C).

To simplify the notation, we suppress the indices that identify the trajectory along which an SEP is produced.

Each formula satisfies four sanity checks, as follows. (i) Each $\langle\sigma\rangle$ has a clear physical interpretation. (ii) Each σ satisfies a fluctuation theorem (Sec. II D). Any corrections depend on the commutators of the charges. (iii) If the charges commute, all three SEPs coincide. (iv) Suppose that no current flows: $[U, Q_\alpha^{\mathtt{X}}] = 0 \; \forall \alpha$. As expected physically, the average entropy production vanishes: $\langle\sigma\rangle = 0$. Also, the fluctuation theorems lack corrections: $\langle e^{-\sigma}\rangle = 1$.

A. Charge stochastic entropy production

First, we motivate the definition of the charge SEP (Sec. III A 1). σ_{chrg} portrays entropy as an extensive thermodynamic quantity (Sec. III A 2). Furthermore, σ_{chrg} satisfies a fluctuation theorem, the corrections of which depend on commutators of the Q_α (Sec. III A 3). Corrections arise because noncommuting charges enable individual stochastic trajectories to violate a "microscopic," or "detailed," notion of charge conservation. [Nevertheless, charge conservation as defined in Eq. (3) is not violated.]

1. Charge-SEP formula

The fundamental relation of statistical mechanics [118] motivates the definition of σ_{chrg}. In this paragraph, we reuse quantum notation (Sec. II A) to denote classical objects, for simplicity. The fundamental relation governs large, classical systems $\mathtt{X} = \mathtt{A}, \mathtt{B}$ that have extensive charges $Q_\alpha^{\mathtt{X}}$ and intensive parameters $\beta_\alpha^{\mathtt{X}}$. Let an infinitesimal interaction conserve each $Q_\alpha^{\mathtt{A}} + Q_\alpha^{\mathtt{B}}$. Since $dQ_\alpha^{\mathtt{B}} = -dQ_\alpha^{\mathtt{A}}$, the total entropy changes by

$$dS^{\mathtt{AB}} = \sum_\alpha \left(\beta_\alpha^{\mathtt{A}}\, dQ_\alpha^{\mathtt{A}} + \beta_\alpha^{\mathtt{B}}\, dQ_\alpha^{\mathtt{B}}\right) \tag{5}$$

$$= \sum_\alpha \Delta\beta_\alpha\, dQ_\alpha^{\mathtt{A}}. \tag{6}$$

According to the second law of thermodynamics, $dS^{\mathtt{AB}} \geq 0$ during spontaneous processes [119]. We posit that $\langle\sigma_{\text{chrg}}\rangle$ should assume the form given in Eq. (6). We reverse-engineer such a formula, using the eigenvalues of the charges:

$$\sigma_{\text{chrg}} := \sum_\alpha \left[\beta_\alpha^{\mathtt{A}}\left(\lambda_{\alpha, f_\alpha^{\mathtt{A}}} - \lambda_{\alpha, i_\alpha^{\mathtt{A}}}\right) + \beta_\alpha^{\mathtt{B}}\left(\lambda_{\alpha, f_\alpha^{\mathtt{B}}} - \lambda_{\alpha, i_\alpha^{\mathtt{B}}}\right)\right]. \tag{7}$$

2. Average of charge SEP

By design, the charge SEP averages to

$$\langle\sigma_{\text{chrg}}\rangle = \sum_\alpha \Delta\beta_\alpha\, \Delta\langle Q_\alpha\rangle. \tag{8}$$

This average is non-negative, equaling a relative entropy [52]:

$$\langle\sigma_{\text{chrg}}\rangle = D(\rho_f \,||\, \rho) \geq 0. \tag{9}$$

This inequality echoes the second-law statement written just below Eq. (6).

3. Fluctuation theorem for charge SEP

σ_{chrg} obeys the fluctuation theorem

$$\begin{aligned}\langle e^{-\sigma_{\text{chrg}}}\rangle = \text{Tr}(U^\dagger &\left[e^{-\Delta\beta_1 Q_1^{\mathtt{A}}} \dots e^{-\Delta\beta_c Q_c^{\mathtt{A}}}\right] U \\ &\times \left[e^{\Delta\beta_c Q_c^{\mathtt{A}}} \dots e^{\Delta\beta_1 Q_1^{\mathtt{A}}}\right] \rho) \\ &+ (c - 1 \text{ terms dependent on commutators}).\end{aligned} \tag{10}$$

We prove the theorem and present the form of the correction in Appendix C 1. Below, we show that the right-hand side evaluates to 1 in the commuting case. In the noncommuting case, corrections arise from two physical sources: (i) $\rho^{\mathtt{A}}$ and $\rho^{\mathtt{B}}$ are non-Abelian thermal states. (ii) Individual stochastic trajectories can violate charge conservation.

In the commuting case, the first term in Eq. (10) equals 1. The reason is that, in $\rho = \rho_{\text{GGE}}^{\mathtt{A}} \otimes \rho_{\text{GGE}}^{\mathtt{B}}$, each $\rho_{\text{GGE}}^{\mathtt{X}} \propto \exp\left(-\sum_\alpha \beta_\alpha^{\mathtt{X}} Q_\alpha^{\mathtt{X}}\right) \propto \prod_\alpha \exp\left(-\beta_\alpha^{\mathtt{X}} Q_\alpha^{\mathtt{X}}\right)$. The $\mathtt{A}$ exponentials cancel the $e^{\beta_\alpha^{\mathtt{A}} Q_\alpha^{\mathtt{A}}}$ factors in Eq. (10). No such cancellation occurs in the noncommuting case, since $\rho_{\text{GGE}}^{\mathtt{X}} \not\propto \prod_\alpha \exp\left(-\beta_\alpha^{\mathtt{X}} Q_\alpha^{\mathtt{X}}\right)$. The first term in Eq. (10) can therefore deviate from 1, quantifying the noncommutation of charges in $\rho_{\text{GGE}}^{\mathtt{X}}$.

The second term vanishes in the commuting case, since all commutators of charges vanish. This second term can deviate from 0 in the noncommuting case, due to *nonconserving trajectories*, which we introduce now. Define a trajectory $(i_1^{\mathtt{A}}, i_1^{\mathtt{B}}, i_2^{\mathtt{A}}, i_2^{\mathtt{B}}, \dots, i_c^{\mathtt{B}}) \mapsto (f_c^{\mathtt{A}}, f_c^{\mathtt{B}}, f_{c-1}^{\mathtt{A}}, f_{c-1}^{\mathtt{B}}, \dots, f_1^{\mathtt{B}})$ as *conserving* if the corresponding charge eigenvalues satisfy

$$\lambda_{\alpha, i_\alpha^{\mathtt{A}}} + \lambda_{\alpha, i_\alpha^{\mathtt{B}}} = \lambda_{\alpha, f_\alpha^{\mathtt{A}}} + \lambda_{\alpha, f_\alpha^{\mathtt{B}}} \quad \forall\, \alpha. \tag{11}$$

We call any trajectory that violates this condition *nonconserving*. Loosely speaking, under Eq. (11), $\mathtt{AB}$ has the same amount of α-type charge at the start and end of the trajectory.

In the commuting case, $\tilde{p}_F = 0$ when evaluated on nonconserving trajectories. We call this vanishing *detailed charge conservation*. Earlier work has relied on detailed charge conservation [12,57]. In the noncommuting case, $\tilde{p}_F$ need not vanish when evaluated on nonconserving trajectories (Appendix C 2). The mathematical reason is, different charges' eigenprojectors in $\tilde{p}_F$ [Eq. (4)] can fail to commute. A physical interpretation is that measuring any Q_α^X disturbs any later measurements of noncommuting $Q_{\alpha'}^X$. Nonconserving trajectories resemble classically forbidden trajectories in the path-integral formulation of quantum mechanics.

We now show that nonconserving trajectories underlie the final term in Eq. (10). Every stochastic function $g(i_1, i_2, \ldots, i_c\,; f_c, f_{c-1}, \ldots, f_1)$ averages to $\langle g \rangle = \langle g \rangle_{\text{cons}} + \langle g \rangle_{\text{noncons}}$. Each term equals an average over just the conserving or nonconserving trajectories. For example, the average in Eq. (8) decomposes as $\langle \sigma_{\text{chrg}} \rangle = \langle \sigma_{\text{chrg}} \rangle_{\text{cons}} + \langle \sigma_{\text{chrg}} \rangle_{\text{noncons}}$. The second term on the right-hand side of Eq. (10) takes the form $\langle g \rangle_{\text{noncons}}$ (Appendix C 2 c). In the commuting case, all trajectories are conserving, so the second term equals zero—as expected, since the term depends on commutators $[Q_\alpha^A, Q_{\alpha'}^A]$. Therefore, the fluctuation theorem's final term (second correction) stems from violations of detailed charge conservation. The average in Eq. (8) contains contributions from conserving and nonconserving trajectories.

We have identified two corrections to the fluctuation theorem of Eq. (10). On the right-hand side of the equation, the first term can deviate from 1 and the second term can deviate from 0. The first deviation originates in the noncommutation of charges in ρ_{GGE}^X. The second deviation stems from nonconserving trajectories. An example illustrates the distinction between the influences of noncommuting charges on the initial conditions and dynamical trajectories. Let $c = 3$, and let $[Q_1, Q_2] \neq 0$, while $[Q_1, Q_3], [Q_2, Q_3] = 0$. Let the noncommuting charges correspond to uniform β: $\beta_1^A = \beta_1^B$ and $\beta_2^A = \beta_2^B$. Thus, there exists no temperature gradient that directly drives noncommuting-charge currents. Accordingly, the first term of the fluctuation theorem equals 1. Yet the second term—an average over nonconserving trajectories—is nonzero.

B. Surprisal stochastic entropy production

σ_{surp} casts entropy as missing information (Sec. III B 1). The average $\langle \sigma_{\text{surp}} \rangle$ can be expressed in terms of relative entropies (Sec. III B 2), as one might expect from precedent [52]. Yet initial coherences, relative to the product bases of the charges, can render $\langle \sigma_{\text{surp}} \rangle$ negative. If ρ is a product $\rho_{\text{GGE}}^A \otimes \rho_{\text{GGE}}^B$—as across much of thermodynamics—ρ has such coherences only if the Q_α fail to commute. Furthermore, positive $\langle \sigma_{\text{surp}} \rangle$ values accompany the arrow of time. Hence the noncommutation of charges enables a resource, similar to work, for effecting a seeming reversal of time's arrow. The noncommutation of charges also engenders a correction to the σ_{surp} fluctuation theorem (Sec. III B 3).

1. Surprisal-SEP formula

Information theory motivates the surprisal-SEP formula. Averaging the surprisal $-\log(p_j)$ yields the Shannon entropy (Sec. II C), so the surprisal is a stochastic (associated-with-one-trial) entropic quantity. A difference of two surprisals forms our σ_{surp} formula. The probabilities follow from preparing ρ and projectively measuring the α^{th} product basis, for any α. Outcome $i_\alpha := (i_\alpha^A, i_\alpha^B)$ obtains with a probability $p_\alpha(i_\alpha^A, i_\alpha^B) := \text{Tr}(\Pi_{\alpha, i_\alpha} \rho)$; and outcome $f_\alpha := (f_\alpha^A, f_\alpha^B)$, with a probability $p_\alpha(f_\alpha^A, f_\alpha^B) := \text{Tr}(\Pi_{\alpha, f_\alpha} \rho)$. Appendix D 1 shows how these probabilities generalize those in the conventional surprisal-SEP formula [52]. The surprisal SEP quantifies the information gained if we expect to observe i_α but we obtain f_α:

$$\sigma_{\text{surp}} := \log\left(\frac{p_\alpha(i_\alpha^A, i_\alpha^B)}{p_\alpha(f_\alpha^A, f_\alpha^B)}\right). \tag{12}$$

All results below hold for arbitrary α. Nevertheless, Appendix F introduces a variation on Eq. (12)—an alternative definition that contains an average over all α. Appendix D 2 confirms that σ_{surp} reduces to σ_{chrg} if the Q_α commute.

2. Average of surprisal SEP

$\langle \sigma_{\text{surp}} \rangle$ demonstrates that the noncommutation of charges can enable a seeming reversal of time's arrow. Time's arrow manifests in, e.g., spontaneous flows of heat from hot to cold bodies. This arrow accompanies positive average entropy production. Hence negative $\langle \sigma \rangle$ simulate reversals of time's arrow. These simulations cost resources, such as the work traditionally used to pump heat from colder to hotter bodies. Quantum phenomena, such as entanglement, serve as such resources too [8,120]. We identify another such resource: initial coherences relative to the product bases of the charges, present in the common initial state [Eq. (1)] only if charges fail to commute.

To prove this result, we denote by Φ_α the channel that dephases states ω with respect to the αth product basis: $\Phi_\alpha(\omega) := \sum_k \Pi_{\alpha,k}\, \omega\, \Pi_{\alpha,k}$. σ_{surp} averages to

$$\langle \sigma_{\text{surp}} \rangle = D(\rho_f \,||\, \Phi_\alpha(\rho)) - D(\rho || \Phi_\alpha(\rho)) \tag{13}$$

(Appendix D 3). The relative entropy is non-negative (Sec. II C). Therefore, initial coherences relative to the product bases of the charges can reduce $\langle \sigma_{\text{surp}} \rangle$. Such coherences can even render $\langle \sigma_{\text{surp}} \rangle$ negative. Since $\langle \sigma_{\text{chrg}} \rangle \geq 0$ [Eq. (9)], σ_{surp} is sensitive to the resource of coherence, while σ_{chrg} is not.

This result progresses beyond three existing results. First, coherences engender a correction to a heat-exchange fluctuation theorem [12]. Those coherences are relative to an eigenbasis of the only charge in Ref. [12], energy. If the dynamics conserve only one charge, or only commuting charges, then the thermal product $\rho_{\text{GGE}}^A \otimes \rho_{\text{GGE}}^B$ [Eq. (1)] lacks the necessary coherences. $\rho_{\text{GGE}}^A \otimes \rho_{\text{GGE}}^B$ has those coherences only if charges fail to commute. Across thermodynamics, $\rho_{\text{GGE}}^A \otimes \rho_{\text{GGE}}^B$ is ubiquitous as an initial state. Hence noncommuting charges underlie a resource for effectively reversing time's arrow in a common thermodynamic setup.

Second, Ref. [28] shows that noncommuting charges can reduce entropy production in the linear-response regime. Our dynamics U can be arbitrarily far from equilibrium. Third, just as we attribute $\langle \sigma_{\text{surp}} \rangle < 0$ to initial coherences, so do Refs. [8,110,120,121] attribute negative average entropy production to initial correlations. Our framework recapitulates such a correlation result, incidentally: if ρ encodes correlations but retains GGE marginals, $\langle \sigma_{\text{chrg}} \rangle$ [Eq. (8)] shares the form of Eq. (13), to within one alteration. The decorrelated state $\rho^{\text{A}} \otimes \rho^{\text{B}}$ replaces the dephased state $\Phi_\alpha(\rho)$: $\langle \sigma_{\text{chrg}} \rangle = D(\rho_f || \rho^{\text{A}} \otimes \rho^{\text{B}}) - D(\rho || \rho^{\text{A}} \otimes \rho^{\text{B}})$. Initial correlations can therefore render $\langle \sigma_{\text{chrg}} \rangle$ negative. Just as initial correlations can render a $\langle \sigma \rangle$ negative, so can coherences attributable to noncommuting charges, σ_{surp} reveals.

3. Fluctuation theorem for surprisal SEP

To formulate the fluctuation theorem, we define the coherent difference $\Delta\rho_\alpha := \Phi_\alpha(\rho)^{-1} - \rho^{-1}$. It quantifies the coherences of ρ with respect to the α^{th} product basis. If and only if ρ is diagonal with respect to this basis, $\Delta\rho_\alpha = 0$. The surprisal SEP obeys the fluctuation theorem

$$\langle e^{-\sigma_{\text{surp}}} \rangle = 1 + \text{Tr}(U^\dagger \Phi_\alpha(\rho) U \, \Delta\rho_\alpha \rho) \tag{14}$$

(Appendix D 4). The second term—the correction—arises from the coherences of ρ relative to the product eigenbases of the charges. If $\rho = \rho^{\text{A}}_{\text{GGE}} \otimes \rho^{\text{B}}_{\text{GGE}}$, as throughout much of thermodynamics, then ρ can have such coherences only if charges fail to commute. Our correction resembles that in Ref. [12] but arises from distinct physics: noncommuting charges, rather than initial correlations.

C. Trajectory stochastic entropy production

σ_{traj} evokes how entropy accompanies irreversibility (Sec. III C 1). σ_{traj} can assume nonreal values, signaling contextuality in a noncommuting-current experiment (Sec. III C 2). Despite the unusualness of nonreal entropy production, σ_{traj} satisfies two sanity checks: $\langle \sigma_{\text{traj}} \rangle$ has a sensible physical interpretation (Sec. III C 3) and σ_{traj} obeys a correction-free fluctuation theorem (Sec. III C 4). Complex-valued entropy production has appeared also in Ref. [11].

1. Trajectory-SEP formula

σ_{traj} generalizes the conventional trajectory-SEP formula, which we now review. Recall the classical experiment in Sec. I: classical systems A and B begin in grand canonical ensembles, then exchange energy and particles. In each trial, AB undergoes the trajectory $(E^{\text{A}}_i, N^{\text{A}}_i, E^{\text{B}}_i, N^{\text{B}}_i) \mapsto (E^{\text{A}}_f, N^{\text{A}}_f, E^{\text{B}}_f, N^{\text{B}}_f)$ with some joint probability. Let us add a subscript F to the notation for that probability: $p_F(E^{\text{A}}_i, N^{\text{A}}_i, E^{\text{B}}_i, N^{\text{B}}_i \,;\, E^{\text{A}}_f, N^{\text{A}}_f, E^{\text{B}}_f, N^{\text{B}}_f)$. Imagine preparing the grand canonical ensembles, then implementing the time-reversed dynamics. One observes the reverse trajectory, $(E^{\text{A}}_f, N^{\text{A}}_f, E^{\text{B}}_f, N^{\text{B}}_f) \mapsto (E^{\text{A}}_i, N^{\text{A}}_i, E^{\text{B}}_i, N^{\text{B}}_i)$, with a probability $p_R(E^{\text{A}}_f, N^{\text{A}}_f, E^{\text{B}}_f, N^{\text{B}}_f \,;\, E^{\text{A}}_i, N^{\text{A}}_i, E^{\text{B}}_i, N^{\text{B}}_i)$. The log-ratio of the probabilities forms the conventional trajectory-SEP formula [1–3,6]: $\log(p_F/p_R)$. In an illustrative forward trajectory, heat and particles flow from a hotter higher-chemical-potential A to a colder lower-chemical-potential B. This forward trajectory is more likely than its reverse: $p_F > p_R$. Hence $\log(p_F/p_R) > 0$, as expected from the second law of thermodynamics.

Let us extend this formula to quasiprobabilities. Section II B has established a forward protocol suitable for potentially noncommuting Q_α. That section has attributed to the forward trajectory $(i_1, i_2, \ldots, i_c) \mapsto (f_c, f_{c-1}, \ldots, f_1)$ the KDQ $\tilde{p}_F(i_1, i_2, \ldots, i_c \,;\, f_c, f_{c-1}, \ldots, f_1)$ [Eq. (4)]. The reverse protocol features $U^\dagger$, rather than U, in step 3, with a reversed list of measurement outcomes. The reverse trajectory $(f_1, f_2, \ldots, f_c) \mapsto (i_c, i_{c-1}, \ldots, i_1)$ corresponds to the quasiprobability $\tilde{p}_{\text{R}}(f_1, f_2, \ldots, f_c \,;\, i_c, i_{c-1}, \ldots, i_1) := \text{Tr}([\Pi_{1,f_1} \ldots \Pi_{c,f_c}] \, U [\Pi_{c,i_c} \ldots \Pi_{1,i_1}] U^\dagger \rho)$. This definition captures the notion of time reversal, we argue in Appendix E 1, while enabling σ_{traj} to agree with σ_{chrg} and σ_{surp} in the commuting case (Appendix E 2). Both quasiprobabilities feature in the trajectory SEP:

$$\sigma_{\text{traj}} := \log\left(\frac{\tilde{p}_F(i_1, i_2, \ldots, i_c \,;\, f_c, f_{c-1}, \ldots, f_1)}{\tilde{p}_R(f_1, f_2, \ldots, f_c \,;\, i_c, i_{c-1}, \ldots, i_1)}\right) \tag{15}$$

$$= \log\left(\frac{\text{Tr}\left(U^\dagger \left[\Pi_{1,f_1} \ldots \Pi_{c,f_c}\right] U \left[\Pi_{c,i_c} \ldots \Pi_{1,i_1}\right] \rho\right)}{\text{Tr}\left(\left[\Pi_{1,f_1} \ldots \Pi_{c,f_c}\right] U \left[\Pi_{c,i_c} \ldots \Pi_{1,i_1}\right] U^\dagger \rho\right)}\right)$$

$$= \log\left(\frac{\langle i_1 | \, \rho U^\dagger \, | f_1 \rangle}{\langle i_1 | \, U^\dagger \rho \, | f_1 \rangle}\right). \tag{16}$$

The final equality follows from the nondegeneracy of the local charges Q^{X}_α: the projectors $\Pi_{\alpha,k} = |\alpha_k\rangle\langle\alpha_k|$, so factors cancel between the numerator and denominator. The $\langle i_1|$ and $|f_1\rangle$ distinguish Q_1 from the other charges. However, Eq. (16) holds for every possible labeling of the Q_α (holds under the labeling of any charge as 1) and for every ordering of the projectors in Eq. (4). Moreover, Appendix F introduces a variation on Eq. (15)—a definition that contains an average over all measurement orderings, removing the dependence on the ordering.

2. Nonreal trajectory SEP witnesses nonclassicality

Nonreal σ_{traj} values signal nonclassicality in a noncommuting-current experiment. To prove this result, we review weak values (conditioned expectation values) and contextuality (provable nonclassicality). We then

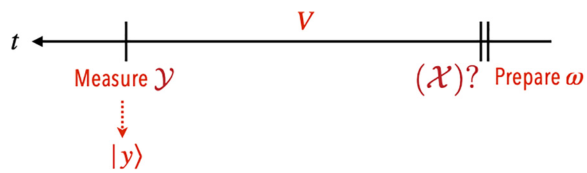

FIG. 2. Weak value: the weak value serves as a "conditioned expectation value" in the protocol depicted. Time runs from right to left, as reading a weak value from right to left translates into the procedure depicted: prepare ω, evolve the state under V, measure $\mathcal{Y}$, and postselect on outcome y. Which value is retrodictively most reasonably attributable to $\mathcal{X}$ immediately after the preparation procedure? Arguably, this value is the weak value [122–125].

express σ_{traj} in terms of weak values. Finally, we prove that nonreal σ_{traj} values herald contextuality in an instance of the forward or reverse protocol.

Figure 2 motivates the form of the weak value [59,126]. Consider preparing a quantum system in a state ω at a time $t = 0$. The system evolves under a unitary V. An observable $\mathcal{Y}$ is then measured, yielding an outcome y. Denote by $\mathcal{X}$ an observable that neither commutes with ω nor shares the $\mathcal{Y}$ eigenstate $|y\rangle$. Which value is retrodictively most reasonably attributable to $\mathcal{X}$ immediately after the state preparation? Arguably, that value is the *weak value* [122–125] $\text{Tr}(\Pi'_y \mathcal{X}\omega)/\text{Tr}(\Pi'_y \omega)$, wherein $\Pi'_y := V^\dagger |y\rangle\langle y| V$. Weak values can be *anomalous*, lying outside the spectrum of $\mathcal{X}$. Anomalous weak values actuate metrological advantages [79,127–131] and signal contextuality [82,90,132].

Contextuality is a strong form of nonclassicality [98,133]. One can model quantum systems as being in unknown microstates akin to classical statistical-mechanical microstates. One might expect to model operationally indistinguishable procedures identically. However, no such model reproduces all quantum-theory predictions. This impossibility is quantum theory's contextuality, which underlies quantum-computational speedups [134]. Anomalous weak values signal contextuality in the process *prepare ω, measure $\mathcal{X}$ weakly, evolve with V, measure $\mathcal{Y}$ strongly, and postselect on y* [82,90,132].

Having introduced the relevant background, we prove that σ_{traj} depends on weak values and signals contextuality. Define the evolved projectors $\Pi'_{1,i_1} := U\Pi_{1,i_1}U^\dagger$ and $\Pi''_{1,f_1} := U^\dagger \Pi_{1,f_1} U$. Define also the weak values

$$_{f_1}\langle \Pi_{1,i_1}\rangle_\rho := \text{Tr}(\Pi''_{1,f_1}\Pi_{1,i_1}\rho)/\text{Tr}(\Pi''_{1,f_1}\rho) \quad \text{and} \tag{17}$$

$$_{i_1}\langle \Pi_{1,f_1}\rangle_\rho := \text{Tr}(\Pi'_{1,i_1}\Pi_{1,f_1}\rho)/\text{Tr}(\Pi'_{1,i_1}\rho). \tag{18}$$

Each is a complex number with a phase ϕ: $_{f_1}\langle \Pi_{1,i_1}\rangle_\rho = |_{f_1}\langle \Pi_{1,i_1}\rangle_\rho| e^{i\phi_{\text{F}}}$, and $_{i_1}\langle \Pi_{1,f_1}\rangle_\rho = |_{i_1}\langle \Pi_{1,f_1}\rangle_\rho| e^{-i\phi_{\text{R}}}$. We suppress the indices of the phases for conciseness. Equation (16) becomes

$$\sigma_{\text{traj}} = \log\left(\left|_{f_1}\langle \Pi_{1,i_1}\rangle_\rho\right| / \left|_{i_1}\langle \Pi_{1,f_1}\rangle_\rho\right|\right) + i(\phi_{\text{F}} - \phi_R) + \log\left(\text{Tr}(\Pi''_{1,f_1}\rho)/\text{Tr}(\Pi'_{1,i_1}\rho)\right). \tag{19}$$

The final log is of mere probabilities. The phase difference is defined modulo 2π. For convenience, we assume that the branch cut of the complex logarithm lies along the negative real axis [135]. Appendix E 3 explains how to choose the value of the complex logarithm if ρ is pure and describes subtleties concerning mixed states ρ.

If $\text{Im}(\sigma_{\text{traj}}) \neq 0$, we call σ_{traj} *anomalous* and at least one weak value is anomalous. Hence at least one of two protocols is contextual:

(1) *Forward compressed protocol.* Prepare ρ. Measure Π_{1,i_1} weakly [136]. Evolve under U. Measure the Q_1 product basis strongly. Postselect on f_1.
(2) *Reverse compressed protocol.* Prepare ρ. Measure Π_{1,f_1} weakly. Evolve under $U^\dagger$. Measure the Q_1 product basis strongly. Postselect on i_1.

The forward compressed protocol is a simplification of the forward protocol in Sec. II B: only measurements pertaining to charge Q_1 are performed. Analogous statements concern the reverse compressed protocol. Hence σ_{traj} joins a sparse set of thermodynamic quantities known to signal contextuality [12,66].

The signaling of contextuality by σ_{traj} exhibits irreversibility—fittingly for an entropic phenomenon—algebraically and geometrically. First, for σ_{traj} to signal contextuality—to become nonreal—nonreality of a weak value does not suffice. Rather, the phases of the weak values must fail to cancel: $\phi_{\text{F}} \neq \phi_{\text{R}}$ [137]. This failure mirrors how, conventionally, entropy is produced only when $p_F \neq p_R$.

Second, suppose that ρ is pure. $\phi_{\text{F}} - \phi_{\text{R}}$ equals the geometric phase imprinted on a state manipulated as follows: ρ is prepared, the forward compressed protocol is performed, the state is reset to ρ, the reverse compressed protocol is performed, and the state is reset to ρ [138,139]. All measurements here are performed in the strong limit. The state acquires the phase $e^{i\phi_{\text{F}}}$ during the forward step and acquires $e^{-i\phi_{\text{R}}}$ during the reverse. Only if the forward and reverse steps fail to cancel does the geometric phase $\neq 1$—does σ_{traj} signal contextuality. Hence σ_{traj} heralds contextuality in the presence of irreversibility, appropriately for a thermodynamic quantity.

3. Average of trajectory SEP

Formally, averaging σ_{traj} [Eq. (15)] with respect to $\tilde{p}_F$ yields a quasiprobabilistic relative entropy of Sec. II C

[140]:

$$\langle\sigma_{\text{traj}}\rangle = D(\tilde{p}_F(i_1,i_2,\ldots,i_c\,;f_c,f_{c-1},\ldots,f_1) \\ ||\,\tilde{p}_R(f_1,f_2,\ldots,f_c\,;\,i_c,i_{c-1},\ldots,i_1)). \qquad (20)$$

The average can be negative and even nonreal. Yet $\langle\sigma_{\text{traj}}\rangle$ has a particularly crisp physical interpretation when ρ is a pure state that retains GGE marginals, as in Eq. (1) [141].

A pure ρ is not as restricted as it may seem: thermodynamics often features pure global states, the reduced states of which are thermal [8,101,120,142,143]. The average becomes

$$\langle\sigma_{\text{traj}}\rangle = \frac{1}{2}\left[D(\rho||\Phi_1(U^\dagger\rho U)) + D(\rho||U^\dagger\Phi_1(\rho)U) \right. \\ \left. -D(\rho||\Phi_1(\rho)) - D(\rho_f||\Phi_1(\rho_f))\right] \\ + i\langle\phi_{\text{F}} - \phi_R\rangle \qquad (21)$$

(Appendix E 3). Each ϕ implicitly depends on indices i_1 and f_1. The real and imaginary components of $\langle\sigma_{\text{traj}}\rangle$ have physical significances that we now elucidate.

In Appendix E 3, we prove that $\langle\phi_{\text{F}} - \phi_R\rangle$ is real [144]. Hence, if $\text{Im}(\langle\sigma_{\text{traj}}\rangle) \neq 0$, at least one ϕ_{F} [associated with one tuple (i_1,f_1)] or one ϕ_{R} is nonzero. Therefore, at least one weak value—at least one ${}_{f_1}\langle\Pi_{1,i_1}\rangle_\rho$ or ${}_{i_1}\langle\Pi_{1,f_1}\rangle_\rho$—is anomalous. At least one instance of the forward or reverse compressed protocol is therefore contextual. In conclusion, $\langle\sigma_{\text{traj}}\rangle$, beyond σ_{traj}, witnesses contextuality.

$\text{Re}(\langle\sigma_{\text{traj}}\rangle)$ has two familiar properties. First, $\text{Re}(\langle\sigma_{\text{traj}}\rangle) \geq 0$, suggestively of the second law of thermodynamics. Second, $\text{Re}(\langle\sigma_{\text{traj}}\rangle)$ depends on relative-entropy differences, similarly to Eq. (9).

Pairs of relative entropies have recognizable physical significances. Each negated D is a relative entropy of coherence, comparing a state (ρ or ρ_f) to its dephased counterpart [145]. Hence the coherences of states relative to $\{\Pi_{1,k}\}$ reduce $\langle\sigma_{\text{traj}}\rangle$. This reduction resembles the reduction of $\langle\sigma_{\text{surp}}\rangle$ by initial coherence (Sec. III B 2). Not only initial coherences, though, but also final coherences reduce $\langle\sigma_{\text{traj}}\rangle$.

The first two relative entropies in Eq. (21) imprint noncommutation on $\langle\sigma_{\text{traj}}\rangle$. In each such D, the compared-to state (the final argument) results from a dephasing and a time-reversed evolution. The ordering of the operations differs between the relative entropies. The $1/2$ in Eq. (21) averages over the orderings. Hence $\langle\sigma_{\text{traj}}\rangle$ translates into sensible physics.

4. Fluctuation theorem for trajectory SEP

Passing another sanity check, σ_{traj} satisfies the correction-free fluctuation theorem

$$\langle e^{-\sigma_{\text{traj}}}\rangle = 1. \qquad (22)$$

The proof follows from the normalization of the KDQ.

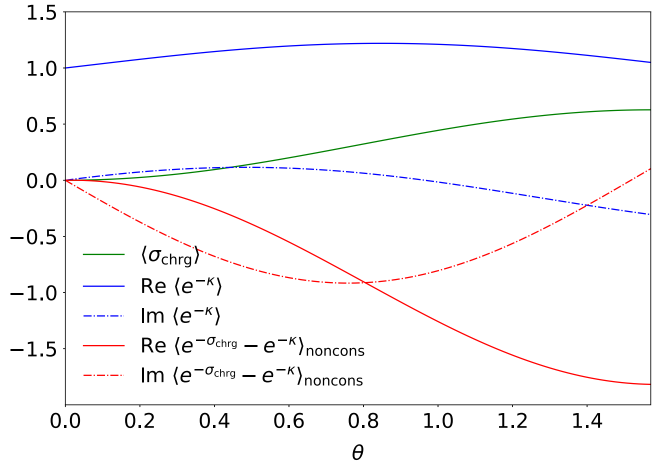

FIG. 3. The components of the σ_{chrg} fluctuation theorem, and $\langle\sigma_{\text{chrg}}\rangle$, versus θ. The generalized inverse temperatures are $\beta_x^{\text{A}} = 0.7$, $\beta_x^{\text{B}} = 0.1$, $\beta_y^{\text{A}} = 1$, $\beta_y^{\text{B}} = 0.2$, $\beta_z^{\text{A}} = 0.5$, and $\beta_z^{\text{B}} = 0.6$.

IV. TWO-QUBIT EXAMPLE

This section numerically illustrates the key properties of the SEP definitions. First, we introduce the simulated system. Afterward, we analyze the calculated SEPs using generic parameter choices.

In our example system, A and B are qubits. The charges are the Pauli operators $Q_1 = \sigma_z$, $Q_2 = \sigma_y$, and $Q_3 = \sigma_x$. By the Schur-Weyl duality, the most general charge-conserving unitary is a linear combination of the permutations of two objects—a linear combination of the identity and SWAP operators [47,117]. The SWAP operator acts on states $|\psi\rangle_{\text{A}}$ and $|\phi\rangle_{\text{B}}$ as SWAP $|\psi\rangle_{\text{A}} \otimes |\phi\rangle_{\text{B}} = |\phi\rangle_{\text{A}} \otimes |\psi\rangle_{\text{B}}$. We parametrize the unitary with an angle θ:

$$U_\theta = \cos(\theta)\,\mathbb{1} + i\sin(\theta)\,\text{SWAP}. \qquad (23)$$

A. Charge SEP

Section III A 3 has introduced nonconserving trajectories and the following results. On the right-hand side of the fluctuation theorem Eq. (10) are two terms. The first, notated as $\langle e^{-\kappa}\rangle$ (Appendix C 1), encodes the noncommutation of charges in the initial state [Eqs. (1) and (2)]. The final term of the fluctuation theorem, notated as $\langle e^{-\sigma_{\text{chrg}}} - e^{-\kappa}\rangle_{\text{noncons}}$ (Appendix C 1), is an average over nonconserving trajectories.

We support these claims by showing how the two terms change as θ varies from 0 to $\pi/2$ in Eq. (23). In Fig. 3, we show the real and imaginary parts of the terms, as well as the average entropy production $\langle\sigma_{\text{chrg}}\rangle$. The values of the generalized inverse temperatures (listed in the caption of Fig. 3) ensure that a strong thermodynamic force pushes the σ_x and σ_y charges from B to A, whereas a weak force pushes σ_z oppositely.

The unitary parameter θ increases along the x axis. As per a sanity check in Sec. III, when $\theta = 0$, the terms in the fluctuation theorem sum to one. The first term, $\langle e^{-\kappa}\rangle$, equals one; and the second term, $\langle e^{-\sigma_{\text{chrg}}} - e^{-\kappa}\rangle_{\text{noncons}}$, vanishes. As θ increases, charges flow more, as evidenced by the increasing $\langle\sigma_{\text{chrg}}\rangle$. $\langle e^{-\kappa}\rangle$ changes little. This near-constancy reflects the origination of $\langle e^{-\kappa}\rangle$ in the noncommutation of charges in the initial state, which remains constant as θ changes. In contrast, as θ grows, $\langle e^{-\sigma_{\text{chrg}}} - e^{-\kappa}\rangle_{\text{noncons}}$ increases in magnitude—due to both its real and imaginary parts. This growth reflects the growing contribution of the nonconserving trajectories to the right-hand side of the fluctuation theorem.

B. Surprisal SEP

The initial state ρ can have coherences relative to the product basis of each charge. As discussed in Sec. III B 2, these coherences can reduce $\langle\sigma_{\text{surp}}\rangle$, even rendering it negative. σ_{surp} is defined in terms of an arbitrary charge index α, which we choose to be 1: $Q_1 = \sigma_z$.

In Fig. 4, we show $\langle\sigma_{\text{surp}}\rangle$ as a function of β_x^{A} and β_z^{A}. If $\beta_z^{\text{A}} \gg \beta_x^{\text{A}}$, ρ^{A} is nearly diagonal relative to the σ_z eigenbasis. Hence $\langle\sigma_{\text{surp}}\rangle$ is positive, as evidenced in the top left-hand corner of the plot. In the opposite regime ($\beta_x^{\text{A}} \gg \beta_z^{\text{A}}$), ρ^{A} has large coherences relative to the σ_z eigenbasis. These coherences drive $\langle\sigma_{\text{surp}}\rangle$ below zero, as evidenced in the bottom right-hand corner.

C. Trajectory SEP

As shown in Sec. III C 2, a nonreal σ_{traj} implies contextuality in a noncommuting-charge experiment. σ_{traj} carries indices i_1 and f_1, by the definition Eq. (15). We numerically calculate the σ_{traj} evaluated on the trajectory defined by $|i_1\rangle = |0\rangle^{\text{A}} \otimes |1\rangle^{\text{B}}$ and $|f_1\rangle = |0\rangle^{\text{A}} \otimes |0\rangle^{\text{B}}$.

In Fig. 5, we show the imaginary part of $\sigma_{\text{traj}}(i_1,f_1)$ plotted against β_x^{A} and β_y^{A}. σ_{traj} typically has a nonzero imaginary component (of a magnitude similar to that of the real part), signaling contextuality. The magnitude of the imaginary component grows particularly large when $\beta_y^{\text{A}} \approx 0$. Furthermore, the imaginary component exhibits stability, changing smoothly with the swept parameters.

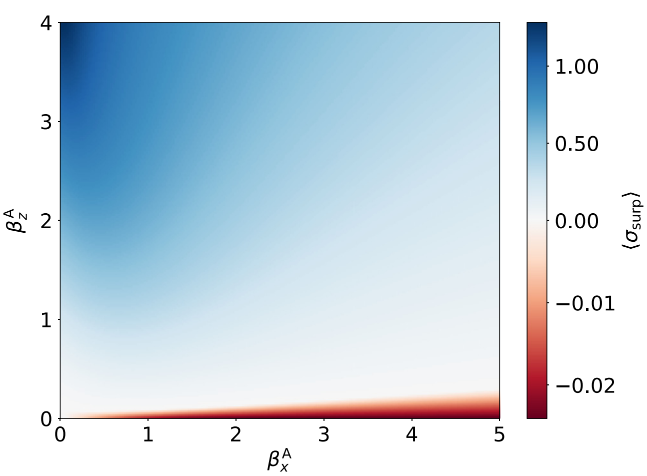

FIG. 4. $\langle\sigma_{\text{surp}}\rangle$ as a function of the generalized inverse temperatures β_x^{A} and β_z^{A}. The unswept parameters are $\beta_y^{\text{A}} = 0$, $\beta_x^{\text{B}} = 0$, $\beta_y^{\text{B}} = 1.6$, $\beta_z^{\text{B}} = 0.1$, and $\theta = \pi/5$.

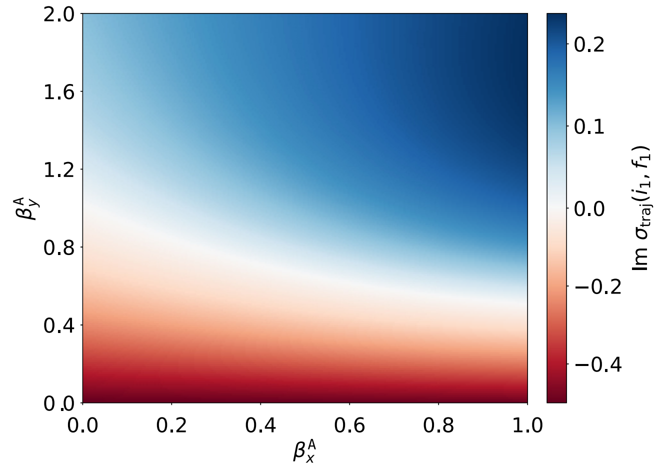

FIG. 5. The imaginary part of σ_{traj}, plotted against β_x^{A} and β_y^{A}. The unswept parameters are $\beta_z^{\text{A}} = 0.01$, $\beta_x^{\text{B}} = 0.01$, $\beta_y^{\text{B}} = 1$, $\beta_z^{\text{B}} = 0.01$, and $\theta = 0.5$.

V. EXPERIMENTAL SKETCH

Our results can be tested experimentally. Several pieces of evidence indicate the feasibility of such an experiment. First, a trapped-ion experiment has recently initiated the experimental testing of noncommuting-charge thermodynamics [48]. Second, other platforms have been argued to support such tests [27,47]. Examples include superconducting qubits, neutral atoms, and possibly nuclear-magnetic-resonance systems. Third, sequential weak measurements have been realized with trapped ions [146], superconducting qubits [147], and photonics [148–152]. Fourth, we now sketch a trapped-ion experiment inspired by Sec. IV. We outline the setup, preparation procedure, evolution, measurement, and data processing. For concreteness, we tailor the proposal to the platform reported on in Ref. [153].

The platform consists of $^{171}Yb^{+}$ ions in a linear Paul trap. Each ion encodes a qubit in two hyperfine ground states (two energy levels that result from splitting a ground space with a hyperfine interaction). Our proposal calls for ten qubits: two form the system of interest, two ancillas enable state preparation, and six ancillas enable weak measurements. The system of interest consists of a qubit A and a qubit B. These qubits will exchange charges σ_x, σ_y, and σ_z. However, tracking just two noncommuting charges suffices for an initial experiment. We choose σ_x and σ_z.

A and B must be prepared in a tensor product of GGEs [Eq. (2)]. One procedure involves two ancilla qubits, as follows. Prepare A and an ancilla in a thermofield-double state (a purification of a GGE), using the trapped-ion protocol in Ref. [153]. Discard the ancilla qubit. Repeat these two steps with qubit B and another ancilla. The generalized inverse temperatures $\beta_\alpha^{\mathrm{X}}$ parametrize the initial state. One chooses the parameter values as in Sec. IV, to observe the three results listed two paragraphs below.

After the state preparation, one weakly measures σ_x^{A} and σ_x^{B}, then σ_z^{A} and σ_z^{B}. One can implement a weak measurement using a qubit ancilla, using the circuit shown in Ref. [154, Fig. 1(a)]. Hence the initial weak measurements require four ancillas total.

After these weak measurements, A and B evolve under a charge-preserving unitary U_θ [Eq. (23)]. The trapped-ion platform under consideration offers a gate set formed from arbitrary single-qubit rotations and XX gates [153,155]. The universality of the gate set implies that U_θ can be implemented, if the ions retain coherence for long enough. The two-qubit gate requires the most time—between one and hundreds of microseconds [155]. However, coherence times range from hundreds of milliseconds to hundred of seconds. The time scales are significantly separated, although gate errors will further restrict circuit depth [156].

After the evolution, one weakly measures σ_x^{A} and σ_x^{B}. Our abstract protocol (Sec. II B) ends with weak measurements of σ_z^{A} and σ_z^{B}. An experimentalist can replace these weak measurements with strong measurements, without hindering the reconstruction of $\tilde{p}_F$ from the experimental data [64]. Furthermore, the replacement spares us the need for two extra ancillas.

One repeats the foregoing protocol many times. From the measurement outcomes, we infer the probability distribution over the possible measurement outcomes. One reconstructs the KDQ $\tilde{p}_F$ via the procedure in Ref. [Appendix A][64]. Analogously, one infers $\tilde{p}_{\mathrm{R}}$ from another batch of trials, guided by the reverse protocol of Sec. III C 1. Since our theoretical results are deductive, the proposed experiment essentially checks the accuracy of quantum theory. However, observing three phenomena would highlight quantum features exhibited by the SEPs when charges fail to commute: (i) Observe a violation of detailed charge conservation. (ii) Observe a negative $\langle \sigma_{\mathrm{surp}} \rangle$. (iii) Observe an imaginary component of σ_{traj}.

VI. OUTLOOK

Noncommuting charges challenge common expectations about entropy production. Three common SEP formulas, though equal when charges commute, separate when charges do not. The formulas also offer different physical insights into how noncommuting charges impact entropy production. First, the noncommutation enables stochastic trajectories to violate charge conservation individually. We introduce these nonconserving trajectories, which are possible only if charges fail to commute, as quantum phenomena in stochastic thermodynamics. The violations of detailed charge conservation underlie commutator-dependent corrections to a fluctuation theorem. Second, initial coherences relative to the eigenbases of the charges can render $\langle \sigma_{\mathrm{surp}} \rangle$ negative. A common (two-thermal-reservoir) setup can entail such coherences only if the charges fail to commute. Hence, the noncommutation of charges sources a resource that can, in a sense, effectively reverse time's arrow. Third, nonreality of σ_{traj} signals contextuality—provable nonclassicality—in a noncommuting-current experiment. Such thermodynamic signatures of contextuality—a stringent criterion for nonclassicality—are rare. These results hold arbitrarily far from equilibrium. In addition to proving these results deductively, we have illustrated them numerically and sketched a trapped-ion test.

Our work introduces noncommuting charges into stochastic thermodynamics [99]. All results in the field now merit reevaluation, in case the noncommutation of charges alters them. For example, thermodynamic uncertainty relations bound the relative variance of a current with entropy production [157–160]. Lowering entropy production, noncommuting charges may increase the relative variance, increasing the unpredictability of the currents. Our work therefore motivates the derivation of thermodynamic uncertainty relations that highlight exchanges of noncommuting charges, using KDQs. Such relations may follow as extensions of Ref. [159].

As another avenue opened up by our work within stochastic thermodynamics, nonconserving trajectories provide a new tool for unearthing genuinely quantum effects. Consider any charge exchange modeled with a KDQ. The KDQ decomposes into a conserving and nonconserving part. The former is the only piece that survives when the process has a classical (probabilistic) description. The average of every stochastic physical variable (analogous to entropy production), with respect to the KDQ, decomposes likewise. Hence the contribution of charge noncommutation to the average can be delineated clearly. For example, this technique could be applied to decompose the averaged stochastic work performed by a monitored quantum engine operating between noncommuting-charge reservoirs.

Quantum engines offer another possible application [38]: The more entropy an engine produces, the lesser the engine's efficiency. We have shown that noncommutation of charges can lower entropy production even on average: coherences relative to the eigenbases of the charges serve as a resource for reducing average entropy production (Sec. III B). Hence engines might leverage such coherences. Such an engine could exchange not only heat but also noncommuting charges with reservoirs. One could extend the engine, proposed in Ref. [161], that leverages a spin reservoir in place of a heat reservoir.

To put the charges on an even more equal footing, one could average over them in the definitions of the KDQ and the SEPs (Appendix F). Finally, calculating a closed form for the average trajectory SEP, for mixed global states, remains an open problem.

Experimental opportunities complement the theoretical ones. In Sec. V, we have sketched a trapped-ion experiment for testing our results. Such a test would highlight the quantum features manifested by SEPs when charges fail to commute.

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APPENDIX A: MEASURING THE KIRKWOOD-DIRAC QUASIPROBABILITY VIA THE FORWARD PROTOCOL

Here, we show how the forward protocol (Sec. II A) leads to the KDQ $\tilde{p}_F$ [Eq. (4)]. One can infer $\tilde{p}_F$ from experiments by performing the forward protocol and simpler protocols [162]. The proof hinges on weak measurements.

We briefly review a model for weak measurements [64,68,125,126,163]. During any measurement, one prepares a detector, couples the detector to the system $\mathcal{S}$ of interest, and projects the detector (measures it strongly). The outcome implies information about $\mathcal{S}$. How much information depends on the strength and duration of the coupling. The entire measurement process evolves the state of $\mathcal{S}$ under Kraus operators.

Kraus operators K_j model general quantum operations [117]. They satisfy the normalization condition $\sum_j K_j^\dagger K_j = \mathbb{1}$. Modeling a measurement that yields outcome j, the operators evolve a measured state ω as $\omega \mapsto K_j \omega K_j^\dagger / \mathrm{Tr}(K_j \omega K_j^\dagger)$. For example, the first weak measurement of the forward protocol effects a Kraus operator

$$K_{1,i_1} \approx (\text{const.})\, \mathbb{1} + g_{1,i_1} \Pi_{1,i_1}. \tag{A1}$$

The dimensionless coupling strength $g_{1,i_1} \in \mathbb{C}$ has a magnitude much smaller than 1 [164]. Hence the forward protocol evolves ρ to the (unnormalized) conditional state

$$\left[K_{1,f_1} K_{2,f_2} \ldots K_{c,f_c}\right] U \left[K_{c,i_c} \ldots K_{2,i_2} K_{1,i_1}\right] \rho \times \left[K_{c,i_c} \ldots K_{2,i_2} K_{1,i_1}\right]^\dagger U^\dagger \left[K_{1,f_1} K_{2,f_2} \ldots K_{c,f_c}\right]^\dagger . \tag{A2}$$

The trace of this expression equals the probability that upon projecting all the detectors, one obtains the outcomes associated with i_1, i_2, etc. We can substitute in for each K from equations of the form given in Eq. (A1). Then, we multiply out the factors. In the resulting sum, one term contains $2c$ projectors Π leftward of ρ and $2c$ identity operators $\mathbb{1}$ rightward of ρ. That term is the real or imaginary part of $\tilde{p}_F$ [Eq. (4)], depending on whether the coupling strengths are real or imaginary. $\tilde{p}_F$ is an *extended KDQ*, containing > 2 projectors [68]. However, we call $\tilde{p}_F$ a KDQ for conciseness.

One can replace the final weak measurement with a strong measurement, for experimental convenience. The outermost Kraus operators in Eq. (A2)—the K_{1,f_1} and $K_{1,f_1}^\dagger$—will become projectors Π_{1,f_1}. The trace will contain a term $\mathrm{Tr}([\Pi_{1,f_1} \Pi_{2,f_2} \ldots \Pi_{c,f_c}] U [\Pi_{c,i_c} \ldots \Pi_{2,i_2} \Pi_{1,i_1}]\, \rho U^\dagger \Pi_{1,f_1})$. The rightmost projector can cycle around to become the leftmost. Since $\Pi_{1,f_1} \Pi_{1,f_1} = \Pi_{1,f_1}$, $\tilde{p}_F$ [Eq. (4)] again results.

APPENDIX B: DEGENERATE CHARGES

This appendix concerns generalizations of our results to degenerate charges Q_α. Charge degeneracies would affect the definitions of the KDQ in Eq. (4), $\tilde{p}_F$, and the surprisal SEP in Eq. (12), σ_{surp}. Each quantity is defined in terms of projectors—the product basis of at least one charge, $\{\Pi_{\alpha,k}\}$. If a Q_α is degenerate, at least one of its eigenprojectors $\Pi_{\alpha,j}$ will have rank > 1. We have two choices of projectors to use in defining $\tilde{p}_F$ and σ_{surp}: We can use degenerate projectors or pick one-dimensional projectors. Each strategy has a drawback, although apparently not due to noncommutation of charges: the drawbacks arise even in the commuting and classical cases. Future work can elucidate degeneracies in greater detail and identify whether degeneracies can play a special role in the noncommuting case.

According to the first strategy, we continue to use the eigenprojectors of the charges, regardless of ranks. $\tilde{p}_F$ and σ_{surp} would retain their definitions, given in Eqs. (4) and (12). Awkwardly, the SEP formulas would no longer equal each other in the commuting case, even if ρ were diagonal with respect to the shared eigenbasis of the charges.

To illustrate, we suppose that the dynamics conserve only one charge. We drop its index 1 from eigenvalues $\lambda_{1,k}$ and from eigenprojectors. According to Eq. (7), the charge SEP is $\sigma_{\rm chrg} = \beta^{\rm A}\left(\lambda_{f^{\rm A}} - \lambda_{i^{\rm A}}\right) + \beta^{\rm B}\left(\lambda_{f^{\rm B}} - \lambda_{i^{\rm B}}\right)$. In contrast, the surprisal SEP is

$$\sigma_{\rm surp} = \log\left(\frac{\mathrm{Tr}\left(\left[\Pi^{\rm A}_{i^{\rm A}} \otimes \Pi^{\rm B}_{i^{\rm B}}\right]\rho\right)}{\mathrm{Tr}\left(\left[\Pi^{\rm A}_{f^{\rm A}} \otimes \Pi^{\rm B}_{f^{\rm B}}\right]\rho\right)}\right) \tag{B1}$$

$$= \log\left(\exp\left(\beta^{\rm A}\left[\mathrm{rank}(\Pi_{f^{\rm A}})\lambda_{f^{\rm A}} - \mathrm{rank}(\Pi_{i^{\rm A}})\lambda_{i^{\rm A}}\right]\right)\right. \left.\exp\left(\beta^{\rm B}\left[\mathrm{rank}(\Pi_{f^{\rm B}})\lambda_{f^{\rm B}} - \mathrm{rank}(\Pi_{i^{\rm B}})\lambda_{i^{\rm B}}\right]\right)\right) \tag{B2}$$

$$= \beta^{\rm A}\left[\mathrm{rank}(\Pi_{f^{\rm A}})\lambda_{f^{\rm A}} - \mathrm{rank}(\Pi_{i^{\rm A}})\lambda_{i^{\rm A}}\right] + \beta^{\rm B}\left[\mathrm{rank}(\Pi_{f^{\rm B}})\lambda_{f^{\rm B}} - \mathrm{rank}(\Pi_{i^{\rm B}})\lambda_{i^{\rm B}}\right]. \tag{B3}$$

Due to the rank factors, $\sigma_{\rm surp} \neq \sigma_{\rm chrg}$.

Second, we can define $\tilde{p}_F$ and $\sigma_{\rm surp}$ in terms of rank-1 projectors only. If a Q_α has a degenerate eigenspace, we must choose an eigenbasis for the space. The SEP formulas will remain equal in the commuting case. However, different choices of projectors engender different correction terms in the $\sigma_{\rm chrg}$ fluctuation theorem given in Eq. (10) and in the $\sigma_{\rm surp}$ fluctuation theorem given in Eq. (14). The varying of the corrections with the choice of basis suggests unphysicality.

For example, let each of A and B be a qubit. We express operators relative to an arbitrary basis: $Q_1 = \left(\begin{smallmatrix}1&0\\0&1\end{smallmatrix}\right)$ and $Q_2 = \left(\begin{smallmatrix}1&0\\0&2\end{smallmatrix}\right)$. Choosing $\Pi_{1,1} = \left(\begin{smallmatrix}1&0\\0&0\end{smallmatrix}\right)$ and $\Pi_{1,2} = \left(\begin{smallmatrix}0&0\\0&1\end{smallmatrix}\right)$ engenders different correction terms than $\Pi_{1,1} = \frac{1}{\sqrt{2}}\left(\begin{smallmatrix}1&1\\1&1\end{smallmatrix}\right)$ and $\Pi_{1,2} = \frac{1}{\sqrt{2}}\left(\begin{smallmatrix}1&-1\\-1&1\end{smallmatrix}\right)$.

APPENDIX C: CHARGE STOCHASTIC ENTROPY PRODUCTION

This appendix concerns $\sigma_{\rm chrg}$ (Sec. III A 1). We prove the fluctuation theorem [Eq. (10)] in Appendix C 1 and explain detailed charge conservation in Appendix C 2.

1. Proof of the charge fluctuation theorem

Here, we prove the $\sigma_{\rm chrg}$ fluctuation theorem [Eq. (10)] in Sec. III A 3:

$$\langle e^{-\sigma_{\rm chrg}}\rangle = \mathrm{Tr}(U^\dagger e^{-\Delta\beta_1 Q_1^{\rm A}} \ldots e^{-\Delta\beta_c Q_c^{\rm A}} U e^{\Delta\beta_c Q_c^{\rm A}} \ldots e^{\Delta\beta_1 Q_1^{\rm A}}\rho) + (c-1 \text{ terms dependent on commutators})\,. \tag{C1}$$

Let us add and subtract $\sum_{\alpha=1}^{c}\beta_\alpha^{\rm B}(\lambda_{\alpha,i_\alpha^{\rm A}} - \lambda_{\alpha,f_\alpha^{\rm A}})$ to and from the right-hand side of Eq. (7):

$$\sigma_{\rm chrg} = -\sum_{\alpha=1}^{c}\left[\beta_\alpha^{\rm B}(\lambda_{\alpha,i_\alpha^{\rm A}} + \lambda_{\alpha,i_\alpha^{\rm B}} - \lambda_{\alpha,f_\alpha^{\rm A}} - \lambda_{\alpha,f_\alpha^{\rm B}}) + \Delta\beta_\alpha(\lambda_{\alpha,i_\alpha^{\rm A}} - \lambda_{\alpha,f_\alpha^{\rm A}})\right]. \tag{C2}$$

We first calculate the right-hand side of the fluctuation theorem in the commuting case. The first parenthesized term in Eq. (C2) vanishes when evaluated on conserving trajectories (Appendix C 2). If the charges commute, therefore,

$$\begin{aligned}
\langle e^{-\sigma_{\rm chrg}}\rangle &= \langle e^{\sum_{\alpha=1}^{c}\Delta\beta_\alpha\left(\lambda_{\alpha,i_\alpha^{\rm A}} - \lambda_{\alpha,f_\alpha^{\rm A}}\right)}\rangle \\
&= \sum_{\substack{i_1^{\rm A}, i_1^{\rm B},\ldots,i_c^{\rm A}, i_c^{\rm B},\\ f_1^{\rm A}, f_1^{\rm B},\ldots,f_c^{\rm A}, f_c^{\rm B}}} \mathrm{Tr}\left(U^\dagger\left[\Pi_{1,f_1^{\rm A}} \otimes \Pi_{1,f_1^{\rm B}}\right]\ldots\left[\Pi_{c,f_c^{\rm A}} \otimes \Pi_{c,f_c^{\rm B}}\right]U\left[\Pi_{c,i_c^{\rm A}} \otimes \Pi_{c,i_c^{\rm B}}\right]\ldots\right. \\
&\quad \times \left.\left[\Pi_{1,i_1^{\rm A}} \otimes \Pi_{1,i_1^{\rm B}}\right]\rho\right) e^{\sum_{\alpha=1}^{c}\Delta\beta_\alpha\left(\lambda_{\alpha,i_\alpha^{\rm A}} - \lambda_{\alpha,f_\alpha^{\rm A}}\right)} \\
&= \sum_{\substack{i_1^{\rm A}, i_2^{\rm A},\ldots,i_c^{\rm A},\\ f_1^{\rm A}, f_2^{\rm A},\ldots,f_c^{\rm A}}} \mathrm{Tr}(U^\dagger\left[\Pi_{1,f_1^{\rm A}} \otimes \mathbb{1}^{\rm B}\right]\ldots\left[\Pi_{c,f_c^{\rm A}} \otimes \mathbb{1}^{\rm B}\right]U\left[\Pi_{c,i_c^{\rm A}} \otimes \mathbb{1}^{\rm B}\right]\ldots\left[\Pi_{1,i_1^{\rm A}} \otimes \mathbb{1}^{\rm B}\right]\rho)e^{\sum_{\alpha=1}^{c}\Delta\beta_\alpha\left(\lambda_{\alpha,i_\alpha^{\rm A}} - \lambda_{\alpha,f_\alpha^{\rm A}}\right)} \\
&= \sum_{\substack{i_1^{\rm A}, i_2^{\rm A},\ldots,i_c^{\rm A},\\ f_1^{\rm A}, f_2^{\rm A},\ldots,f_c^{\rm A}}} \mathrm{Tr}\left(U^\dagger\left[e^{-\Delta\beta_1\lambda_{1,f_1^{\rm A}}}\Pi_{1,f_1^{\rm A}} \otimes \mathbb{1}^{\rm B}\right]\ldots\left[e^{-\Delta\beta_c\lambda_{c,f_c^{\rm A}}}\Pi_{c,f_c^{\rm A}} \otimes \mathbb{1}^{\rm B}\right]U\left[e^{\Delta\beta_c\lambda_{c,i_c^{\rm A}}}\Pi_{c,i_c^{\rm A}} \otimes \mathbb{1}^{\rm B}\right]\right. \\
&\quad \left.\ldots\left[e^{\Delta\beta_1\lambda_{1,i_1^{\rm A}}}\Pi_{1,i_1^{\rm A}} \otimes \mathbb{1}^{\rm B}\right]\rho\right)
\end{aligned} \tag{C3}$$

$$= \mathrm{Tr}(U^\dagger \left\{ \left[e^{-\Delta\beta_1 Q_1^{\mathrm{A}}} \ldots e^{-\Delta\beta_c Q_c^{\mathrm{A}}} \right] \otimes \mathbb{1}^{\mathrm{B}} \right\} U \left\{ \left[e^{\Delta\beta_c Q_c^{\mathrm{A}}} \ldots e^{\Delta\beta_1 Q_1^{\mathrm{A}}} \right] \otimes \mathbb{1}^{\mathrm{B}} \right\} \rho). \tag{C4}$$

This expression is the right-hand side of the fluctuation theorem in the commuting case (and equals 1 when ρ is the usual tensor product of thermal states).

We now compute $\langle e^{-\sigma_{\mathrm{chrg}}} \rangle$ in the noncommuting case. To identify a correction, we separate out a term of the form given in Eq. (C4). All other terms will be commutator-dependent corrections. First, we insert the definitions of σ_{chrg} [Eq. (7)] and $\tilde{p}_F$ [Eq. (4)] into the left-hand side of the fluctuation theorem. For conciseness, we suppress the indices $(i_1^{\mathrm{A}}, i_1^{\mathrm{B}}, \ldots, i_c^{\mathrm{A}}, i_c^{\mathrm{B}} \,;\, f_1^{\mathrm{A}}, f_1^{\mathrm{B}}, \ldots, f_c^{\mathrm{A}}, f_c^{\mathrm{B}})$ in the sum:

$$\langle e^{-\sigma_{\mathrm{chrg}}} \rangle = \sum \mathrm{Tr}(U^\dagger \Pi_{1,f_1} \ldots \Pi_{c,f_c} U \Pi_{c,i_c} \ldots \Pi_{1,i_1} \rho) e^{\sum_{\alpha=1}^{c} \beta_\alpha^{\mathrm{A}} \lambda_{\alpha,i_\alpha^{\mathrm{A}}} + \beta_\alpha^{\mathrm{B}} \lambda_{\alpha,i_\alpha^{\mathrm{B}}} - \beta_\alpha^{\mathrm{A}} \lambda_{\alpha,f_\alpha^{\mathrm{A}}} - \beta_\alpha^{\mathrm{B}} \lambda_{\alpha,f_\alpha^{\mathrm{B}}}} \tag{C5}$$

$$= \sum \mathrm{Tr} \left(U^\dagger \left[e^{-\beta_1^{\mathrm{A}} \lambda_{1,f_1^{\mathrm{A}}} - \beta_1^{\mathrm{B}} \lambda_{1,f_1^{\mathrm{B}}}} \Pi_{1,f_1} \right] \ldots \left[e^{-\beta_c^{\mathrm{A}} \lambda_{c,f_c^{\mathrm{A}}} - \beta_c^{\mathrm{B}} \lambda_{c,f_c^{\mathrm{B}}}} \Pi_{c,f_c} \right] U \left[e^{\beta_c^{\mathrm{A}} \lambda_{c,i_c^{\mathrm{A}}} + \beta_c^{\mathrm{B}} \lambda_{c,i_c^{\mathrm{B}}}} \Pi_{c,i_c} \right] \ldots \left[e^{\beta_1^{\mathrm{A}} \lambda_{1,i_1^{\mathrm{A}}} + \beta_1^{\mathrm{B}} \lambda_{1,i_1^{\mathrm{B}}}} \Pi_{1,i_1} \right] \rho \right)$$

$$= \mathrm{Tr}(U^\dagger e^{-\beta_1^{\mathrm{A}} Q_1^{\mathrm{A}} - \beta_1^{\mathrm{B}} Q_1^{\mathrm{B}}} \ldots e^{-\beta_c^{\mathrm{A}} Q_c^{\mathrm{A}} - \beta_c^{\mathrm{B}} Q_c^{\mathrm{B}}} U e^{\beta_c^{\mathrm{A}} Q_c^{\mathrm{A}} + \beta_c^{\mathrm{B}} Q_c^{\mathrm{B}}} \ldots e^{\beta_1^{\mathrm{A}} Q_1^{\mathrm{A}} + \beta_1^{\mathrm{B}} Q_1^{\mathrm{B}}} \rho). \tag{C6}$$

We now massage this expression to bring out the commutator-dependent corrections. As always, $\mathbb{1}$ operators are implicitly tensored on wherever necessary. We replace the expressions $-\beta_\alpha^{\mathrm{A}} Q_\alpha^{\mathrm{A}} - \beta_\alpha^{\mathrm{B}} Q_\alpha^{\mathrm{B}}$ with $-\Delta\beta_\alpha^{\mathrm{A}} Q_\alpha^{\mathrm{A}} - \beta_\alpha^{\mathrm{B}} Q_\alpha^{\mathrm{tot}}$ in Eq. (C6):

$$\langle e^{-\sigma_{\mathrm{chrg}}} \rangle = \mathrm{Tr}(U^\dagger \left[e^{-\Delta\beta_1 Q_1^{\mathrm{A}} - \beta_1^{\mathrm{B}} Q_1^{\mathrm{tot}}} \ldots e^{-\Delta\beta_c Q_c^{\mathrm{A}} - \beta_c^{\mathrm{B}} Q_c^{\mathrm{tot}}} \right] U \left[e^{\Delta\beta_c Q_c^{\mathrm{A}} + \beta_c^{\mathrm{B}} Q_c^{\mathrm{tot}}} \ldots e^{\Delta\beta_1 Q_1^{\mathrm{A}} + \beta_1^{\mathrm{B}} Q_1^{\mathrm{tot}}} \right] \rho). \tag{C7}$$

Now, we commute each $e^{-\beta_\alpha^{\mathrm{B}} Q_\alpha^{\mathrm{tot}}}$ from the left of U to the right, until the exponential cancels with its counterpart, $e^{\beta_\alpha^{\mathrm{B}} Q_\alpha^{\mathrm{tot}}}$. Here are the first few manipulations, starting with the $e^{-\beta_{c-1}^{\mathrm{B}} Q_{c-1}^{\mathrm{tot}}}$ in the leftmost half of the argument of the trace:

$$\langle e^{-\sigma_{\mathrm{chrg}}} \rangle = \mathrm{Tr} \left(U^\dagger e^{-\Delta\beta_1 Q_1^{\mathrm{A}} - \beta_1^{\mathrm{B}} Q_1^{\mathrm{tot}}} \ldots e^{-\Delta\beta_{c-1} Q_{c-1}^{\mathrm{A}} - \beta_{c-1}^{\mathrm{B}} Q_{c-1}^{\mathrm{tot}}} e^{-\Delta\beta_c Q_c^{\mathrm{A}}} U e^{\Delta\beta_c Q_c^{\mathrm{A}}} e^{\Delta\beta_{c-1} Q_{c-1}^{\mathrm{A}} + \beta_{c-1}^{\mathrm{B}} Q_{c-1}^{\mathrm{tot}}} \ldots e^{\Delta\beta_1 Q_1^{\mathrm{A}} + \beta_1^{\mathrm{B}} Q_1^{\mathrm{tot}}} \rho \right)$$

$$= \mathrm{Tr}(U^\dagger e^{-\Delta\beta_1 Q_1^{\mathrm{A}} - \beta_1^{\mathrm{B}} Q_1^{\mathrm{tot}}} \ldots e^{-\Delta\beta_{c-1} Q_{c-1}^{\mathrm{A}}} e^{-\Delta\beta_c Q_c^{\mathrm{A}}} U e^{\Delta\beta_c Q_c^{\mathrm{A}}} e^{\Delta\beta_{c-1} Q_{c-1}^{\mathrm{A}}} \ldots e^{\Delta\beta_1 Q_1^{\mathrm{A}} + \beta_1^{\mathrm{B}} Q_1^{\mathrm{tot}}} \rho)$$

$$+ \mathrm{Tr} \left(U^\dagger e^{-\Delta\beta_1 Q_1^{\mathrm{A}} - \beta_1^{\mathrm{B}} Q_1^{\mathrm{tot}}} \ldots e^{-\Delta\beta_{c-1} Q_{c-1}^{\mathrm{A}}} \left[e^{-\beta_{c-1}^{\mathrm{B}} Q_{c-1}^{\mathrm{tot}}}, e^{-\Delta\beta_c Q_c^{\mathrm{A}}} U e^{\Delta\beta_c Q_c^{\mathrm{A}}} \right] e^{\Delta\beta_{c-1} Q_{c-1}^{\mathrm{A}} + \beta_{c-1}^{\mathrm{B}} Q_{c-1}^{\mathrm{tot}}} \ldots e^{\Delta\beta_1 Q_1^{\mathrm{A}} + \beta_1^{\mathrm{B}} Q_1^{\mathrm{tot}}} \rho \right). \tag{C8}$$

To arrive at the second line, we have canceled the exponentials that contained Q_c^{tot}. In the third line, canceling the exponentials involving Q_{c-1}^{tot}, we have had to swap $e^{-\beta_{c-1}^{\mathrm{B}} Q_{c-1}^{\mathrm{tot}}}$ and $e^{-\Delta\beta_c Q_c^{\mathrm{A}}} U e^{\Delta\beta_c Q_c^{\mathrm{A}}}$. This swap has induced the commutator-containing summand. Continuing in this fashion—bringing all the Q_α^{tot}-dependent exponentials together and inducing a commutator each time—we arrive at the desired form:

$$\langle e^{\sum_{\alpha=1}^{c} \beta_\alpha^{\mathrm{A}} \lambda_{\alpha,i_\alpha^{\mathrm{A}}} + \beta_\alpha^{\mathrm{B}} \lambda_{\alpha,i_\alpha^{\mathrm{B}}} - \beta_\alpha^{\mathrm{A}} \lambda_{\alpha,f_\alpha^{\mathrm{A}}} - \beta_\alpha^{\mathrm{B}} \lambda_{\alpha,f_\alpha^{\mathrm{B}}}} \rangle = \mathrm{Tr}(U^\dagger e^{-\Delta\beta_1 Q_1^{\mathrm{A}}} \ldots e^{-\Delta\beta_c Q_c^{\mathrm{A}}} U e^{\Delta\beta_c Q_c^{\mathrm{A}}} \ldots e^{\Delta\beta_1 Q_1^{\mathrm{A}}} \rho) \tag{C9}$$

$$+ (c-1 \text{ commutator-dependent terms}). \tag{C10}$$

We now expand on how the right-hand side simplifies to 1 in the commuting case. First, the $c-1$ commutator-dependent terms vanish. For example, consider the commutator $\left[e^{-\beta_{c-1}^{\mathrm{B}} Q_{c-1}^{\mathrm{tot}}},\, e^{-\Delta\beta_c Q_c^{\mathrm{A}}} U e^{\Delta\beta_c Q_c^{\mathrm{A}}} \right]$. The first argument commutes with $e^{\pm\Delta\beta_c Q_c^{\mathrm{A}}}$ because the charges commute. Also, the first argument commutes with U because of charge conservation. Hence the commutator vanishes.

Second, the first term in Eq. (C9) equals 1. The thermal state [Eq. (1)] expands as a product, so the term simplifies as

$$\mathrm{Tr}(U^\dagger e^{-\Delta\beta_1 Q_1^{\mathrm{A}}} \ldots e^{-\Delta\beta_c Q_c^{\mathrm{A}}} U e^{\Delta\beta_c Q_c^{\mathrm{A}}} \ldots e^{\Delta\beta_1 Q_1^{\mathrm{A}}} \rho) = \mathrm{Tr}(U^\dagger \prod_\gamma e^{-\Delta\beta_\gamma Q_\gamma^{\mathrm{A}}} U \prod_\delta e^{\Delta\beta_\delta Q_\delta^{\mathrm{A}}} \frac{1}{Z} \prod_\alpha e^{-\beta_\alpha^{\mathrm{A}} Q_\alpha^{\mathrm{A}} - \beta_\alpha^{\mathrm{B}} Q_\alpha^{\mathrm{B}}}) \tag{C11}$$

$$= \mathrm{Tr}\Big(U^\dagger \prod_\gamma e^{-\Delta\beta_\gamma Q_\gamma^{\mathrm{A}}} U \frac{1}{Z} \prod_\alpha e^{-\beta_\alpha^{\mathrm{B}} Q_\alpha^{\mathrm{tot}}}\Big) \tag{C12}$$

$$= 1. \tag{C13}$$

The third equality follows from charge conservation.

2. Detailed charge conservation

The KDQ obeys detailed charge conservation if $\tilde{p}_F$ is nonzero only when evaluated on indices that satisfy

$$\lambda_{\alpha,i_\alpha^{\mathrm{A}}} + \lambda_{\alpha,i_\alpha^{\mathrm{B}}} = \lambda_{\alpha,f_\alpha^{\mathrm{A}}} + \lambda_{\alpha,f_\alpha^{\mathrm{B}}}, \quad \forall\alpha. \tag{C14}$$

If the dynamics conserve just one charge, the KDQ obeys detailed charge conservation, as we show in Appendix C 2 a. Appendix C 2 b generalizes the argument to multiple commuting charges.

a. Detailed charge conservation in the presence of only one charge

Here, we prove that the KDQ obeys detailed charge conservation in the presence of only one charge. We omit the index of the charge to simplify notation. The total charge eigendecomposes as $Q^{\mathrm{A}} + Q^{\mathrm{B}} = \sum_k \lambda_k \Pi_k$. The eigenprojectors decompose as $\Pi_k = \sum_{i^{\mathrm{A}},i^{\mathrm{B}}:\lambda_{i^{\mathrm{A}}}+\lambda_{i^{\mathrm{B}}}=\lambda_k} \Pi_{i^{\mathrm{A}}} \otimes \Pi_{i^{\mathrm{B}}}$. Since U commutes with Q, U has the same block-diagonal structure: $U = \sum_k B_k$, wherein B_k has support only on the subspace projected onto by Π_k.

The relevant KDQ is $\tilde{p}_F(i^{\mathrm{A}}, i^{\mathrm{B}}; f^{\mathrm{A}}, f^{\mathrm{B}}) = \mathrm{Tr}(U^\dagger \Pi_f U \Pi_i \rho)$. By the orthogonality of the projectors, $\Pi_f U = \Pi_f B_k$, wherein k satisfies $\lambda_k = \lambda_{f^{\mathrm{A}}} + \lambda_{f^{\mathrm{B}}}$. By the same logic, $B_k \Pi_i = 0$, unless $\lambda_k = \lambda_{i^{\mathrm{A}}} + \lambda_{i^{\mathrm{B}}}$. Hence $\Pi_{f^{\mathrm{A}} f^{\mathrm{B}}} U \Pi_i$ and so $\tilde{p}(i^{\mathrm{A}}, i^{\mathrm{B}}; f^{\mathrm{A}}, f^{\mathrm{B}})$ is nonzero only if $\lambda_{f^{\mathrm{A}}} + \lambda_{f^{\mathrm{B}}} = \lambda_k = \lambda_{i^{\mathrm{A}}} + \lambda_{i^{\mathrm{B}}}$, satisfying detailed charge conservation.

b. Detailed charge conservation in the presence of commuting charges

Suppose that the dynamics conserve multiple charges that commute with each other. We show that the KDQ satisfies detailed charge conservation. Recall the form of $\tilde{p}_F$ in Eq. (4). Since the charges commute, every eigenprojector in $\tilde{p}_F$ commutes with every other. Thus, rearranging the projectors does not alter the quasiprobability. We bring the initial and final charge-α eigenprojectors beside U:

$$\tilde{p}_F(i_1^{\mathrm{A}}, i_1^{\mathrm{B}}, \ldots, i_c^{\mathrm{A}}, i_c^{\mathrm{B}}\,;\, f_c^{\mathrm{A}}, f_c^{\mathrm{B}}, \ldots, f_1^{\mathrm{A}}, f_1^{\mathrm{B}})$$

$$= \mathrm{Tr}\big(U^\dagger \big[\Pi_{1,f_1} \ldots \Pi_{c,f_c}\big] U \big[\Pi_{c,i_c} \ldots \Pi_{1,i_1}\big] \rho\big) \tag{C15}$$

$$= \mathrm{Tr}(U^\dagger \ldots \Pi_{\alpha,f_\alpha} U \Pi_{\alpha,i_\alpha} \ldots \rho). \tag{C16}$$

By the reasoning for one charge, unless $\lambda_{\alpha,i_\alpha^{\mathrm{A}}} + \lambda_{\alpha,i_\alpha^{\mathrm{B}}} = \lambda_{\alpha,f_\alpha^{\mathrm{A}}} + \lambda_{\alpha,f_\alpha^{\mathrm{B}}}$, the projected unitary $\Pi_{\alpha,f_\alpha} U \Pi_{\alpha,i_\alpha} = 0$ and hence $\tilde{p}_F = 0$. This conclusion governs an arbitrary α, so $\tilde{p}_F$ satisfies detailed charge conservation.

c. Connection of Fluctuation theorem to nonconserving trajectories

We now show how the two terms in the σ_{chrg} fluctuation theorem [Eq. (C1)] are related to (non)conserving trajectories. According to Appendix C 1, the first term on the right-hand side of the fluctuation theorem is $\langle e^{-\kappa}\rangle$, wherein $\kappa := \sum_{\alpha=1}^{c} \Delta\beta_\alpha(\lambda_{\alpha,f_\alpha^{\mathrm{A}}} - \lambda_{\alpha,i_\alpha^{\mathrm{A}}})$ [Eq. (C3)]. Since the average decomposes as $\langle\cdot\rangle = \langle\cdot\rangle_{\mathrm{cons}} + \langle\cdot\rangle_{\mathrm{noncons}}$, the first term of the fluctuation theorem can contain contributions from conserving and nonconserving trajectories.

To identify the relation of the second term to nonconserving trajectories, we rewrite the fluctuation theorem:

$$\langle e^{-\sigma_{\mathrm{chrg}}}\rangle = \langle e^{-\kappa}\rangle + \langle e^{-\sigma_{\mathrm{chrg}}} - e^{-\kappa}\rangle \tag{C17}$$

$$= \langle e^{-\kappa}\rangle + \langle e^{-\sigma_{\mathrm{chrg}}} - e^{-\kappa}\rangle_{\mathrm{cons}} + \langle e^{-\sigma_{\mathrm{chrg}}} - e^{-\kappa}\rangle_{\mathrm{noncons}} \tag{C18}$$

$$= \langle e^{-\kappa}\rangle + \langle e^{-\sigma_{\mathrm{chrg}}} - e^{-\kappa}\rangle_{\mathrm{noncons}}. \tag{C19}$$

The third line follows because $\sigma_{\mathrm{chrg}} = \kappa$ on conserving trajectories, by the σ_{chrg} definition given in Eq. (7) and the definition in Eq. (11) of conserving trajectories. Therefore, the second term of the fluctuation theorem equals the average, over nonconserving trajectories, of $e^{-\sigma_{\mathrm{chrg}}} - e^{-\kappa}$.

APPENDIX D: SURPRISAL STOCHASTIC ENTROPY PRODUCTION

This appendix supports claims made about σ_{surp} in Sec. III B 1. First, we complete the motivation for the definition of σ_{surp} (Appendix D 1). We show that the charge and surprisal formulas equal each other in the commuting case (Appendix D 2); we calculate $\langle\sigma_{\mathrm{surp}}\rangle$, proving Eq. (13) (Appendix D 3); and we prove the fluctuation theorem given in Eq. (14) for σ_{surp} (Appendix D 4).

1. Motivation for the suprisal SEP formula

Section III B 1 has partially motivated the σ_{surp} definition given in Eq. (12). Information theory suggests that the SEP depends on surprisals. The surprisals are of particular probabilities. Why those probabilities? This appendix motivates the choice.

We build on the first paragraph in Sec. III C 1. For simplicity, we suppose that only energy is ever measured. A classical thermodynamic story has motivated the conventional SEP formula,

$$\log\Big(p_F(E_i^{\mathrm{A}}, E_i^{\mathrm{B}}\,;\, E_f^{\mathrm{A}}, E_f^{\mathrm{B}}) / p_R(E_f^{\mathrm{A}}, E_f^{\mathrm{B}}\,;\, E_i^{\mathrm{A}}, E_i^{\mathrm{B}})\Big). \tag{D1}$$

The p_F denotes the probability of observing the forward trajectory—the probability of observing E_i^{A} and E_i^{B}, times the probability of observing E_f^{A} and E_f^{B}, conditioned on the initial observations and on the forward dynamics:

$$p_F(E_i^{\mathbb{A}}, E_i^{\mathbb{B}}\,;\, E_f^{\mathbb{A}}, E_f^{\mathbb{B}}) = p(E_i^{\mathbb{A}}, E_i^{\mathbb{B}}) \times p(E_f^{\mathbb{A}}, E_f^{\mathbb{B}} \,|\, E_i^{\mathbb{A}}, E_i^{\mathbb{B}}, \text{forward dynamics}). \tag{D2}$$

The reverse probability decomposes analogously:

$$p_R(E_f^{\mathbb{A}}, E_f^{\mathbb{B}}\,;\, E_i^{\mathbb{A}}, E_i^{\mathbb{B}}) = p(E_f^{\mathbb{A}}, E_f^{\mathbb{B}},) \times p(E_i^{\mathbb{A}}, E_i^{\mathbb{B}}, \,|\, E_f^{\mathbb{A}}, E_f^{\mathbb{B}}, \text{reverse dynamics}). \tag{D3}$$

The dynamics are reversible, so the conditional probabilities cancel in Eq. (D1) [52]. The trajectory-SEP formula reduces to $\log\left(p(E_i^{\mathbb{A}}, E_i^{\mathbb{B}})/p(E_f^{\mathbb{A}}, E_f^{\mathbb{B}})\right)$. This SEP formula is the difference of two surprisals. Each is evaluated on the probability of observing some outcome, upon preparing each system and measuring its energy. The analogue, in the noncommuting case, is Eq. (12).

2. Equivalence of σ_{surp} and σ_{chrg} in the commuting case

Throughout this appendix, we assume that the charges commute with each other: $[Q_\alpha, Q_{\alpha'}] = 0\ \forall \alpha, \alpha'$. We establish that σ_{surp} and σ_{chrg} agree: $\sigma_{\text{surp}} = \sigma_{\text{chrg}}$ *when evaluated on any trajectory for which* $\tilde{p}_F \neq 0$. The restriction on trajectories is a technicality; on a trajectory that never occurs, the values of the SEPs are irrelevant to any calculation.

For convenience, we assume that the eigenvalues of the charges are ordered as follows. The eigenvalues of Q_1 are ordered arbitrarily. The eigenvalues of each other Q_α are ordered so that the j^{th} eigenvalue, $\lambda_{\alpha,j}$, corresponds to the same eigenvalue as $\lambda_{1,j}$. This ordering is possible due to the nondegeneracy of the charges: they all have the same number of eigenspaces.

$\tilde{p}_F \neq 0$ only on trajectories in which all initial indices equal each other, as do all final indices: $i_1 = i_2 = \ldots = i_c$, and $f_1 = f_2 = \ldots = f_c$. This claim follows from the ordering stipulated in the last paragraph: up to a relabeling of eigenspaces, $\Pi_{\alpha,i_\alpha}\Pi_{\zeta,i_\zeta} = 0$, unless $i_\alpha = i_\zeta$. The claim now follows immediately from the definition of the KDQ [Eq. (4)]:

$$\tilde{p}_F(i_1, i_2, \ldots, i_c\,;\, f_c, f_{c-1}, \ldots, f_1) := \operatorname{Tr}\left(U^\dagger\left[\Pi_{1,f_1}\Pi_{2,f_2}\ldots\Pi_{c,f_c}\right]U\left[\Pi_{c,i_c}\ldots\Pi_{2,i_2}\Pi_{1,i_1}\right]\rho\right). \tag{D4}$$

On the trajectories on which $\tilde{p}_F \neq 0$, we can simplify the σ_{chrg} formula [Eq. (7)] by equating the $i^{\mathbb{A}}$ indices of all the charges, equating the $i^{\mathbb{B}}$ indices of the charges, equating the $f^{\mathbb{A}}$ indices of the charges, and equating the $f^{\mathbb{B}}$ indices of the charges:

$$\sigma_{\text{chrg}} = \sum_{\zeta=1}^{c}\left[\beta_\zeta^{\mathbb{A}}\left(\lambda_{\zeta,f_\alpha^{\mathbb{A}}} - \lambda_{\zeta,i_\alpha^{\mathbb{A}}}\right) + \beta_\zeta^{\mathbb{B}}\left(\lambda_{\zeta,f_\alpha^{\mathbb{B}}} - \lambda_{\zeta,i_\alpha^{\mathbb{B}}}\right)\right], \quad \text{if } \tilde{p}_F \neq 0. \tag{D5}$$

Now consider the surprisal SEP, which is defined in terms of measurement probabilities [Eq. (12)]. These probabilities simplify in the commuting case. Consider strongly measuring the shared eigenbasis of the charges of system $\mathbb{X}$. Outcome $i_\alpha^{\mathbb{X}}$ obtains with a probability

$$\operatorname{Tr}(\Pi^{\mathbb{X}}_{\alpha,i_\alpha^{\mathbb{X}}}\rho^{\mathbb{X}}) = \frac{1}{Z^{\mathbb{X}}}\operatorname{Tr}(\Pi^{\mathbb{X}}_{\alpha,i_\alpha^{\mathbb{X}}}e^{-\sum_{\zeta=1}^{c}\beta_\zeta^{\mathbb{X}}Q_\zeta^{\mathbb{X}}}) = \frac{1}{Z^{\mathbb{X}}}e^{-\sum_\zeta\beta_\zeta^{\mathbb{X}}\lambda_{\zeta,i_\alpha^{\mathbb{X}}}}\operatorname{Tr}(\Pi^{\mathbb{A}}_{\alpha,i_\alpha^{\mathbb{A}}}) = \frac{1}{Z^{\mathbb{X}}}e^{-\sum_\zeta\beta_\zeta^{\mathbb{X}}\lambda_{\zeta,i_\alpha^{\mathbb{X}}}}. \tag{D6}$$

The last equality follows from the nondegeneracy of the charges: the eigenprojectors are rank-1. The choice of α is arbitrary, because all the charges have the same product bases. The surprisal SEP is therefore

$$\sigma_{\text{surp}} = \log\left(\frac{e^{-\sum_\zeta\beta_\zeta^{\mathbb{A}}\lambda_{\zeta,i_\alpha^{\mathbb{A}}}}\,e^{-\sum_\zeta\beta_\zeta^{\mathbb{A}}\lambda_{\zeta,i_\alpha^{\mathbb{A}}}}}{e^{-\sum_\zeta\beta_\zeta^{\mathbb{A}}\lambda_{\zeta,f_\alpha^{\mathbb{A}}}}\,e^{-\sum_\zeta\beta_\zeta^{\mathbb{A}}\lambda_{\zeta,f_\alpha^{\mathbb{A}}}}}\right) \tag{D7}$$

$$= \sum_\zeta\left[\beta_\zeta^{\mathbb{A}}\left(\lambda_{\zeta,f_\alpha^{\mathbb{A}}} - \lambda_{\zeta,i_\alpha^{\mathbb{A}}}\right) + \beta_\zeta^{\mathbb{B}}\left(\lambda_{\zeta,f_\alpha^{\mathbb{B}}} - \lambda_{\zeta,i_\alpha^{\mathbb{B}}}\right)\right], \tag{D8}$$

in agreement with Eq. (D5).

3. Calculation of $\langle\sigma_{\text{surp}}\rangle$

Here, we prove Eq. (13),

$$\langle\sigma_{\text{surp}}\rangle = D(\rho_f\,||\,\Phi_\alpha(\rho)) - D(\rho||\Phi_\alpha(\rho)). \tag{D9}$$

σ_{surp} [Eq. (12)] depends implicitly on fewer indices than $\tilde{p}_F$ depends on [Eq. (4)]. Therefore, some of the indices disappear (yield factors of unity) when summed over in $\langle\sigma_{\text{surp}}\rangle$. Let us substitute the definition of σ_{surp} into the left-hand side of Eq. (D9) and then substitute in the definition of each probability. Finally, we rearrange terms:

$$\langle\sigma_{\text{surp}}\rangle = \left\langle\log\left(\frac{p_\alpha(i_\alpha^{\mathbb{A}}, i_\alpha^{\mathbb{B}})}{p_\alpha(f_\alpha^{\mathbb{A}}, f_\alpha^{\mathbb{B}})}\right)\right\rangle = \sum_{i_\alpha, f_\alpha}\operatorname{Tr}(U^\dagger\Pi_{\alpha,f_\alpha}U\Pi_{\alpha,i_\alpha}\rho) \times\log\left(\frac{\operatorname{Tr}(\Pi_{\alpha,i_\alpha}\rho)}{\operatorname{Tr}(\Pi_{\alpha,f_\alpha}\rho)}\right)$$

$$= \sum_{i_\alpha}\operatorname{Tr}(\Pi_{\alpha,i_\alpha}\rho)\log\left(\operatorname{Tr}(\Pi_{\alpha,i_\alpha}\rho)\right) - \sum_{f_\alpha}\operatorname{Tr}(\Pi_{\alpha,f_\alpha}\rho_f)\log\left(\operatorname{Tr}(\Pi_{\alpha,f_\alpha}\rho)\right) \tag{D10}$$

$$= \mathrm{Tr}\left(\left[\sum_{i_\alpha} \log\left(\mathrm{Tr}(\Pi_{\alpha,i_\alpha}\rho)\right)\Pi_{\alpha,i_\alpha}\right]\rho\right) - \mathrm{Tr}\left(\left[\sum_{f_\alpha} \Pi_{\alpha,f_\alpha} \log\left(\mathrm{Tr}(\Pi_{\alpha,f_\alpha}\rho)\right)\right]\rho_f\right). \quad \text{(D11)}$$

To simplify the traces, we recall the channel that dephases ρ with respect to the product basis of Q_α: $\Phi_\alpha(\rho) := \sum_{i_\alpha} \Pi_{\alpha,i_\alpha}\rho\Pi_{\alpha,i_\alpha} = \sum_{i_\alpha} \mathrm{Tr}(\Pi_{\alpha,i_\alpha}\rho)\,\Pi_{\alpha,i_\alpha}$. In terms of this channel,

$$\log\left(\Phi_\alpha(\rho)\right) = \sum_{i_\alpha} \log\left(\mathrm{Tr}(\Pi_{\alpha,i_\alpha}\rho)\right)\Pi_{\alpha,i_\alpha}. \quad \text{(D12)}$$

Substituting into Eq. (D11) yields $\langle\sigma_{\mathrm{surp}}\rangle = \mathrm{Tr}(\rho\log(\Phi_\alpha(\rho))) - \mathrm{Tr}(\rho_f\log(\Phi_\alpha(\rho)))$. This expression can be rewritten in terms of relative entropies. By the unitary invariance of the von Neumann entropy, $0 = S_{\mathrm{vN}}(\rho) - S_{\mathrm{vN}}(\rho_f) = \mathrm{Tr}(\rho_f\log(\rho_f)) - \mathrm{Tr}(\rho\log(\rho))$. Adding this 0 onto our $\langle\sigma_{\mathrm{surp}}\rangle$ expression yields Eq. (D9).

4. Proof of fluctuation theorem for σ_{surp}

Here, we prove the fluctuation theorem given in Eq. (14),

$$\langle e^{-\sigma_{\mathrm{surp}}}\rangle = 1 + \mathrm{Tr}(U^\dagger\Phi_\alpha(\rho)U\Delta\rho_\alpha\rho). \quad \text{(D13)}$$

Also, we present the form of the correction.

Recall the definition of the coherent difference $\Delta\rho_\alpha = \Phi_\alpha(\rho)^{-1} - \rho^{-1}$. We substitute into $\langle e^{-\sigma_{\mathrm{surp}}}\rangle$ the definitions of σ_{surp} [Eq. (12)] and $\tilde{p}_F$ [Eq. (4)]. As with the derivation of $\langle\sigma_{\mathrm{surp}}\rangle$, some of the indices are marginalized over. Rearranging factors,

$$\langle e^{-\sigma_{\mathrm{surp}}}\rangle = \sum_{i_1^{\mathrm{A}},i_2^{\mathrm{A}},\ldots,i_c^{\mathrm{A}},f_1^{\mathrm{A}},f_2^{\mathrm{A}},\ldots,f_c^{\mathrm{A}}} \mathrm{Tr}(U^\dagger\Pi_{1,f_1}\ldots\Pi_{c,f_c}U\Pi_{c,i_c}\ldots\Pi_{1,i_1}\rho)\left(\frac{p_\alpha(f_\alpha^{\mathrm{A}},f_\alpha^{\mathrm{B}})}{p_\alpha(i_\alpha^{\mathrm{A}},i_\alpha^{\mathrm{B}})}\right) \quad \text{(D14)}$$

$$= \sum_{i_\alpha^{\mathrm{A}},i_\alpha^{\mathrm{B}},\ f_\alpha^{\mathrm{A}},f_\alpha^{\mathrm{B}}} \mathrm{Tr}\left(U^\dagger\left[\Pi^{\mathrm{A}}_{\alpha,f_\alpha^{\mathrm{A}}}\otimes\Pi^{\mathrm{B}}_{\alpha,f_\alpha^{\mathrm{B}}}\right]U\left[\Pi^{\mathrm{A}}_{\alpha,i_\alpha^{\mathrm{A}}}\otimes\Pi^{\mathrm{B}}_{\alpha,i_\alpha^{\mathrm{B}}}\right]\rho\right)\left(\frac{p_\alpha(f_\alpha^{\mathrm{A}},f_\alpha^{\mathrm{B}})}{p_\alpha(i_\alpha^{\mathrm{A}},i_\alpha^{\mathrm{B}})}\right) \quad \text{(D15)}$$

$$= \mathrm{Tr}\left(U^\dagger\left\{\sum_{f_\alpha^{\mathrm{A}},f_\alpha^{\mathrm{B}}}\left[\Pi^{\mathrm{A}}_{\alpha,f_\alpha^{\mathrm{A}}}\otimes\Pi^{\mathrm{B}}_{\alpha,f_\alpha^{\mathrm{B}}}\right]p_\alpha(f_\alpha^{\mathrm{A}},f_\alpha^{\mathrm{B}})\right\}U\left\{\sum_{i_\alpha^{\mathrm{A}},i_\alpha^{\mathrm{B}}}\left[\Pi^{\mathrm{A}}_{\alpha,i_\alpha^{\mathrm{A}}}\otimes\Pi^{\mathrm{B}}_{\alpha,i_\alpha^{\mathrm{B}}}\right]p_\alpha(i_\alpha^{\mathrm{A}},i_\alpha^{\mathrm{B}})^{-1}\right\}\rho\right). \quad \text{(D16)}$$

The summands simplify to dephased states and inverses thereof: $\sum_{f_\alpha^{\mathrm{A}},f_\alpha^{\mathrm{B}}}(\Pi^{\mathrm{A}}_{\alpha,f_\alpha^{\mathrm{A}}}\otimes\Pi^{\mathrm{B}}_{\alpha,f_\alpha^{\mathrm{B}}})\,p_\alpha(f_\alpha^{\mathrm{A}},f_\alpha^{\mathrm{B}}) = \Phi_\alpha(\rho)$ and $\sum_{i_\alpha^{\mathrm{A}},i_\alpha^{\mathrm{B}}}(\Pi^{\mathrm{A}}_{\alpha,i_\alpha^{\mathrm{A}}}\otimes\Pi^{\mathrm{B}}_{\alpha,i_\alpha^{\mathrm{B}}})\quad p_\alpha(i_\alpha^{\mathrm{A}},i_\alpha^{\mathrm{B}})^{-1} = \Phi_\alpha(\rho)^{-1} = \rho^{-1} + \Delta\rho_\alpha$. We substitute into Eq. (D16), multiply out, and simplify:

$$\langle e^{-\sigma_{\mathrm{surp}}}\rangle = \mathrm{Tr}(U^\dagger\Phi_\alpha(\rho)U\left[\rho^{-1}+\Delta\rho_\alpha\right]\rho)$$

$$= \mathrm{Tr}(U^\dagger\Phi_\alpha(\rho)U\rho^{-1}\rho) + \mathrm{Tr}(U^\dagger\Phi_\alpha(\rho)U\Delta\rho_\alpha\rho) \quad \text{(D17)}$$

$$= 1 + \mathrm{Tr}(U^\dagger\Phi_\alpha(\rho)U\Delta\rho_\alpha\rho). \quad \text{(D18)}$$

The second term is the correction sourced by coherences. It vanishes if $\Delta\rho_\alpha = 0$.

APPENDIX E: TRAJECTORY STOCHASTIC ENTROPY PRODUCTION

This appendix concerns the trajectory-SEP formula (Sec. III C 1). We further motivate our choice of reverse quasiprobability, $\tilde{p}_{\mathrm{R}}$, in Appendix E 1. We prove that $\sigma_{\mathrm{traj}} = \sigma_{\mathrm{chrg}}$ in the commuting case (Sec. III C 1) in Appendix C 2. In Appendix E 3, we calculate $\langle\sigma_{\mathrm{traj}}\rangle$ [prove Eq. (21)].

1. Choice of reverse quasiprobability

Section II B has introduced the forward quasiprobability [Eq. (4)],

$$\tilde{p}_F(i_1,i_2,\ldots,i_c\,;f_c,f_{c-1},\ldots,f_1) := \mathrm{Tr}\left(U^\dagger\left[\Pi_{1,f_1}\Pi_{2,f_2}\ldots\Pi_{c,f_c}\right]U\left[\Pi_{c,i_c}\ldots\Pi_{2,i_2}\Pi_{1,i_1}\right]\rho\right), \quad \text{(E1)}$$

and Sec. III C 1 has introduced the reverse quasiprobability,

$$\tilde{p}_{\mathrm{R}}(f_1,f_2,\ldots,f_c\,;i_c,i_{c-1},\ldots,i_1) := \mathrm{Tr}\left(\left[\Pi_{1,f_1}\Pi_{2,f_2}\ldots\Pi_{c,f_c}\right]U\left[\Pi_{c,i_c}\ldots\Pi_{2,i_2}\Pi_{1,i_1}\right]U^\dagger\rho\right). \quad \text{(E2)}$$

We have motivated the definition of $\tilde{p}_{\rm R}$ operationally in Sec. III C 1. However, other possible definitions could satisfy the constraint that, in the commuting case, $\sigma_{\rm traj}$ must reduce to $\sigma_{\rm chrg}$ and $\sigma_{\rm surp}$. The prior literature features nonunique reverse distributions (of probabilities, rather than quasiprobabilities) [52,165]. The authors there have distinguished one reverse distribution by specifying one of multiple possible reverse protocols. Similarly, we specify a reverse protocol from which $\tilde{p}_{\rm R}$ can be inferred experimentally. We therefore regard $\tilde{p}_{\rm R}$ as capturing the notion of time reversal.

We can associate each KDQ with a protocol—the key stage of an experiment used to infer the quasiprobability (see Appendix A and Ref. [68]). One begins at one end of the argument of the trace and proceeds toward the opposite end. If a projector appears on just one side of ρ, that projector corresponds to a weak measurement. We show that the $\tilde{p}_R$ protocol is a time reverse of the $\tilde{p}_F$ protocol.

We associate $\tilde{p}_F$ with a protocol by reading the indices in Eq. (E1) from right to left: one measures charges 1 through c weakly, evolves the state forward in time, and then measures charges c through 1 weakly. Before interpreting $\tilde{p}_R$, we cycle ρ to the left-hand side of the trace:

$$\tilde{p}_{\rm R}(f_1,f_2,\ldots,f_c\,;\,i_c,i_{c-1},\ldots,i_1) := {\rm Tr}\left(\rho\left[\Pi_{1,f_1}\ldots\Pi_{c,f_c}\right]U\left[\Pi_{c,i_c}\ldots\Pi_{1,i_1}\right]U^\dagger\right). \quad \text{(E3)}$$

Then, we read from left to right. In the associated protocol, one measures charges 1 through c weakly, evolves the state backward in time (under $U^\dagger$), and then measures charges c through 1 weakly. Relative to the forward protocol, the time evolution is reversed, as is the list of measurement outcomes.

2. Equivalence of $\sigma_{\rm traj}$ and $\sigma_{\rm surp}$ in the commuting case

In this appendix, we show that $\sigma_{\rm traj}=\sigma_{\rm surp}$ in the commuting case. Equation (16) defines the trajectory SEP:

$$\sigma_{\rm traj}=\log\left(\langle i_1|\,\rho U^\dagger\,|f_1\rangle\,/\,\langle i_1|\,U^\dagger\rho\,|f_1\rangle\right). \quad \text{(E4)}$$

Since the initial state is diagonal with respect to the 1st product basis, $\langle i_1|\,\rho={\rm Tr}(\Pi_{i_1}\rho)\,\langle i_1|$, and $\rho\,|f_1\rangle={\rm Tr}(\Pi_{f_1}\rho)\,|f_1\rangle$. Therefore,

$$\sigma_{\rm traj}=\log\left(\frac{{\rm Tr}(\Pi_{i_1}\rho)\,\langle i_1|\,U^\dagger\,|f_1\rangle}{{\rm Tr}(\Pi_{f_1}\rho)\,\langle i_1|\,U^\dagger\,|f_1\rangle}\right)=\log\left(\frac{{\rm Tr}(\Pi_{i_1}\rho)}{{\rm Tr}(\Pi_{f_1}\rho)}\right). \quad \text{(E5)}$$

The final expression is $\sigma_{\rm surp}$ [Eq. (12)] with $\alpha=1$. (The choice of α is irrelevant in the commuting case, since all the product bases coincide.) We have already established the equivalence of $\sigma_{\rm surp}$ and $\sigma_{\rm chrg}$ in the commuting case (Appendix D 2). Therefore, we have shown that all three SEP formulas agree when charges commute.

3. Calculation of $\langle\sigma_{\rm traj}\rangle$ when the initial state ρ is pure

Let the initial state in Sec. II A be pure: $\rho=|\psi\rangle\langle\psi|$. Under this assumption, we derive Eq. (21):

$$\langle\sigma_{\rm traj}\rangle=\frac{1}{2}\left[D(\rho||\Phi^1(U^\dagger\rho U))+D(\rho||U^\dagger\Phi^1(\rho)U)-D(\rho||\Phi^1(\rho))-D(\rho_f||\Phi^1(\rho_f))\right]+i\langle\phi_{\rm F}-\phi_R\rangle. \quad \text{(E6)}$$

Our proof consists of three steps. First, we express $\sigma_{\rm traj}$ in terms of weak values, slightly rewriting Eq. (19):

$$\sigma_{\rm traj}=\log\left(\frac{\left|{}_{f_1}\langle\Pi_{1,i_1}\rangle_\rho\right|}{\left|{}_{i_1}\langle\Pi_{1,f_1}\rangle_\rho\right|}\frac{{\rm Tr}\left(\Pi''_{1,f_1}\rho\right)}{{\rm Tr}\left(\Pi_{1,i_1}\rho\right)}\right)+i(\phi_{\rm F}-\phi_R). \quad \text{(E7)}$$

Second, we prove that $i\langle\phi_{\rm F}-\phi_{\rm R}\rangle$ is imaginary. Finally, we prove that the average of the logarithm is real and equals the relative-entropy sum in Eq. (E6). By implication, $i\langle\phi_{\rm F}-\phi_{\rm R}\rangle={\rm Im}(\langle\sigma_{\rm traj}\rangle)$. This result supports the claim in the main text that ${\rm Im}(\langle\sigma_{\rm traj}\rangle)\neq 0$ signals contextuality.

Let us show that $i\langle\phi_{\rm F}-\phi_R\rangle$ is imaginary. Let z denote any complex number. We denote the principal value of its argument (of its complex phase) by ${\rm Arg}(z)$ and the multivalued argument function by ${\rm arg}(z)$. $\phi_{\rm F}-\phi_{\rm R}$ equals an argument by Eq. (16) and the polar forms in Sec. III C 1: For each index pair (i_1,f_1), there is a branch of arg such that

$$\begin{aligned}\phi_{\rm F}-\phi_{\rm R}&={\rm arg}\left(\frac{\langle i_1|\psi\rangle\langle\psi|U^\dagger|f_1\rangle}{\langle i_1|U^\dagger|\psi\rangle\langle\psi|f_1\rangle}\right)\\&={\rm Arg}\left(\langle i_1|\psi\rangle\right)+{\rm Arg}\left(\langle\psi|U^\dagger|f_1\rangle\right)\\&\quad-{\rm Arg}\left(\langle i_1|U^\dagger|\psi\rangle\right)-{\rm Arg}\left(\langle\psi|f_1\rangle\right).\end{aligned} \quad \text{(E8)}$$

Each summand in the right-hand side of Eq. (E8) depends on one index, i_1 or f_1. (If ρ is mixed, $\sigma_{\rm traj}$ does not decompose in this manner. Hence new techniques are required to compute the average.) Therefore, averaging $\phi_{\rm F}-\phi_{\rm R}$ with respect to $\tilde{p}_F$ yields separate averages with respect to probability distributions. Hence $\langle\phi_{\rm F}-\phi_{\rm R}\rangle$ is real and $i\langle\phi_{\rm F}-\phi_{\rm R}\rangle$ is imaginary.

Our task reduces to showing that

$$\left\langle\log\left(\frac{\left|{}_{f_1}\langle\Pi_{1,i_1}\rangle_\rho\right|}{\left|{}_{i_1}\langle\Pi_{1,f_1}\rangle_\rho\right|}\frac{{\rm Tr}\left(\Pi''_{1,f_1}\rho\right)}{{\rm Tr}\left(\Pi'_{1,i_1}\rho\right)}\right)\right\rangle=\frac{1}{2}\left[D(\rho||\Phi^1(U^\dagger\rho U))+D(\rho||U^\dagger\Phi^1(\rho)U)-D(\rho||\Phi^1(\rho))-D(\rho_f||\Phi^1(\rho_f))\right]. \quad \text{(E9)}$$

The weak values have magnitudes of

$$\left|{}_{f_1}\langle \Pi_{1,i_1}\rangle_\rho\right| = \frac{\left[\mathrm{Tr}(\Pi''_{1,f_1}\Pi_{1,i_1}\rho)\mathrm{Tr}(\rho\Pi_{1,i_1}\Pi''_{1,f_1})\right]^{\frac{1}{2}}}{\mathrm{Tr}(\Pi''_{1,f_1}\rho)} \quad \text{and}$$
$$\left|{}_{i_1}\langle \Pi_{1,f_1}\rangle_\rho\right| = \frac{\left[\mathrm{Tr}(\Pi'_{1,i_1}\Pi_{1,f_1}\rho)\mathrm{Tr}(\rho\Pi_{1,f_1}\Pi'_{1,i_1})\right]^{\frac{1}{2}}}{\mathrm{Tr}(\Pi'_{1,i_1}\rho)}. \tag{E10}$$

When we insert these expressions into Eq. (E9), the denominators in Eq. (E10) cancel. To simplify the left-hand side of Eq. (E9) further, we express ρ and the rank-1 projectors as outer products: $\rho = |\psi\rangle\langle\psi|$, $\Pi_{1,i_1} = |i_1\rangle\langle i_1|$, etc. Factors $\langle f_1|U|i_1\rangle$ and $\langle i_1|U^\dagger|f_1\rangle$ appear in the numerator and denominator. Canceling the factors, we compute the left-hand side of Eq. (E9):

$$\left\langle \log\left(\frac{\left[\mathrm{Tr}(\Pi''_{1,f_1}\Pi_{1,i_1}\rho)\mathrm{Tr}(\rho\Pi_{1,i_1}\Pi''_{1,f_1})\right]^{\frac{1}{2}}}{\left[\mathrm{Tr}(\Pi'_{1,i_1}\Pi_{1,f_1}\rho)\mathrm{Tr}(\rho\Pi_{1,f_1}\Pi'_{1,i_1})\right]^{\frac{1}{2}}}\right)\right\rangle = \left\langle \frac{1}{2}\log\left(\frac{\mathrm{Tr}(\Pi_{1,f_1}U\rho U^\dagger)\mathrm{Tr}(\Pi_{1,i_1}\rho)}{\mathrm{Tr}(\Pi_{1,f_1}\rho)\mathrm{Tr}(\Pi_{1,i_1}U^\dagger\rho U)}\right)\right\rangle \tag{E11}$$

$$= \sum_{i_1,\ldots,i_c,f_1,\ldots,f_c} \frac{1}{2}\mathrm{Tr}(U^\dagger\Pi_{1,f_1}\ldots\Pi_{1,f_c}U\Pi_{c,i_c}\ldots\Pi_{1,i_1}\rho)\log\left(\frac{\mathrm{Tr}(\Pi_{1,f_1}U\rho U^\dagger)\mathrm{Tr}(\Pi_{1,i_1}\rho)}{\mathrm{Tr}(\Pi_{1,f_1}\rho)\mathrm{Tr}(\Pi_{1,i_1}U^\dagger\rho U)}\right) \tag{E12}$$

$$= \frac{1}{2}\Bigg[\sum_{f_1}\mathrm{Tr}(\Pi_{1,f_1}\rho_f)\log\left(\mathrm{Tr}(\Pi_{1,f_1}\rho_f)\right) + \sum_{i_1}\mathrm{Tr}(\Pi_{1,i_1}\rho)\log\left(\mathrm{Tr}(\Pi_{1,i_1}\rho)\right)$$
$$- \sum_{f_1}\mathrm{Tr}(\Pi_{1,f_1}\rho_f)\log\left(\mathrm{Tr}(\Pi_{1,f_1}\rho)\right) - \sum_{i_1}\mathrm{Tr}(\Pi_{1,i_1}\rho)\log\left(\mathrm{Tr}(\Pi_{1,i_1}U^\dagger\rho U)\right)\Bigg] \tag{E13}$$

$$= \frac{1}{2}\left[\mathrm{Tr}\left(\rho_f\log\left(\Phi_1(\rho_f)\right)\right) + \mathrm{Tr}\left(\rho\log\left(\Phi_1(\rho)\right)\right) - \mathrm{Tr}\left(\rho_f\log\left(\Phi_1(\rho)\right)\right) - \mathrm{Tr}\left(\rho\log\left(\Phi_1(U^\dagger\rho U)\right)\right)\right]. \tag{E14}$$

The final equality follows from Eq. (D12).

By the unitary invariance of the von Neumann entropy, $\frac{1}{2}[S_{\mathrm{vN}}(\rho) - S_{\mathrm{vN}}(\rho) + S_{\mathrm{vN}}(\rho) - S_{\mathrm{vN}}(\rho_f)] = 0$. We add this zero to Eq. (E13). By the cyclicality of the trace, $\mathrm{Tr}\left(\rho\log\left(U^\dagger\Phi_1(\rho)U\right)\right) = \mathrm{Tr}\left(U\rho U^\dagger\log\left(\Phi_1(\rho)\right)\right)$ in Eq. (E13). Rearranging terms yields the right-hand side of Eq. (E9). $\mathrm{Re}(\langle\sigma_{\mathrm{traj}}\rangle)$ is non-negative because it can be written as $\frac{1}{2}\left[D(\Phi^1(\rho)||\Phi^1(U^\dagger\rho U)) + D(\Phi^1(\rho_f)||\Phi^1(\rho))\right]$.

When ρ is pure, Eq. (E6) points, for each index pair (i_1,f_1), to a choice of branch of the complex logarithm in the definition of σ_{traj}. This choice enables $\langle\sigma_{\mathrm{traj}}\rangle$ to signal contextuality. If ρ is mixed, in the absence of a more explicit expression for $\langle\sigma_{\mathrm{traj}}\rangle$, it is not clear what choice enables $\langle\sigma_{\mathrm{traj}}\rangle$ to signal contextuality.

APPENDIX F: SYMMETRIZED DEFINITIONS

In defining the KDQ and some SEPs, we choose projectors and the order in which to arrange them. Here, we discuss alternative KDQ and SEP definitions based on symmetrizing over these choices. We present the corresponding averages $\langle\sigma\rangle$. Via arguments similar to the ones for unsymmetrized SEPs σ, one can derive fluctuation theorems.

1. Symmetrized Kirkwood-Dirac quasiprobability

A primary motivation for using the KDQ is a desire to describe charges flowing in the absence of measurement disturbance. Though based on weak measurements, the KDQ depends on the ordering of the measurements, i.e., how the charges are labeled. But if the systems interact unitarily without being measured, relabeling the charges does not change any physical observables. Also the stochastic description of this process should respect this symmetry. We take this for granted in the commuting case, in which the ordering of the measurements does not change the joint probability distribution. We can enforce this symmetry in the noncommuting case by averaging over all possible orderings of the initial projectors. (Once the initial projectors are ordered, the ordering of the final projectors is fixed by the fourth sanity check in Sec. III.) We define the *symmetrized KDQ* (SKDQ) as

$$\tilde{p}_F^{\text{symm}} := \frac{1}{c!}\sum_{\tau\in S_c} \text{Tr}(U^\dagger \left[\Pi_{\tau(1),f_{\tau(1)}} \dots \Pi_{\tau(c),f_{\tau(c)}}\right] U\left[\Pi_{\tau(c),i_{\tau(c)}} \dots \Pi_{\tau(1),i_{\tau(1)}}\right]\rho). \tag{F1}$$

S_c is the symmetric group of degree c, i.e., the set of all permutations of $\mathbb{Z}_c$. $\tilde{p}_F^{\text{symm}}$ is invariant under every possible relabeling of the charges, respecting a fundamental symmetry of the undisturbed-charge-flow process. The single-index marginals of the SKDQ are those of $\tilde{p}_F$. In the commuting case, $\tilde{p}_F^{\text{symm}} = \tilde{p}_F$.

2. Charge stochastic entropy production

The charge SEP is already symmetric under every possible relabeling of the charges. Since the SKDQ has the same marginals as the KDQ, σ_{chrg} has the same average:

$$\langle\sigma_{\text{chrg}}\rangle_{\text{symm}} = \langle\sigma_{\text{chrg}}\rangle = \sum_\alpha \Delta\beta_\alpha\, \Delta\langle Q_\alpha\rangle. \tag{F2}$$

3. Surprisal stochastic entropy production

To obtain the symmetrized surprisal SEP, we average over the different bases:

$$\sigma_{\text{surp}}^{\text{symm}} := \frac{1}{c}\sum_{\alpha=1}^{c} \log\left(\frac{p_\alpha(i_\alpha^{\text{A}}, i_\alpha^{\text{B}})}{p_\alpha(f_\alpha^{\text{A}}, f_\alpha^{\text{B}})}\right). \tag{F3}$$

The average now involves dephasing in all bases:

$$\langle\sigma_{\text{surp}}^{\text{symm}}\rangle_{\text{symm}} = \frac{1}{c}\sum_{\alpha=1}^{c}\left[D(\rho_f\,||\Phi_\alpha(\rho)) - D(\rho||\Phi_\alpha(\rho))\right]. \tag{F4}$$

4. Trajectory stochastic entropy production

A natural definition for the symmetrized trajectory SEP is

$$\sigma_{\text{traj}}^{\text{symm}} = \frac{1}{c}\left(\sum_{\alpha=1}^{c} \log\frac{\langle i_\alpha|\,\rho U^\dagger\,|f_\alpha\rangle}{\langle i_\alpha|\,U^\dagger\rho\,|f_\alpha\rangle}\right). \tag{F5}$$

This symmetrized SEP is closely related to the SKDQ. As in the unsymmetrized case, we define the trajectory SEP as the ratio of the forward and reverse quasiprobabilities. However, we perform the averaging after taking the ratio:

$$\sigma_{\text{traj}}^{\text{symm}} := \frac{1}{c!}\sum_{\tau\in S_c}\log\left(\frac{\tilde{p}_F(\tau)}{\tilde{p}_{\text{R}}(\tau)}\right) = \frac{1}{c!}\sum_{\tau\in S_c}\log\left(\frac{\text{Tr}(U^\dagger\left[\Pi_{\tau(1),f_{\tau(1)}}\dots\Pi_{\tau(c),f_{\tau(c)}}\right]U\left[\Pi_{\tau(c),i_{\tau(c)}}\dots\Pi_{\tau(1),i_{\tau(1)}}\right]\rho)}{\text{Tr}(\left[\Pi_{\tau(1),f_{\tau(1)}}\dots\Pi_{\tau(c),f_{\tau(c)}}\right]U\left[\Pi_{\tau(c),i_{\tau(c)}}\dots\Pi_{\tau(1),i_{\tau(1)}}\right]U^\dagger\rho)}\right) \tag{F6}$$

$$= \frac{1}{c}\sum_{\alpha=1}^{c}\log\left(\frac{\langle i_\alpha|\,\rho U^\dagger\,|f_\alpha\rangle}{\langle i_\alpha|\,U^\dagger\rho\,|f_\alpha\rangle}\right). \tag{F7}$$

The cancellation of the factors simplifies the sum to be only over c charges, rather than $c!$ permutations. If ρ is pure, the average is

$$\langle\sigma_{\text{traj}}\rangle = \frac{1}{c}\sum_{\alpha=1}^{c}\left\{\frac{1}{2}\left[D(\rho||\Phi_\alpha(U^\dagger\rho U)) + D(\rho||U^\dagger\Phi_1(\rho)U) - D(\rho||\Phi_1(\rho)) - D(\rho_f\,||\Phi_1(\rho_f\,))\right] + i\langle\phi_{\text{F}}^\alpha - \phi_R^\alpha\rangle_{\text{symm}}\right\}. \tag{F8}$$

The weak-value phases for general α are defined analogously to the weak-value phases in Sec. III C 2.

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