Quantum-classical correspondence principles for locally nonequilibrium driven systems

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Many of the core concepts and (especially field-theoretic) tools of statistical mechanics have developed within the context of thermodynamic equilibrium, where state variables are all taken to be *charges*, meaning that their values are inherently preserved under reversal of the direction of time. A principle concern of nonequilibrium statistical mechanics is to understand the emergence and stability of *currents*, quantities whose values change sign under time reversal. Whereas the correspondence between classical charge-valued state variables and their underlying statistical or quantum ensembles is quite well understood, the study of currents away from equilibrium has been more fragmentary, with classical descriptions relying on the asymmetric auxiliary-field formalism of Martin, Siggia, and Rose (and often restricted to the Markovian assumption of Doi and Peliti), while quantum descriptions employ a symmetric two-field formalism introduced by Schwinger and further clarified by Keldysh. In this paper we demonstrate that for quantum ensembles in which superposition is not violated by very strong conditions of decoherence, there is a large natural generalization of the principles and tools of equilibrium, which not only admits but *requires* the introduction of current-valued state variables. For these systems, not only do Martin-Siggia-Rose (MSR) and Schwinger-Keldysh (SK) field methods both exist, in some cases they provide inequivalent classical and quantum descriptions of identical ensembles. With these systems for examples, we can both study the correspondence between classical and quantum descriptions of currents, and also clarify the nature of the mapping between the structurally homologous but interpretationally different MSR and SK formalisms.

DOI: [10.1103/PhysRevE.77.021109](http://dx.doi.org/10.1103/PhysRevE.77.021109)

PACS number(s): 05.70.Ln, 02.50.Ey, 03.65.Sq, 05.30.-d

I. INTRODUCTION

The early development of field-theoretic techniques for statistical mechanics seemed to suggest that many of the tools and principles applicable to equilibrium were inherently unsuited to nonequilibrium phenomena. Reliance on time-reversal invariance, analyticity, and dimensionality and renormalization led to the powerful ideas of effective field theory—the understanding that many low-dimensional theories could be derived from symmetries and renormalizationgroup relevance without further assumptions $[1]$ $[1]$ $[1]$ —and Ginzburg-Landau effective potentials—direct potentials for the classical state variables of a statistical system $[2]$ $[2]$ $[2]$. These, together with maximum-entropy (MaxEnt) principles, produced the phenomenological theory of equilibrium phase transitions, critical scaling, and universality $[3,4]$ $[3,4]$ $[3,4]$ $[3,4]$. Meanwhile, the set of tools available to study nonequilibrium statistical mechanics (NESM) was more limited, and frequently phenomenological $[5-8]$ $[5-8]$ $[5-8]$.

In the last five decades, this apparent qualitative divide has been eroding, as a growing list of techniques have been freed from assumptions that entail equilibrium, and have found application to dynamical and even irreversible processes. Field-theoretic methods have been central to this advancement, as these directly represent collective and cooperative effects among multiple excitations, and serve as a basis for iterative schemes of coarse-graining and phenomenological description. Stationary-point expansions of field theories directly link the outcomes of renormalization to effective potentials for classical state variables. Irreversible

processes have come to be associated with a structurally homologous class of "two-field" methods, one inherently quantum mechanical and developed primarily by Schwinger $[9]$ $[9]$ $[9]$ and Keldysh $[10]$ $[10]$ $[10]$, the other classical (in a variety of interpretations) and developed primarily by Doi $[11,12]$ $[11,12]$ $[11,12]$ $[11,12]$ and Peliti [$13,14$ $13,14$], Eyring $[15]$ $[15]$ $[15]$, and Martin, Siggia, and Rose (MSR) $\lfloor 16 \rfloor$ $\lfloor 16 \rfloor$ $\lfloor 16 \rfloor$.

At the same time as coarse-graining methods have been extended to nonequilibrium systems with two-field approaches, the use and calculation of entropies has been somewhat freed from equilibrium restrictions, to include both time-local nonequilibrium ensembles $[17,18]$ $[17,18]$ $[17,18]$ $[17,18]$, and ensembles on spaces of paths rather than merely of configurations [19–](#page-23-5)[22](#page-23-6). Both extensions lead naturally to principled derivations of entropies, which depend on currents among their extensive state-variable arguments, and in special cases to a limited class of well-founded maximum-entropy production (MaxEP) principles.

Despite these advancements, current-valued state variables are not nearly as well understood as the charge-valued state variables of equilibrium thermodynamics. Most theoretical approaches to NESM $[5-8,21,22]$ $[5-8,21,22]$ $[5-8,21,22]$ $[5-8,21,22]$ $[5-8,21,22]$ —and also most interesting applications $[23-25]$ $[23-25]$ $[23-25]$ —continue to represent single moments of time with the approximation of *local equilibrium*: the assumption that the state variables and statistics of the nonequilibrium system remain well approximated by those of equilibria, with currents introduced (if at all) secondarily as auxiliary fields to reflect constraints. When the underlying system is quantum mechanical, the passage between microscopic and classical effective theories is poorly understood, because in many cases the classical theory assumes commuting observables $\lceil 11-14 \rceil$ $\lceil 11-14 \rceil$ $\lceil 11-14 \rceil$, which rule out direct correspondence with the coherent dynamics that the quantum *FAX: 505-982-0565; desmith@santafe.edu transport theory was invented to preserve. Yet this absence of

1539-3755/2008/77(2)/021109(24)

correspondence principles is surprising, because a central feature of two-field methods is a representation of causality in a distinctive tridiagonal Green's function structure, which is more fundamental than the distinction between MSR (classical) and SK (quantum) interpretations of the Hilbert spaces on which the fundamental excitations of the theories are defined $\lceil 26 \rceil$ $\lceil 26 \rceil$ $\lceil 26 \rceil$.

The purpose of this paper is to clarify the interpretation of current-valued state variables in two-field models for NESM, focusing particularly on the passage back and forth between classical MSR and quantum SK representations for quantum systems with locally *nonequilibrium* structure, and on the representation of current-dependent entropies. Much of the work of the paper will be the derivation of operator and field correspondences between MSR and SK representations, but the conceptual core of the paper is the idea of *kinematic symmetry* arising from superposition. The most important arguments that current-dependent entropies are not only possible, but often required, can be understood on the basis of symmetry alone, and many features of the quantum-classical correspondence and relations among time structures in MSR and SK follow from symmetry properties of the state variables.

Perhaps most important, kinematic symmetries introduce a new class of maximum-entropy ensembles, which are richer than any classical descriptions that use commuting observables, but which nonetheless involve no quantum information, so that both classical MSR and quantum SK representations are formally exact and interconvertible. These ensembles will be used as the basis to understand classical or quantum correspondence principles, both physically and in the formal structure of two-field theories.

The introductory statements up to this point have been intended to place the particular problem of two-field correspondence principles in the larger context of building a conceptual foundation for the use of current-valued state variables in NESM, and to deemphasize the more technical aspects relative to the concepts of symmetry, coarsegraining, and effective potentials including the entropy. The remainder of the Introduction will fill in the necessary history of two-field methods, in particular, their association with commuting observables in classical theories, and will explain more fully the limitations of the local-equilibrium approximation that often accompanies these.

A. History of two-field methods

Quantum two-field methods for NESM may be viewed as an extension of field-theoretic representations of the equilibrium partition function. The Matsubara field representation $[27]$ $[27]$ $[27]$ of the trace of the Boltzmann factor exp{-Hamiltonian/*k_BT*} as a path integral over a "Euclidean action" on a loop in imaginary time $\lceil 28 \rceil$ $\lceil 28 \rceil$ $\lceil 28 \rceil$ enables computation, by analytic continuation of the time variable to real values, of time-dependent correlations of fluctuations about equilibrium backgrounds. The equivalent of the analytic continuation of thermal Green's functions in the Matsubara theory is achieved by Schwinger's explicit insertion of the time-loop *S* matrix $[9]$ $[9]$ $[9]$, which effectively deforms the imaginary time loop into the real half-plane, by evolving the basis states in the density matrix with real-time path integrals.

By embedding the Schrödinger-picture evolution of states in the Matsubara sum over Boltzmann factors, the time loop represents time-dependent correlations in both vacuum and finite-temperature systems as functions of initial data alone. It further permits evaluation of correlation functions about dynamically varying backgrounds; a stationary point expansion of the time-loop action can even be used to generalize the equilibrium free energy to a dynamical functional of Ginzburg-Landau form for the spontaneous symmetry breaking of thermodynamically reversible self-organizing states $[29,30]$ $[29,30]$ $[29,30]$ $[29,30]$.

One of the interesting observations from stationary-point expansion of the time-loop thermal effective action for the ideal gas $\lceil 29 \rceil$ $\lceil 29 \rceil$ $\lceil 29 \rceil$ was that the full adiabatic equations of motion can be recovered—including time-varying temperature from conformal modes that dilate and contract the circumference of the Matsubara imaginary-time cycle. An unresolved feature of that continuation of the Euclidean effective action, however, was the appearance of logarithmic terms representing the entropy, which entailed a departure from the analytic (polynomial) expansions usually assumed for vacuum effective actions $[1]$ $[1]$ $[1]$. The current paper will revisit this issue, showing how to consistently propagate such entropy terms and their generalizations to local nonequilibrium—at a classical level of description.

Time-loop structure was originally introduced to define time-dependent inner products of states from initial data in a thermal density matrix, but because the two (bra and ket) state histories evolve in parallel, it is also possible to incrementally implement partial traces between them (a so-called "super operator" on the density matrix) to represent dissipation. Thus the time-loop structure provides a means for defining and renormalizing dynamical dissipative phenomena in quantum mechanics. The general causal structure of renormalized dissipative *S* matrices was clarified by Keldysh $[10]$ $[10]$ $[10]$, who introduced "classical" and "quantum" superpositions of fields on the forward and backward legs of the time loop, and showed that causal dynamics arises from the now familiar tridiagonal form of the two-field Green's function, whose blocks are the correlation function of classical components and the response functions of classical to quantum components. While it might be expected that the close connection of the Schwinger-Keldysh (SK) time loop to the Matsubara representation of the free energy is the source of dynamical Ginzburg-Landau potentials, Kamenev has remarked $[26]$ $[26]$ $[26]$, and we shall see below, that only the Keldysh causal structure is really needed for such potentials to be possible.

Dissipation converts the time-loop *S* matrix for unitary evolution into a topology that could be called a "time trellis" (the figures below will explain this choice of description), after which the Keldysh field rotation effectively replaces the trellis entirely by a pair-field structure on a simple time line. Martin, Siggia, and Rose $[16]$ $[16]$ $[16]$ recognized that the Keldysh fields and causal structure define an effective-field prescription for general dissipative systems; they introduced by hand a field homologous to Keldysh's "quantum" component to create a tridiagonal Green's function for the study of quite general classical stochastic processes. A full suite of algebraic and path-integral methods with causal structure equivalent to Keldysh's quantum field theory was subsequently developed for classical reaction-diffusion systems by Doi $[11,12]$ $[11,12]$ $[11,12]$ $[11,12]$ (operator methods) and Peliti $[13,14]$ $[13,14]$ $[13,14]$ $[13,14]$ (path integral through insertion of coherent states in the Doi Hilbert space). Doi's operator representation of Markovian transfer matrices, and Hilbert-space representation of their associated generating functions, leads to an expression for the Liouville operator (acting on the generating function) as a symplectic pseudopotential with many of the properties of a Hamiltonian $[15,31]$ $[15,31]$ $[15,31]$ $[15,31]$, hence the Liouville operator is the actual source of dynamical Ginzburg-Landau potentials. The MSR homologue to the effective action may be used as the basis not only for perturbative renormalization $[32,33]$ $[32,33]$ $[32,33]$ $[32,33]$, but also for the nonperturbative estimation of large-deviation probabilities $[34,35]$ $[34,35]$ $[34,35]$ $[34,35]$, a particularly valuable use of effective potentials in equilibrium theories $[36]$ $[36]$ $[36]$ (Chap. 7).

MSR methods have since been derived for stochastic partial differential equations by Hochberg *et al.* [[37](#page-23-21)], and for Lorentz-invariant operators by Cooper *et al.* [[38](#page-23-22)]. The isomorphism of the field structures and Green's functions between the Schwinger-Keldysh (SK) and Doi-Peliti (DP)-or more generally the MSR—field theories has been emphasized $\lceil 26 \rceil$ $\lceil 26 \rceil$ $\lceil 26 \rceil$, and provides a clue to linking these levels of description despite their arising from quite different Hilbert spaces. It is this relation of the underlying operators and inner products that has not to date been clarified.

B. Parallel treatments of dissipative quantum systems

Both SK and MSR methods were created to treat the combined effects of transport and dissipation. In principle they therefore have overlapping domains of applicability, in which the two approaches generate *inequivalent* (quantum and classical) representations of the same ensembles. The emphasis on SK to treat dissipation as a correction to unitary quantum evolution, and of MSR as an effective theory for classical processes, has apparently caused neglect of this area of overlap, and no attention seems to have been given to the transformation back and forth between SK and MSR representations where both exist, and where a "correspondence principle" between the two representations would be most informative. In particular, the DP construction of MSR field theories for Markov processes assumes the existence of a classical probability distribution. If this assumption is taken to define the "classical limit" of an underlying quantum process, decoherence is assumed to be so strong that the classical state variables can at most correspond to expectations within a complete set of commuting observables (CSCO) in the quantum theory, generally excluding currents which are the canonical conjugates to the classical state variables of equilibrium. Thus classical MSR theories are usually studied precisely where they rule out the expression of Hamiltonian transport, which is the key structural element in the SK representation.

The purpose of the current paper is to study SK and MSR field theories in the more interesting region where the full set of *classical state variables* needed to describe a dissipatively evolving quantum density matrix cannot be represented within any CSCO of the underlying quantum theory, where the structure of Hamiltonian transport is still expressed in the classical equation of state and equation of motion, and where important phenomena are lost in the naïve Markovian description. The most common way such a situation arises is that observables corresponding to canonically conjugate charges and currents are superpositions of the same set of quantum operators. One may think of standing and traveling waves, which are the two linearly independent superpositions of the real and imaginary solutions to a second-order mode equation. When these solutions carry dimensions, clearly no more than one superposition may be taken without creating a dimensional redundancy, which would overconstrain the Legendre duality between dimensionally complementary intensive and extensive state variables in an equilibrium ensemble, a point we briefly reconsider in Sec. II A.) Therefore any CSCO must exclude either the charges or the currents, and no consistent Markov process exists in the variables that are retained, which correctly reproduces the oscillations of the quantum system $\lceil 39 \rceil$ $\lceil 39 \rceil$ $\lceil 39 \rceil$.

While this region lies outside the formal assumption by Doi of a conventional probability distribution and Markovian evolution, it may be understood as a generalization of the DP construction to arbitrary complex-valued generating functions for nonstationary quantum ensembles. For the ensembles actually studied here, the role of a classical probability is recovered in the form of a probability density, in the Glauber-Sudarshan "*P* representation" for quantum ensembles $[18]$ $[18]$ $[18]$, so it is not surprising that the DP construction goes through.)

The paper will focus on particular quantum ensembles for which both the SK and DP constructions provide *complete* specifications. The motivation is that the correspondence between quantum and classical descriptions is clearest where the classical description does not offer merely an approximation of the underlying quantum system, but rather an alternative representation of it. In other words, the quantum ensemble must be specified by maximum entropy subject only to the values of its *classical* state variables, but at the same time those state variables must contain nonequilibrium information not specifiable within any CSCO.

Such ensembles have been used to model dissipative cavity resonances in quantum optics $[40]$ $[40]$ $[40]$, and have been studied in their own right as sources of history-dependent entropies $[17]$ $[17]$ $[17]$, and as models in which the dual structure of thermodynamics is preserved even when the local distribution is not that of equilibrium $[18]$ $[18]$ $[18]$. They have been recognized as a structurally stable set under a lowest-order Fokker-Planck equation $[40]$ $[40]$ $[40]$, and in that sense enjoy the status of effectivefield solutions. In this paper a slight further clarification will be given of their status as a universality class. The main observation will be that, as long as decoherence does not break the superposition symmetries of the quantum kinematics in passing to the classical state description, those symmetries permit the classical equation of state to depend on currents as well as the charges usually taken as equilibrium state variables, without implying any additional *information* in the underlying quantum correlations. The universality class so defined corresponds to the phenomenological class of Ohm's or Fourier's laws of linear transport, and differs from ensembles that make use only of conservation laws based on classical symmetries.

The idea of a universality class defined by quantum kinematic symmetries allows us to start with an equilibrium classical theory, and merely by imposition of symmetry—with no explicitly quantum information—to arrive at a richer suite of classical theories for which the well-defined entropy is a function of currents as well as charges. Further knowledge about the quantum system, such as its Hamiltonian or dissipative structure, then allows identification of a particular nonequilibrium equation of state and equation of motion.

C. MaxEnt and MaxEP

It appears not to have been appreciated for a long time that the notion of entropy is applicable in this way to driven systems, but that the entropy function itself is generally not the same for a driven system as the equilibrium entropy. The equilibrium form will generally be a *coarse-graining* [[41](#page-23-25)] of the true entropy for a driven ensemble, predicated on the Markovian approximation of the classical limit. This particular coarse graining removes the currents that are the distinguishing feature of the driven state, precluding any possible application of entropy maximization to account for these currents $\lfloor 17 \rfloor$ $\lfloor 17 \rfloor$ $\lfloor 17 \rfloor$.

Onsager attempted to work around this problem by reintroducing currents as classical auxiliary fields, to be related to the gradients of the equilibrium state variables by means of classical dissipation coefficients $\lceil 5 \rceil$ $\lceil 5 \rceil$ $\lceil 5 \rceil$. He showed that values for these fields could be derived by minimizing a "rate of production" of the equilibrium-form entropy relative to a quadratic "dissipation function" of currents defined from the phenomenological coefficients. In certain limiting cases, this interpretation is exact $[7,19]$ $[7,19]$ $[7,19]$ $[7,19]$, but such cases require asymptotically equilibrium boundaries. Exact treatment of more general driven quantum ensembles $[17,18]$ $[17,18]$ $[17,18]$ $[17,18]$, without the imposition of the Markovian approximation, shows that maximization of a true excess entropy defined from kinematic symmetries), which is the logarithm of the driven partition function, accounts correctly for the spontaneous emergence of steady-state currents, and leads to Onsager's principle as a phenomenological approximation $\lceil 18 \rceil$ $\lceil 18 \rceil$ $\lceil 18 \rceil$. Other applications of the phenomenological equations of motion, outside the basin of attraction of the equilibrium state, have been found to lead to maximization, rather than minimization, of the so-called entropy production in the stable state $[7,8]$ $[7,8]$ $[7,8]$ $[7,8]$.

More recent approaches $\left[19-22\right]$ $\left[19-22\right]$ $\left[19-22\right]$ to first-principles definition of current-dependent classical entropies may be seen as falling within the same local equilibrium approximation as Onsager's, and in this respect they differ from the approach presented here. The principle assumption leading to MaxEP is that the state variables and entropy function remain those of equilibrium. The only new piece of knowledge that defines a path ensemble—besides its nonequilibrium boundary conditions—is the equation of conservation of flux (of en-ergy, particle number, etc.) [[21](#page-23-7)],

$$
\frac{\partial q}{\partial t} = -\nabla \cdot j,\tag{1}
$$

in which *q* is one of the charge-valued classical state variables, and *j* is an auxiliary field introduced as a free variable.

Jaynes introduced the notion of *caliber* [[19,](#page-23-5)[20](#page-22-11)] in the path ensemble characterized by (q, j) , to replace the entropy of a configurational macrostate (characterized by q alone) in equilibrium. The set of phase-space histories with the largest caliber, consistent with the historical macrotrajectory, replaces the macrostate containing the largest number of typical configurations, as the basis for stable observables. When the only knowledge of the constitutive relations of a system is the conservation law (1) (1) (1) , a general result $[21,22]$ $[21,22]$ $[21,22]$ $[21,22]$ is that the most likely macrohistory corresponds to gradient flow, with the gradient being that of the equilibrium entropy, leading to MaxEP. The result is important, as it explains the success of many phenomenological MaxEP principles $[23-25]$ $[23-25]$ $[23-25]$. However, in this class of examples the approximation of local equilibrium has relegated the current *j* to being an argument of the path entropy but not of the local entropy density.

Both the path-entropy approach and the work in this paper may be seen as efforts to identify and remove conventional, but needless, assumptions from the structure of statistical mechanics, and thus to extend it to the widest possible domain of phenomena. Just as Jaynes observed that statistical physics is *nothing* more than the application of unbiased statistical inference to incompletely determined physical systems $\left[42,43\right]$ $\left[42,43\right]$ $\left[42,43\right]$ $\left[42,43\right]$ —and that nothing precludes the same principles's being applied to nonequilibrium systems—this paper observes that the restriction of classical state variables to a CSCO follows from a strong assumption of decoherence, which violates underlying quantum kinematic symmetries and is not required by the dual structure of thermodynamics anyway. The nonequilibrium entropies generated in this paper from kinematic symmetries may even be embedded in path ensembles, thus incorporating both local and nonlocal current dependence in a MaxEnt principle. The correspondence principle between SK and DP representations of the resulting entropy-maximizing ensembles then expresses these classical theories in terms of their underlying quantum ensembles.

D. Layout and main results

The first two main results of the paper involve only elementary observations about symmetry in quantum systems, or algebraic properties of generating functions and their representation by vectors in Hilbert space. These results therefore do not require the full SK or DP constructions, which are relegated to the Appendixes.

Section II derives the von Neumann entropy as a general state function for classical limits of driven quantum systems, motivated solely by symmetry and entropy maximization. The main observation is that a general classical system composed of *D* independent quantum excitations admits D^2 state variables, of which $D(D-1)/2$ are currents. The quantum ensembles for which the von Neumann state function is the maximizing entropy are introduced, and shown to correspond to a class of linear-dissipative classical transport equations. The raising and lowering operators that generate the quantum Fock space the Hilbert space over which field theories are constructed) are introduced here as well, and the crosslinked structure of operator interactions on the time loop is illustrated from the Fokker-Planck equation for which these ensembles are the general solution.

The symmetry arguments for the classical state variables in Sec. II motivate the general form of classical source fields and their associated Doi operator representation in Sec. III. Here the DP construction is introduced simply as a means to handle generating functions, and is appropriately generalized to state variables which include currents. The Liouville operator for the generating function of the classical equation of state is presented, and from it the operator correspondences are derived between DP operators (or fields) and their timeloop counterparts. The central result of this section is that the noncommutativity of the matrix-valued DP fields allows matrix ordering in the classical Hilbert space to reproduce all possible single-time insertions of the number operator in the underlying quantum time loop. A closely related result is that nonlinearity of the classical Liouville operator is necessary to preserve the fluctuation-dissipation theorem, which is a consequence of linear dissipation together with the time-loop structure in the underlying quantum representation.

To investigate the relation of causal structure in the quantum and classical two-field representations, it is necessary in Sec. IV to bring forward a few results from the explicit SK and DP constructions. The free-field, continuum SK action, in both time-loop and Keldysh variables, is presented here, along with its associated Green's functions. The corresponding action for the classical MSR representation of the same ensemble is then presented, and compared to the Keldysh action both in terms of their isomorphic causal structures, and in terms of the field correspondences presented in Sec. III. The main result of this section, apart from the correspondence between the two representations, is the way in which a classical MSR field theory, constructed from first principles, captures and propagates the von Neumann entropy for driven systems, together with the fluctuations of the $D²$ classical state variables.

II. KINEMATIC SYMMETRIES AND ENTROPIES FOR DRIVEN SYSTEMS

Before descending into details of the two-field representations of dynamical partition functions, we first make clear in a general discussion why the dual structure of classical thermodynamics does *not* entail a restriction to the usual suite of equilibrium state variables, but rather admits a much richer classical description without requiring any assumption of quantum information. The strategy is to start with a conventional equilibrium partition function, and then show that, if it is known to be derived from an underlying quantum system, the usual choice of equilibrium state variables assumes not only the classical limit, but also a form of decoherence that breaks the superposition symmetry in the quantum theory, and which is not necessary to define classical statistics. After examining the properties of the equilibrium classical entropy and its appropriate symmetrized generalization, we will prepare for the two-field constructions by introducing the basis for nonequilibrium equations of state in entropy-maximizing quantum ensembles, and will consider the status of those ensembles as a universality class.

A. Symmetries and the entropy

Because the basis for both SK and DP constructions is free-field theory, we will begin with free-field kinematics, and because the conventional DP construction uses raising and lowering operators with bosonic statistics (occupation numbers $m \in 0, \ldots, \infty$, we will restrict attention to bosonic field theories. We begin with a single simple-harmonic oscillator, as the source of an integer tower of energy states with separation *E*. The entropy-maximizing Boltzmann distribution for an ensemble with a constraint only on the average energy has probabilities

$$
p_m = \frac{1}{Z_1} e^{-\beta Em},\tag{2}
$$

in which $\beta = 1/k_B T$, k_B is Boltzmann's constant, and the partition function for a single degree of freedom is

$$
Z_1 = \sum_{m=0}^{\infty} e^{-\beta Em} = \frac{1}{1 - e^{-\beta E}}.
$$
 (3)

For a single oscillator, since energy and excitation numbers are proportional, a constraint on the excitation number simply offsets the energy by a fixed chemical potential.)

The expected excitation number is

$$
n = \sum_{m=0}^{\infty} m p_m = \frac{1}{e^{\beta E} - 1} = Z_1 - 1, \tag{4}
$$

and the classical single-particle entropy evaluates on the distribution (2) (2) (2) to

$$
S_1 \equiv -\sum_{m=0}^{\infty} p_m \ln p_m = (1+n)\ln(1+n) - n \ln n. \tag{5}
$$

For a single oscillator, there is no further correlation specifiable by a linear constraint involving n , so Eq. (5) (5) (5) is the most general form the entropy can take on an entropy-maximizing ensemble.

For a *D*-dimensional classical oscillator, the number index becomes a vector $\vec{m} \equiv (m_i); i \in 1, ..., D$, and the equilibrium entropy $S = \sum_{i=1}^{D} S_i$, where each S_i is defined from Eq. ([5](#page-4-1)) with respect to its expected number component n_i . If this oscillator is obtained from a CSCO of an underlying quantum system, then we may write each index m_i as the expectation of an operator $\hat{n}_i = a_i^{\dagger} a^i$ (a_i^{\dagger} and a^i are, respectively, the conventional raising and lowering operators for oscillator i) between bra and ket number states $\langle \vec{m} | , | \vec{m} \rangle$, where each such state is a product of the number states over the individual *i*. The independence of the different number components is given by the commutation relations $[a^i, a_j^{\dagger}] \equiv \delta_j^i$.

Now, without yet making any assumption about dynamics, but only supposing that these *D* oscillators are jointly superposable, we imply that the kinematics of the state space is preserved under the symmetry $a \rightarrow Ua$, $a^{\dagger} \rightarrow a^{\dagger} U^{\dagger}$, with *a* and a^{\dagger} regarded as column and row vectors, respectively, and *U* an arbitrary unitary transformation in *D* dimensions with Hermitian conjugate U^{\dagger} . (Note that these unitary transformations preserve the orthogonal commutation relations.) The components \hat{n}_i come to be regarded as diagonal elements in

the matrix operator $\hat{n} \equiv a^{\dagger} a$ (i.e., $[\hat{n}^i_j] \equiv [a^{\dagger}_j a^i]$), and the sum $S = \sum_{i=1}^{D} S_i$ over terms ([5](#page-4-1)) may be understood as a matrix trace, with *n* becoming a diagonal matrix which is the classical expectation value of the $D \times D$ operator matrix \hat{n} .

Under unitary transformations of the state space, the operator \hat{n} transforms as $\hat{n} \rightarrow U \hat{n} U^{\dagger}$, and hence the classical expectation $n \rightarrow UnU^{\dagger}$. The most general entropy function agreeing with the equilibrium form in the diagonalizing basis of *n*, but respecting the unitary symmetry of the kinematics, is the von Neumann form

$$
S = \operatorname{Tr}[(I+n)\ln(I+n) - n \ln n],\tag{6}
$$

in which square brackets denote the matrix trace with respect to the index $i \in 1, \ldots, D$. This *classical* entropy depends, in general, on the $D(D-1)$ off-diagonal entries of a Hermitian *n*, in addition to the *D* diagonal expectation values of any CSCO whose basis need not even have been specified up to this point).

The important observation is that the mere fact that the eigenstates of $D²$ observables cannot be independently specified does *not* imply that classical *expectation values* for these $D²$ observables cannot be independently specified. In general they can be, and unless there is a physical reason that decoherence selects a particular CSCO and forbids the finite average occupancy of off-diagonal states, quantum superposition requires the provision of D^2 state variables to specify the most general classical state defined by entropy maximization and linear constraint. In thermal or electrical conduction, offdiagonal states include transport currents—one may think of traveling-wave solutions to a Klein-Gordon or Schrödinger equation, respectively—so the mere existence of a classical limit clearly is not a general prohibition against quantum coherence of this kind. Thus, the usual assumption of "local equilibrium" in phenomenological approaches to NESM $\lceil 8 \rceil$ $\lceil 8 \rceil$ $\lceil 8 \rceil$ is needlessly restrictive, and the von Neumann entropy (6) (6) (6) provides the foundation for a kinematically natural generalization.

To go beyond kinematics requires specification of dynamical quantities such as the Hamiltonian and whatever (nonunitary) conservation laws are respected by dissipative interactions. Together these couple the currents in n to its charges, and to asymmetries in the boundary conditions. Because elements of unitary evolution from the Hamiltonian may be expressed, beyond those implicit in simple flux conservation laws, the entropy maximization problem for systems which are *not* in local equilibrium may not decompose simply into an equilibrium MaxEnt problem and a MaxEP problem for currents.

For locally nonequilibrium systems, currents are spontaneously generated by the Hamiltonian whenever it does not commute with asymmetries in the boundary conditions. For the free oscillator, the raising and lowering operators transform under a time translation by *t* as $a^{\dagger} \rightarrow a^{\dagger} e^{-iEt}$, $a \rightarrow e^{iEt}a$, where E is now a $D \times D$ Hermitian matrix and the Hamiltonian is $\hat{H} = Tr[E\hat{n}]$. Therefore *n* transforms as *n* →*eiEtne*−*iEt*. Hamiltonian evolution generates a particular fiber of unitary transformations respecting the kinematics of the state space.

If the eigenbasis of the Hamiltonian is used to define the diagonal of *n*—and the CSCO which is the basis for the usual equilibrium classical statistical ensemble—then the imaginary, antisymmetric components of *n* change sign under time reversal, and correspond to classical currents. The symmetric, real off-diagonal components are time-reversal invariant observables (charges), which may couple to asymmetric thermodynamic potentials on the system boundary $\lceil 18 \rceil$ $\lceil 18 \rceil$ $\lceil 18 \rceil$.

The dual, Hermitian intensive state variable to *n* under *S*,

$$
\Lambda = \frac{\delta S}{\delta n} = \ln(I + n^{-1}),\tag{7}
$$

now has both diagonal and off-diagonal components, and an antisymmetric part which is purely imaginary. Driven ensembles are *defined* as those for which $[E, \Lambda] \neq 0$. Equation ([7](#page-5-1)) is the general form of the classical *equation of state*, and the components of Λ are the generalization of the inverse temperature, pressure, or chemical potentials of equilibrium. Thus, for instance, these could be taken to define the local nonequilibrium approximation in a path-entropy ensemble $[21]$ $[21]$ $[21]$.)

In general, extensive quantities such as energy or particle number have dimensions, and the entropy may be taken as dimensionless, in which case the intensive state variables will have opposite dimensions to their extensive duals. The off-diagonal components in a matrix-valued gradient such as Eq. ([7](#page-5-1)) will then have dimensions that are superpositions of those of the equilibrium intensive state variables, and the dissipative structure constants of the system will determine how many of the D^2 independent boundary conditions can be specified consistently with complete description by the en-tropy ([6](#page-5-0)). The Legendre dual to *S*,

$$
Tr[\Lambda n(\Lambda)] - S[n(\Lambda)] = -\ln Z(\Lambda),\tag{8}
$$

is the generalization of β times the equilibrium Helmholtz free energy, and minus the logarithm of the *D*-particle partition function Z . Equation (8) (8) (8) establishes the off-diagonal components of the matrix Λ as the asymmetric boundary conditions that couple to both nonstationary charges and currents. An entire dual structure follows from these currentdependent entropies $[18]$ $[18]$ $[18]$, with the same form as the dual structure of equilibrium, but with the further ability to couple internal currents to nonequilibrium boundary conditions.

B. Maximum-entropy ensembles, unitary evolution, and dissipation

The unitary transformation law $n \rightarrow e^{iEt}ne^{-iEt}$ for *n* allows us to see how classical currents and charges are coupled by the Hamiltonian, but the status of the von Neumann entropy (6) (6) (6) as a most-general form is better clarified when we introduce dissipation.

To do this, we observe $[18]$ $[18]$ $[18]$ that the entropy (6) (6) (6) can also be derived as the state function that results from maximizing the quantum entropy $-Tr(\rho \ln \rho)$ of a density matrix ρ subject to a constraint on $Tr(\hat{n}\rho)$, which generalizes the diagonal matrix of equilibrium to respect the kinematic symmetries. Appendix A defines the overcomplete basis of coherent states for *D*-independent quantum oscillators, in terms of which the entropy-maximizing Gaussian ensembles have the form

$$
\rho = \int d\xi^{\dagger} d\xi \, \text{Det}\left(\frac{K}{\pi}\right) e^{-\xi^{\dagger} K \xi} |\xi\rangle\langle\xi^{\dagger}|. \tag{9}
$$

 $|\xi\rangle$ are the coherent states with vector arguments $\xi = [\xi^{\mu}],$ and *K* is the matrix inverse of *n* as follows:

$$
n \equiv \text{Tr}(\rho \hat{n}) = \langle \xi \xi^{\dagger} \rangle = K^{-1}.
$$
 (10)

[The angle brackets in Eq. (10) (10) (10) stand for expectation in the Gaussian integral that results from tracing Eq. ([9](#page-6-1)).] The coherent state $|\xi\rangle$ is an eigenstate of the lowering operator *a* with eigenvalue ξ , while $\langle \xi^{\dagger} |$ is the eigenstate of a^{\dagger} with eigenvalue ξ^{\dagger} . Thus the action by *a* on the left of ρ results in the insertion of field ξ , while action on the right by a^{\dagger} results in insertion of ξ^{\dagger} . In general, these coherent states no longer factor over any single CSCO, and the basis in which any given $|\xi\rangle$ does diagonalize is not generally preserved in time.

Reference $[18]$ $[18]$ $[18]$ shows that the class (9) (9) (9) of density matrices is preserved under the Fokker-Planck operator equation

$$
\frac{\partial \rho}{\partial t} = iE_{\mu}^{\nu}[a_{\nu}^{\dagger}a^{\mu}, \rho]
$$

$$
+ (r + rn_R)_{\mu}^{\nu}\left(a^{\mu}\rho a_{\nu}^{\dagger} - \frac{1}{2}\{a_{\nu}^{\dagger}a^{\mu}, \rho\}\right)
$$

$$
+ (rn_R)_{\mu}^{\nu}\left(a_{\nu}^{\dagger}\rho a^{\mu} - \frac{1}{2}\{a^{\mu}a_{\nu}^{\dagger}, \rho\}\right), \tag{11}
$$

which is well known from quantum optics $\left[40\right]$ $\left[40\right]$ $\left[40\right]$ to result from treatment of decoherent system-reservoir interactions in the Born approximation. Equation ([11](#page-6-1)) incorporates all tracepreserving bilinear terms in a and a^{\dagger} , and is therefore the lowest-order effective theory for a dissipatively evolving density matrix. When the set of all such Fokker-Planck equations is considered (over all E , r , and rn_R), the complete space of classical equations consistent with the kinematic symmetries of the entropy (6) (6) (6) is covered.

The Fokker-Planck equation is more transparently understood through its effect on the classical number matrix (again, exact),

$$
\frac{dn}{dt} = i[E,n] + rn_R - \left\{\frac{r}{2},n\right\},\tag{12}
$$

the most general linear evolution equation for n , in which rn_R is an external source matrix and r is the dissipation ma-trix to the reservoir. Equation ([12](#page-6-2)) is the *equation of motion* which, together with the equation of state (7) (7) (7) , completely defines the mechanics and thermodynamics of the classical state variables. If rn_R is derived from some average of particle numbers over neighboring sites in a spatial topology, the last two terms in Eq. (11) (11) (11) lead, through the density matrices ([9](#page-6-1)), to the universality class of Fourier's or Ohm's laws for particle diffusion.

To go beyond the expression (6) (6) (6) for entropy, and the classical evolution equation (12) (12) (12) for particle number, it is necessary to represent the time dependence and fluctuations result-

FIG. 1. Hamiltonian evolution of the bra and ket states in the density matrix ([9](#page-6-1)). The open circle represents the field variables ξ and ξ^{\dagger} , and the closed circles represent new fields added to produce the time legs of the *S* matrix. The indexing scheme with values $\pm n$ is defined following Eq. $(B7)$ $(B7)$ $(B7)$ in Appendix B. Fields on the upper (ket) leg evolve "forward" in time and are denoted ξ_n , ξ_n^{\dagger} , and fields on the lower (bra) leg evolve backward in time and are denoted $\xi_{-n}, \xi_{-n}^{\dagger}.$

ing from the Fokker-Planck equation (11) (11) (11) , and this is the domain of the SK and DP constructions. Here we sketch only topological features of these time-dependent theories, and return to their quantitative representation in the next section.

Hamiltonian evolution of the states $|\xi\rangle$ and $\langle \xi^{\dagger}|$ whose outer product is the basis for the density matrix ([9](#page-6-1)) yields the forward and backward legs of the time loop, shown in Fig. [1.](#page-6-3) The ket state evolves forward in time, the bra state effectively evolves backward in time, and under unitary evolution the two are not coupled. The SK construction, whose details are developed in Appendix B but are not needed here, creates a functional integral over (complex vector-valued) histories by inserting coherent states $|\xi_n\rangle$, $\langle \xi_{-n}^{\dagger}|$ and their Hermitian conjugates at intervals *dt* along the Hamiltonian quadrature of the states $|\xi\rangle$ and $\langle \xi^{\dagger}|$. It is in terms of the new *n*-indexed fields that time-dependent correlations are then evaluated.

Dissipation has the same effect as interleaving Hamiltonian evolution with a partial "trace" over the time-evolved density matrix, thus coupling fields on the forward and backward time lines. Figure [2](#page-7-0) shows the topological relations created by the three structural matrices in Eq. (11) (11) (11) . Hamiltonian evolution *(iE)* couples ξ and ξ^{\dagger} fields only along the time lines, dissipation (r) couples the forward to the backward leg, and the source term rn_R creates couplings both ways.

We thus see part of the relation between the time-loop structure of the SK construction and the time-linear structure of the MSR classical theory, to which we return in Sec. IV. Dissipation makes a trellis work of the time loop, with the asymmetry between particle source and sink creating the unidirectional time evolution of the MSR description. The causal structure of this trellis work is revealed by the Keldysh rotation, but that is not conveniently treated in the discrete representation, so we return to it only in the continuum limit.) Before making the explicit map, however, we turn to the general form of the MSR operators induced by kinematic symmetry, in the next section.

III. QUANTUM AND CLASSICAL NUMBER OPERATORS

Section II argued that the symmetry group of superpositions in a quantum system admits—and in the most general case requires—a $D \times D$ Hermitian matrix *n* of classical state

FIG. 2. Couplings of fields created by the three structural ma-trices in Eq. ([11](#page-6-1)). The dots denote fields ξ and ξ^{\dagger} at indices $\pm n$ on the forward or backward time legs of Fig. [1.](#page-6-3) The arrows denote couplings of dyads $\xi \xi^{\dagger}$, with the arrow proceeding from the position of ξ to that of ξ^{\dagger} . (a) Hamiltonian evolution with coupling *iE* respects the time lines. (b) Dissipative particle loss with matrix *r* rescales fields within time lines and couples the forward to the backward leg. (c) Dissipative particle addition from source term rn_R rescales fields within the time lines, and creates bidirectional couplings across the lines.

variables as the most general set of linear constraints that can be independently imposed on a maximum-entropy ensemble for *D* independent harmonic oscillators. We may thus anticipate that the lowering operator in the Doi theory will be a $D \times D$ matrix *A*, and that both it and its dual A^{\dagger} will transform (in the Heisenberg picture) as $e^{iEt}Ae^{-iEt}$, and $e^{iEt}A^{\dagger}e^{-iEt}$. The details and justification for the full DP construction are provided in Appendix C, with only a few results presented in this section.

Whereas, for the usual classical *D*-dimensional Markov process the Doi number states $|\vec{m}|$ would be indexed by vectors of occupation numbers \vec{m} , here, in order to respect the

unitary symmetry of the kinematics they must have $D \times D$ matrix arguments $|m\rangle$, and will be eigenstates of the number operator

$$
A^{\dagger} A | m) = m | m). \tag{13}
$$

Note that Doi number states have round brackets to distinguish them from quantum states with angular brackets.) The quantum density matrix ρ , which takes the place of a classical probability distribution, will be mapped to a state vector $|\Psi\rangle$ which, as for the case of the Markov chain, is the algebraic representation of the generating function of ρ . $|\Psi\rangle$ will therefore evolve linearly in time under the algebraic representation of the Liouville operator for the generating function.

Because the trace of the density matrix is the evaluation of its generating function at the identity argument, the appropriate inner product for the classical two-field construction is taken against the Glauber state $(0|e^{Tr[A]}$. Because this state is normalized against all states $|m$, both of the expectations

$$
(0|e^{\text{Tr}[A]}A^{\dagger}A|\Psi) = (0|e^{\text{Tr}[A]}A|\Psi) = n,\tag{14}
$$

as do an infinite number of other expectations that differ by powers of A^{\dagger} . Under the Peliti insertion (in Appendix C) of coherent states on the basis of eigenstates $|m$, the coherentstate mean field ζ will replace A, and its conjugate ζ^{\dagger} will replace *A*† , in a path integral of MSR form. These fieldoperator maps $A \leftrightarrow \zeta$, $A^{\dagger} \leftrightarrow \zeta^{\dagger}$ are the classical counterpart to the maps $a \leftrightarrow \xi$, $a^{\dagger} \leftrightarrow \xi^{\dagger}$ in the quantum domain.

One question we wish to address, then, is, given that *A* has both the Heisenberg transformation law and the expectation of the dyadic $\xi \xi^{\dagger}$, what is the role of the field A^{\dagger} and of the matrix product in Eq. (14) (14) (14) ? A second, related question is to what extent linear time evolution of $|\Psi\rangle$ can capture the trellislike structure of the time loop in the underlying quantum theory. The second question is equivalent to asking how the very different norms

$$
(0|e^{\text{Tr}[A]}A^{\dagger}A|\Psi) = \int d\xi^{\dagger}d\xi \,\text{Det}\left(\frac{K}{\pi}\right)e^{-\xi^{\dagger}K\xi}\langle\xi^{\dagger}|a^{\dagger}a|\xi\rangle\tag{15}
$$

can be understood to represent the same quantity, and how these mean values are extended to the Green's functions of the classical and quantum theories.

The outcome of the DP construction will be that the field ζ indeed has the expectation of the quantum correlation $\xi \xi^{\dagger}$, and a stationary-point condition corresponding to the equa-tion of motion ([12](#page-6-2)). More important, differently ordered products of ζ and ζ^{\dagger} will have the effect of introducing the quantum number operator at different positions in the time loop. A nonintuitive result is that the bilinear Fokker-Planck equation ([11](#page-6-1)) requires a nonlinear Liouville equation (with both linear and cubic terms), to respect the fluctuationdissipation theorem.

A. Generating function and Liouville operator

As the Doi operator formalism is simply an algebraic representation of a generating function, there is no surprise that it goes through for matrix-valued sources as well as for classical vector-valued sources. Because the logarithms of the classical state variable repeatedly arise at intermediate stages of the calculation, it is indeed more convenient to work with a conventional complex-valued generating function at first, and to convert to the algebraic form later, as we do in Appendix C. A complex-valued $D \times D$ source field *z*, which will correspond to the Doi raising operator *A*† , is traced against the quantum number operator. For technical reasons, the actual source is the matrix logarithm ln *z*, and the generating function is defined as

$$
\Psi(z) \equiv \text{Tr}[e^{a^{\dagger} (\ln z)a} \rho]. \tag{16}
$$

The Doi lowering operator *A* is then the derivative $\partial/\partial z$.

Insertions of the number operator $a^{\dagger}a$ into Ψ are produced by the derivative $\partial/\ln \partial z \sim z \partial/\partial z$. However, when correlations are considered between number operators at different times, the distinct matrix orderings possible between *z* and $\partial/\partial z$ distinguish among different insertions of *a* and a^{\dagger} on the left and right of the density matrix in Eq. (16) (16) (16) . Both orderings are required to produce the complete set of phase-advance and trace-preserving terms in Eq. ([11](#page-6-1)).

Appendix A provides the systematic construction of the Liouville operator under which the density (16) (16) (16) evolves. The particular difficulty of producing the antinormal ordered operators which couple to rn_R is most easily solved by using a pair of generating functions [Eq. ([A13](#page-14-0)) in Appendix A] in which the order of *a* and a^{\dagger} in the exponential of Eq. ([16](#page-8-0)) is reversed, and the transformation between these leads to the linear and cubic terms in the Liouville equation. The result is that Ψ evolves under the differential equation

$$
\frac{\partial \Psi}{\partial t} = \left\{ \text{Tr}[rn_R \epsilon] + \text{Tr} \left[\left(-i[E, \epsilon] + \epsilon rn_R \epsilon - \left\{ \frac{r}{2}, \epsilon \right\} \right) \frac{\partial}{\partial \epsilon} \right] \right\} \Psi
$$

$$
= -\mathcal{L}\Psi,
$$
 (17)

in which $\epsilon \equiv z - I$. Under the Doi algebraic representation $\Psi(z) \rightarrow |\Psi\rangle$ and $\partial/\partial \epsilon \rightarrow A$, while $\epsilon \rightarrow A^{\dagger} - I$. Under the Peliti insertion of (matrix-valued) coherent states, the operator *A* is replaced by the observable field ζ , and A^{\dagger} by the conjugate response field ζ^{\dagger} .

B. Correspondence of time-local operators

We may now observe how the combination of matrix ordering and time-linear evolution in the DP formalism "weaves" the trellis-work of the dissipative time loop in Fig. [2.](#page-7-0) The result of the full DP conversion of the Liouville equation (17) (17) (17) into a field integral is that, between time steps *n*−1 and *n*,

$$
\frac{\partial}{\partial \epsilon} = \frac{\partial}{\partial z} \to \zeta_{n-1},
$$

$$
\epsilon + I = z \to \zeta_n^{\dagger}.
$$
 (18)

In turn, the quantum operators traced together with *iE*, *r*, or rn_R in Eq. ([11](#page-6-1)) map to the field dyadics shown in the respective panels of Fig. [2.](#page-7-0)

A direct comparison of the terms in the Fokker-Planck equation (11) (11) (11) and the Liouville equation (17) (17) (17) coupled, respectively, to $iE+r/2$, $iE-r/2$, *r*, and rn_R , then gives the time-local operator correspondences

$$
\zeta_n^{\dagger} \zeta_{n-1} \leftrightarrow \xi_{-n} \xi_{-(n-1)}^{\dagger},
$$

\n
$$
\zeta_{n-1} \zeta_n^{\dagger} \leftrightarrow \xi_{n-1} \xi_n^{\dagger},
$$

\n
$$
\zeta_{n-1} \leftrightarrow \xi_{n-1} \xi_{-(n-1)}^{\dagger},
$$

\n
$$
\zeta_n^{\dagger} + \zeta_n^{\dagger} \zeta_{n-1} \zeta_n^{\dagger} \leftrightarrow \xi_{-n} \xi_n^{\dagger}.
$$
 (19)

The first three field products correspond, respectively, to the insertions $\rho a^{\dagger}a$, $a^{\dagger}a\rho$, and $a\rho a^{\dagger}$ (acting on ρ at time step *n* -1), and their expectations are accordingly *n* (at time step *n*−1), obtained from the density-matrix trace. The last field product corresponds to the insertion $a^{\dagger} \rho a$, and therefore has expectation *n*+*I*.

In this way, the matrix products in the MSR field theory are capable of generating *all* of the distinct bilinear insertions of *a* and a^{\dagger} in Ψ at a single time. However, the fact that the Fokker-Planck equation ([11](#page-6-1)) depends *only* on these contemporaneous bilinear insertions is what allows the classical equation of motion (12) (12) (12) to depend only on *n*, and the corresponding MSR field theory to make no explicit reference to underlying quantum correlations, except through the equations of motion. What we cannot do in the classical theory is insert arbitrary products of a and a^{\dagger} at different times; we can at most sample correlations of bilinear combinations at different times.

IV. CORRELATIONS AND CAUSAL STRUCTURE

We have thus resolved the puzzle of the time structure of local operator products in the quantum and classical representations of these maximum-entropy ensembles. The other feature that has been raised as a point of correspondence between quantum SK theories and classical DP theories is the isomorphic representation of causality of their Green's functions $[26]$ $[26]$ $[26]$. If there exists a mapping between matrix products of classical fields ζ and ζ^{\dagger} and products of their time-loop antecedents ξ and ξ^{\dagger} , to what extent is this mapping also the basis of the similar tridiagonal Green's functions of the classical MSR and quantum Keldysh fields? We will see that, while the Green's functions of corresponding classical and time-loop operators necessarily coincide, the coincidence does not arise from the products of Keldysh operators that one would naïvely guess on the basis of the causal structure.

A. Continuum limit, Keldysh rotation, and causal structure on the time loop

The result of the SK construction in Appendix B is the representation of the trace of the time-evolved density matrix, from initial condition ρ of Eq. ([9](#page-6-1)), as the path integral

$$
1 = \frac{1}{Z} \int_0^T D\xi^{\dagger} \mathcal{D}\xi e^{-F}.
$$
 (20)

The measure is the limit of the discrete skeletonization

$$
\mathcal{D}\xi^{\dagger}\mathcal{D}\xi \equiv \int \frac{d\xi_1^{\dagger}d\xi_1}{\pi^D} \dots \int \frac{d\xi_{2N}^{\dagger}d\xi_{2N}}{\pi^D},\tag{21}
$$

in which we originally label the points along a time loop with index $n \in 0, ..., 2N$ [see Eq. ([B4](#page-16-1))], before using the fact that time extends only from 0 to $T = N \delta t$ to convert indices on the backward legs to −*n* as in the preceding figures. The path integral is the inverse of the partition function

$$
Z = \text{Det}(I + K^{-1}),\tag{22}
$$

with *K* defined from ρ by Eq. ([9](#page-6-1)).

Allowing *E*, *r*, and rn_R to be functions of the time index n , and interleaving coherent-state insertions with the operator evolution (11) (11) (11) , the time-loop "action" *F* in Eq. (20) (20) (20) evaluates to

$$
F[E,r,rn_R] = \xi_1^{\dagger} e^{(iE + r/2 + rn_R)_1 \delta t} (I - p) \xi_0
$$

+
$$
\sum_{n=1}^{N} \xi_n^{\dagger} \left[\xi_n - \xi_{n-1} - \left(iE - \frac{r}{2} - rn_R \right)_{n} \delta t \xi_{n-1} \right]
$$

+
$$
\xi_{-(n-1)}^{\dagger} \left[\xi_{-(n-1)} - \xi_{-n} + \left(iE + \frac{r}{2} + rn_R \right)_{n} \delta t \xi_{-n} \right]
$$

-
$$
\xi_{-(n-1)}^{\dagger} (r + rn_R)_n \delta t \xi_{n-1} - \xi_n^{\dagger} (rn_R)_n \delta t \xi_{-n}
$$

+
$$
Tr[(rn_R)_n] \delta t.
$$
 (23)

As in the diagram of Fig. [2,](#page-7-0) all time-loop fields are coupled, and the causal structure is not apparent.

The Keldysh rotation on the discrete indexing is defined as

$$
\begin{bmatrix} \phi_n \\ \psi_n \end{bmatrix} = \begin{bmatrix} I/2 & I/2 \\ -I & I \end{bmatrix} \begin{bmatrix} \xi_n \\ \xi_{-n} \end{bmatrix},
$$
(24)

in which ϕ_n is referred to as the *classical* component and ψ_n as the *quantum component*. In passing to the continuum limit, the time index $n \rightarrow t \equiv n \delta t$, and both time-loop and Keldysh fields are simply reindexed $\xi_n \rightarrow \xi_t$, etc. (that is, they are homogeneous of order zero in δt). Then the time-loop action (after taking care with the prescription for evaluating equal-time products of fields) becomes

$$
F \to \xi_{\delta t}^{\dagger} (I - p)\xi_0 + \int_0^T dt \left\{ \left[\xi_t^{\dagger} \xi_{-t}^{\dagger} \right] \left[\begin{array}{cc} \partial_t - iE + r/2 + rn_R & -rn_R \\ -\left(r + rn_R \right) & -\partial_t + iE + r/2 + rn_R \end{array} \right] \left[\begin{array}{c} \xi_t \\ \xi_{-t} \end{array} \right] - \text{Tr} \left[\frac{r}{2} \right] \right\},\tag{25}
$$

and its counterpart in the Keldysh fields becomes

$$
F \rightarrow \left(\phi_{\delta t}^{\dagger} - \frac{1}{2}\psi_{\delta t}^{\dagger}\right)(I - p)\left(\phi_0 + \frac{1}{2}\psi_0\right) + \int_0^T dt \left\{ \left[\phi^{\dagger} \psi^{\dagger}\right] \left[\right. \\ \left. - \partial_t + iE - r/2 \right. \\ \left. - \left(\rho_0 + iE + r/2\right) \right] \left[\phi \right] - \text{Tr}\left[\frac{r}{2}\right] \right\}.
$$
 (26)

The surface terms are marked with indices $\delta t \rightarrow 0$ to resolve operator ordering in the initial conditions for the action, and p is defined relative to K in Appendix B (it is the generalization of a Boltzmann factor). The tridiagonal structure is now apparent in Eq. ([26](#page-9-1)), with no self-interaction of the classical fields ϕ , ϕ^{\dagger} . The time index has also been dropped, as it is no longer needed to distinguish forward from backward time-loop fields.

If the action (26) (26) (26) is written as a bilinear form in fields $[\phi^{\dagger} \psi^{\dagger}]_t$ and their conjugates at time *t'*, the kernel has the form

$$
\delta(t - t') \left[-\partial_{t'} + iE - r/2 - (rn_R + r/2) \right]
$$

=
$$
\left[\left[D^A \right]^{-1} \left[D^{-1} \right]^{K} \right]_{t, t'}
$$
, (27)

while that of the Green's function which is its inverse is then

$$
\left\langle \begin{bmatrix} \phi_t \\ \psi_t \end{bmatrix} [\phi_{t'}^\dagger \ \psi_{t'}^\dagger] \right\rangle = \begin{bmatrix} D^K & D^R \\ D^A & \end{bmatrix}_{t,t'}.
$$
 (28)

In the case that one can write

$$
[D^{-1}]^K = M[D^A]^{-1} - [D^R]^{-1}M \tag{29}
$$

for some matrix M , matrix inversion then implies $[26]$ $[26]$ $[26]$ that the Keldysh Green's function must have the form

$$
D^K = MD^A - D^R M. \tag{30}
$$

For the kernel ([27](#page-9-2)), in which all of $[D^A]^{-1}$, $[D^R]^{-1}$, and $[D^{-1}]^K$ are time local, we may choose $M_{t,t'} = (K^{-1} + I/2)_t$ $\times \delta(t-t')$, for which Eq. ([29](#page-9-3)) translates to

$$
rn_R = \partial_t K^{-1} - [iE, K^{-1}] + \left\{ \frac{r}{2}, K^{-1} \right\}
$$
 (31)

at each time, recovering the equation of motion (12) (12) (12) through the identification (10) (10) (10) .

Restricting to the case *E*, *r* constant to simplify the notation for the purpose of illustrating the structure, the *A*dvanced and *R*etarded response Green's functions are readily evaluated to

$$
D_{t,t'}^{A} = e^{-(iE+r/2)(t'-t)} \theta(t'-t),
$$

\n
$$
D_{t,t'}^{R} = -e^{(iE-r/2)(t-t')} \theta(t-t').
$$
\n(32)

To evaluate the Keldysh correlation function, we note that Eq. (31) (31) (31) is solved by

$$
K_t^{-1} = e^{(iE - r/2)t} \mathcal{K}_t^{-1} e^{-(iE + r/2)t},
$$
\n(33)

in which

$$
\mathcal{K}_t^{-1} \equiv K^{-1} + \int_0^t dt' e^{-(iE_S - r/2)t'} (r n_R)_t' e^{(iE_S + r/2)t'} \qquad (34)
$$

is expressed in terms of initial value K^{-1} from Eq. ([9](#page-6-1)) and the (optionally time-dependent) source rn_R .

Then in terms of the same K_t^{-1} , the Keldysh correlator is

$$
D_{t,t'}^{K} = e^{(iE-r/2)t} [\theta(t-t')\mathcal{K}_{t'}^{-1} + \theta(t'-t)\mathcal{K}_{t}^{-1}]e^{-(iE+r/2)t'} + \frac{1}{2}(D_{t,t'}^{A} - D_{t,t'}^{R}).
$$
\n(35)

At equal times,

$$
D_{t,t}^{K} = e^{(iE - r/2)t} \mathcal{K}_t^{-1} e^{-(iE + r/2)t} + \frac{I}{2} = K_t^{-1} + \frac{I}{2}
$$
 (36)

generalizes the free correlator $(B14)$ $(B14)$ $(B14)$ of Appendix B to the dissipative equation of motion (31) (31) (31) for K^{-1} .

B. Fluctuation-dissipation theorem

We note the forms of the advanced and retarded Greens functions ([32](#page-10-0)) in order to point out that the classical equation of motion ([31](#page-9-4)), slightly rearranged, becomes

$$
\partial_t K_t^{-1} + \left(\frac{r}{2} - iE\right) K_t^{-1} + K_t^{-1} \left(\frac{r}{2} + iE\right) = rn_R,\tag{37}
$$

the standard solution for the covariance matrix (K^{-1}) of a linear Fokker-Planck equation $[[44]$ $[[44]$ $[[44]$, p. 175, Eq. $(5.166)]$, with source rn_R .

At late times $rt \rightarrow \infty$, memory of the initial condition is erased, and the correlator goes to

$$
K_t^{-1} \to \int_0^\infty du \ e^{-(r/2 - iE)u} (r n_R)_{t-u} e^{-(r/2 + iE)u}.\tag{38}
$$

 rn_R is now seen to play the role of a diffusion matrix in the Fokker-Planck equation, a point also manifest in the Glauber-Sudarshan "P representation" in Eq. (8) of Ref. [[18](#page-23-4)]. This diffusivity serves as the kernel of the equivalent Onsager-Machlup form of the time-loop action, derived by integration over half of the time-loop fields to yield Eq. ([B28](#page-19-0)) in the Appendix B. The covariance function (K^{-1}) is expressed through the response functions (32) (32) (32) in terms of the

diffusivity (rn_R) in Eq. ([38](#page-10-1)), in the generalization of the standard fluctuation-dissipation theorem $[[44]$ $[[44]$ $[[44]$, p. 179, Eq. (5.184)] to a time-dependent source.

C. Classical continuum limit and MSR representation

Classical state variables for a driven MSR field theory, like their equilibrium counterparts, are the complete constraints sufficient to specify the entropy, and minimum sufficient statistics for the nonstochastic components of correlation functions. Thus their mean field values equal the nonstochastic components of the Green's functions in the Keldysh description. The generalization of the DP construction to arrive at MSR form, performed in Appendix C, is by quadrature of the Liouville equation (17) (17) (17) , interleaved with insertions of coherent-state representations of unity, to introduce fields ζ_n , ζ_n^{\dagger} at a set of indices $n \in 0, ..., N$, and so times $t \in 0, \ldots, N \delta t$.

In the continuum limit, the generating function (16) (16) (16) , evolved to time *T*, is represented by the path integral

$$
\Psi_T(z) = \int_0^T D\zeta^{\dagger} D\zeta e^{(z-\zeta_T^{\dagger})\zeta_T + \int_0^T dt L_t} \Psi_0(\zeta_0^{\dagger}),
$$
\n(39)

in which the measure

$$
\int_0^T \mathcal{D}\zeta^{\dagger} \mathcal{D}\zeta \leftarrow \prod_{n=0}^N \int \frac{D\zeta_n^{\dagger} D\zeta_n}{\mathrm{Det}(\pi)},
$$
\n(40)

and again $T=N\delta t$ is held fixed as $\delta t \rightarrow 0$.

The action starts as a sum over the discrete Lagrangian with the form

$$
L_n \delta t \equiv \left(\zeta_n^{\dagger} - \zeta_{n-1}^{\dagger}\right) \zeta_{n-1} - \mathcal{L}_n \left(\zeta_n^{\dagger}, \zeta_{n-1}\right) \delta t, \tag{41}
$$

expressed in terms of the Liouville operator from Eq. ([17](#page-8-1)) [also given in Eq. ([A23](#page-15-0)) of Appendix A] with $z \rightarrow \overline{\zeta_n^{\dagger}}$ and $\partial/\partial z \rightarrow \zeta_{n-1}$,

$$
\mathcal{L}_n(\zeta_n^{\dagger}, \zeta_{n-1}) = \text{Tr}\Bigg[\left(iE + \frac{r}{2} + rn_R \right)_n \zeta_n^{\dagger} \zeta_{n-1} + \left(-iE + \frac{r}{2} + rn_R \right)_n \zeta_{n-1} \zeta_n^{\dagger} - \left(r + rn_R \right)_n \zeta_{n-1} - \left(rn_R \right)_n \left(\zeta_n^{\dagger} + \zeta_n^{\dagger} \zeta_{n-1} \zeta_n^{\dagger} \right) + \left(rn_R \right)_n \Bigg]. \tag{42}
$$

A direct comparison of the discrete classical Lagrangian ([42](#page-10-2)) to its quantum counterpart ([23](#page-9-5)) recovers the operator corre-spondences ([19](#page-8-2)) derived previously from the Fokker-Planck and Liouville operators.

Fields ζ and ζ^{\dagger} , as well as the Lagrangian *L*, are again homogeneous of order zero in δt , so the labels $n \rightarrow t \equiv n \delta t$ in the continuum limit, producing

$$
L_t \to \partial_t \zeta_t^\dagger \cdot \zeta_t - \mathcal{L}_t(\zeta_t^\dagger, \zeta_t), \tag{43}
$$

with \mathcal{L}_t defined from Eq. ([42](#page-10-2)), so that now ζ_t^{\dagger} substitutes for *z*, and ζ_t for $\partial/\partial z$ in $\mathcal L$ of Eq. ([17](#page-8-1)).

The trace of the time-evolved generating function Ψ_T \equiv 1 is Eq. ([39](#page-10-3)) evaluated at argument *z*=*I*. The path integral

is conveniently approximated by shifting the response field to $\zeta_n^{\dagger} \to \widetilde{\zeta}_{n-\zeta}^{\dagger} = \zeta_1^{\dagger} - I$, equivalent to the usual convention of commuting $e^{Tr[A]}$ to the right through all insertions in the operator Doi formalism. The result is that

$$
1 = \Psi_T(I) = \int_0^T \mathcal{D}\tilde{\zeta}^{\dagger} \mathcal{D}\zeta e^{-\tilde{\zeta}_T^{\dagger} \zeta_T + \int_0^T dt L_t - \text{Tr}\ln[I - K_0^{-1} \tilde{\zeta}_0^{\dagger}]}.
$$
 (44)

Now $\tilde{\zeta}_t^{\dagger}$ substitutes directly for ϵ , and ζ_t for $\partial/\partial \epsilon$ in $\mathcal L$ of Eq. $(17).$ $(17).$ $(17).$

The main point of interest in Eq. (44) (44) (44) —and the motivation for generalizing the DP construction to noncommuting observables—is that the initial generating function $\Psi_0(\zeta_0^{\dagger})$ takes the place of the usual Poisson distribution $\left[32\right]$ $\left[32\right]$ $\left[32\right]$ as the initial condition for the functional integral. At argument $\tilde{\zeta}_0^+$ =−*I* this is the initial partition function ([22](#page-9-6)). More generally, the trace log which appears as a boundary term in the action is responsible for correctly propagating the nonequilibrium von Neumann entropy ([6](#page-5-0)) dynamically.

The Green's functions which were inconveniently evaluated through the matrix inversion ansatz (29) (29) (29) are here obtained directly from the stationary-point conditions of the classical action,

$$
\partial_t \tilde{\zeta}^{\dagger} = [iE, \tilde{\zeta}^{\dagger}] + \left\{ \frac{r}{2}, \tilde{\zeta}^{\dagger} \right\} - \tilde{\zeta}^{\dagger} (rn_R), \tilde{\zeta}^{\dagger},
$$

$$
\partial_t \zeta = [iE, \zeta] - \left\{ \frac{r}{2}, \zeta \right\} + (rn_R) + (rn_R) \tilde{\zeta}^{\dagger} \zeta + \zeta \tilde{\zeta}^{\dagger} (rn_R).
$$
(45)

Stationary $\tilde{\zeta}^{\dagger}$ solves exactly the evolution equation for a kernel *K*, though its classical value is $\tilde{\zeta}^{\dagger} \equiv 0$, $\forall t$, and it evolves "backward" in time. Meanwhile, ζ evolves forward in time and solves the evolution equation (31) (31) (31) for K^{-1} , perturbed by an additive noise field whose classical expectation is zero. This latter equation is the Langevin equation for the classical fields whose expectations are the state variables of the nonequilibrium theory, and the combinations $(rn_R)\tilde{\zeta}^{\dagger}\zeta$ and $\zeta \tilde{\zeta}^{\dagger}(m_R)$ define the correct form for the Langevin field. Note that the presence of the linear term in the Liouville operator (17) (17) (17) is necessary for the stationary condition (45) (45) (45) to capture the evolution ([37](#page-10-4)) of the covariance matrix at $\tilde{\zeta}^{\dagger} = 0$, which we said is one expression of the fluctuation-dissipation theorem.

If we subtract the stationary part from L_t (and drop the subscripts t), we are left with a Lagrangian for zero-mean fluctuations, which may be called \tilde{L} , and which evaluates to

$$
\widetilde{L} = \partial_t \widetilde{\xi}^\dagger \cdot \widetilde{\zeta} - \operatorname{Tr} \left[\widetilde{\xi} \left(iE + \frac{r}{2} \right) \widetilde{\xi}^\dagger - \widetilde{\xi}^\dagger \left(iE - \frac{r}{2} \right) \widetilde{\zeta}
$$

$$
- (r n_R) \widetilde{\xi}^\dagger K_l^{-1} \widetilde{\xi}^\dagger - (r n_R) \widetilde{\xi}^\dagger \widetilde{\xi} \widetilde{\xi}^\dagger \right], \tag{46}
$$

in which $\widetilde{\zeta}_t = \zeta_t - K_t^{-1}$ and K_t^{-1} stands for the time-dependent stationary value of ζ_t .

The MSR homologue to the Keldysh causal structure is now expressed by the action (46) (46) (46) , through the lack of a $\tilde{\zeta}^2$ interaction, but with an interesting twist. As in the operator correspondence ([19](#page-8-2)), matrix field ordering matters to the interpretation of the causal roles of fields. The kernel in Eq. ([46](#page-11-1)) can be formally cast in tridiagonal form, by writing the matrix products themselves as an inner product as follows:

$$
\text{Tr}\left\{ \big[\widetilde{\zeta}-\widetilde{\zeta}^\dagger\big]\Bigg[\frac{iE+r/2}{iE-r/2}\ \ \textit{rn}_R\ast\big(K_t^{-1}+\widetilde{\zeta}\big)^\ast\ \bigg]\Bigg[\ \widetilde{\zeta}\ \ \Bigg]\right\},
$$

in which the asterisks stand for the positions of the factors of $\pm \tilde{\zeta}_t^{\dagger}$ in the lower-right trace. Depending on its position in the $\frac{d}{dt}$ in the following through the pointing on the position in the trace, the field $\tilde{\zeta}$ can be homologous to either ϕ^{\dagger} or ϕ , while a sign together with position in the trace causes $-\tilde{\zeta}^{\dagger}$ to be homologous to ψ^{\dagger} , while $\tilde{\zeta}^{\dagger}$ is homologous to ψ . These assignments could also be rationalized, and the signs of the quadratic terms in $\tilde{\zeta}^{\dagger}$ made convergent, by the contour rotation on all components that makes $\tilde{\zeta}^{\dagger}$ an *anti*-Hermitian matrix, so that − *˜*† becomes its Hermitian conjugate.

The MSR response functions respect these homology assignments, with

$$
\langle \widetilde{\zeta}_t^{\dagger} \widetilde{\zeta}_{t'} \rangle = e^{-(iE + r/2)(t'-t)} \theta(t'-t) = D_{t,t'}^A = \langle \psi_t \phi_{t'}^{\dagger} \rangle,
$$

$$
-\langle \widetilde{\zeta}_t \widetilde{\zeta}_t^{\dagger} \rangle = -e^{(iE - r/2)(t-t')} \theta(t-t') = D_{t,t'}^R = \langle \phi_t \psi_{t'}^{\dagger} \rangle. \quad (47)
$$

The discrete evaluation of the Liouville operator in Eq. (42) (42) (42) , and the time-loop Lagrangian (23) (23) (23) , made possible a direct comparison of time-local field products, but did not manifest the Keldysh or MSR causal structure. The discrete equivalent to Eq. (46) (46) (46) in shifted fields,

$$
\mathcal{L}_n(\zeta_n^{\dagger}, \zeta_{n-1}) = \text{Tr}\Bigg[\left(iE + \frac{r}{2} \right)_n \Bigg[\tilde{\zeta}_n^{\dagger} \zeta_{n-1} + \frac{1}{2} (\tilde{\zeta}_n^{\dagger} + \tilde{\zeta}_n^{\dagger} \zeta_{n-1} \tilde{\zeta}_n^{\dagger} + I) \Bigg] - \left(iE - \frac{r}{2} \right)_n \Bigg[\zeta_{n-1} \tilde{\zeta}_n^{\dagger} + \frac{1}{2} (\tilde{\zeta}_n^{\dagger} + \tilde{\zeta}_n^{\dagger} \zeta_{n-1} \tilde{\zeta}_n^{\dagger} + I) \Bigg] - \left(r n_R + \frac{r}{2} \right)_n (\tilde{\zeta}_n^{\dagger} + \tilde{\zeta}_n^{\dagger} \zeta_{n-1} \tilde{\zeta}_n^{\dagger}) - \frac{r_n}{2} \Bigg], \tag{48}
$$

can be compared to the Lagrangian (23) (23) (23) under the discrete Keldysh rotation (24) (24) (24) , which has the block-diagonal form of Eq. (26) (26) (26) and discrete index *n* in all of the "potential" terms those terms that do not become time derivatives in the continuum limit). What we find is that the first term in each of the two square-bracketed expressions in Eq. (48) (48) (48) maps to its Keldysh counterpart, accounting for the response functions (47) (47) (47) . The operators, however, differ, and only the vanishing expectation value of the $\tilde{\zeta}^{\dagger}$ is responsible for the agreement of the free response functions. Higher-order operator products would not preserve the agreement.

From this section we learn, then, what are the trade-offs in passing between the classical and quantum descriptions. In the quantum description, the fields are vectors reflecting the *D* independent excitations in the underlying state space. The path-integral action is bilinear, reflecting the bilinearity of the Fokker-Planck equation and the lowest-order effectivefield character of this class of quantum ensembles. However, the state variables of the theory can only be obtained from the correlation and response functions, and propagation of the entropy through time is not transparent.

In contrast, in the classical description, the fields become $D \times D$ matrices, directly reflecting the structure of the state variables and the classical equation of motion. (These can of course be treated as vectors in the adjoint representation, but the kinematic symmetries are better reflected in the matrix representation.) Furthermore, the equations of motion arise directly from the stationary points of the classical action, and the expression for the initial partition function is explicit as a trace-log surface term in that action. However, the classical action necessarily becomes nonlinear, and the calculation of fluctuations about the mean value becomes correspondingly more complicated. Furthermore, matrix ordering matters to the interpretation of correlation and response functions, albeit in a way that preserves some of the intuition from the Keldysh form.

V. CONCLUSIONS

The main result of this paper is its demonstration of a class of exact *classical* field theories for nonequilibrium driven systems defined from first principles by maximization of an *entropy*. These provide a proof of concept—and a collection of free effective-field theories as starting points for perturbative expansion—showing that the taking of classical limits does not inherently exclude currents from roles equivalent to the roles of charges in the classical entropy state function (6) (6) (6) , in Langevin equations (45) (45) (45) , or in the fluctuation-dissipation theorem (37) (37) (37) . The existence of such a general result does not appear to have been known, and the resulting frequent restriction to the local-equilibrium approximation in NESM since the 1950s has led to widespread use of phenomenological "entropy production" methods in place of any proper first principles of statistical inference in most work on nonequilibrium systems.

The series of papers $[17,18,29,30]$ $[17,18,29,30]$ $[17,18,29,30]$ $[17,18,29,30]$ $[17,18,29,30]$ $[17,18,29,30]$ preceding this one have developed a principled way to generalize thermodynamics away from local equilibrium, complementary to the way path entropies $[21,22]$ $[21,22]$ $[21,22]$ $[21,22]$ provide generalizations with nonlocal nonequilibrium structure. For some cases the two approaches overlap enough that nonlocal histories continue immediately to local constraints $[17]$ $[17]$ $[17]$; in other cases local nonequilibrium can be used to generalize the localequilibrium assumption usually used within a coarse-grained path-entropy framework. The current paper has given more explicit attention to the role of symmetries in defining locally nonequilibrium statistical mechanics than did Refs. $[17,18]$ $[17,18]$ $[17,18]$ $[17,18]$, in order to emphasize the classical, effective-field character of the ensembles presented.

The specification of the systems studied in this paper by symmetry and maximum entropy has also allowed us to study a new class of quantum-classical correspondence principle, without introducing the irrelevant feature of approximation. The quantum Schwinger-Keldysh and classical Martin-Siggia-Rose field theories both provide exact specifications of a common density matrix. They are distinguished by the fact that the action in the quantum formulation reflects the bilinear form of the Fokker-Planck equation, while the classical formulation expands directly in the leading nonstochastic component of the Green's function [Eq. (45) (45) (45)], at the cost of nonlinearity in the action/Liouville operator.

The methods derived in this paper could be applied directly to molecular transition states, extending Eyring's original theory of rate processes $[15]$ $[15]$ $[15]$ to a many-particle statistical theory of chemical reactors. A classical stochastic theory is desirable for chemistry, because most quantum dynamics is rendered decoherent by solvent or other environmental factors. However, the configuration space for the transition state itself is inherently quantum mechanical, arising from superposition of the same delocalized manyelectron wave functions as create the bonding and antibonding orbitals in molecules. The transition-state current which is at the heart of chemical reactions results from the same kind of superposition as the currents in the examples of this paper.

In such a field theory, the spontaneous emergence and stability of reaction currents in response to chemical potential gradients would be derived directly from maximization of an excess entropy, restoring the interpretation that stable states are maximally unordered consistent with their constraints, whether they are equilibrated or dynamic. The absence of such a coherent principle up to now has not been much of a limitation in understanding mass-action kinetics of single chemical reactions, but it has been a serious problem in understanding the stability of larger, more complex reaction networks such as the biosphere as a whole. The notorious observation that living matter is a reduced-entropy state by the equilibrium entropy measure $[45,46]$ $[45,46]$ $[45,46]$ $[45,46]$ has left science with no principle by which to understand why it has been stable over geological time scales. The observation that life mediates "entropy production" in the universe has not filled this gap, both because of the unreliability of phenomenological entropy production rules in general $[21,22]$ $[21,22]$ $[21,22]$ $[21,22]$, and more fundamentally because of the incommensurability of entropies (of the living state) and entropy *rates* (in the evolution of the rest of the universe). The existence of a well-defined entropy for driven chemistry does not, of course, ensure the existence of a similar entropy for biology, but it is at least consistent with a maximum-entropy explanation for the stability of the living state, which the local-equilibrium approximation of chemistry was not.

ACKNOWLEDGMENTS

I wish to thank Insight Venture Partners for support of this work, and Tanmoy Bhattacharya for helpful conversations.

APPENDIX A: DENSITY MATRICES AND GENERATING FUNCTIONS

This and the subsequent appendixes derive the SK and DP field theories corresponding to maximum-entropy-driven quantum ensembles subject to linear constraints. Appendix A defines generating functions and derives their associated Liouville operator. Appendix B is devoted to the time-loop path integral, the Keldysh rotation, and the origin of lowestorder dissipative terms in the Born approximation. Appendix C concerns the conversion of the ordinary complex-valued generating function into the state vectors and generating functionals of the MSR representation.

1. Density matrices with structure in noncommuting observables

The Fock space for *D* independent quantum harmonic oscillators is generated from a ground (ket) state $|0\rangle$ by the action of *D* orthogonal raising and lowering operators. The operator commutation relations $[a^{\mu}, a^{\dagger}_{\nu}] = \delta^{\mu}_{\nu}, \mu, \nu \in 1, ..., D$, are preserved under any unitary transformation *U* acting on the column vector $a \equiv [a^{\mu}]$ by $a \rightarrow Ua$, and on the row vector $a^{\dagger} \equiv [a_{\nu}^{\dagger}]$ as $a^{\dagger} \rightarrow a^{\dagger} U^{\dagger}$. In any basis, the diagonal elements of the dyadic matrix operator $\hat{n} \equiv a^{\dagger} a$ (i.e., $[\hat{n}^{\mu}_{\nu}] \equiv [a^{\dagger}_{\nu} a^{\mu}]$) constitute a complete set of independent number components in the Fock space on $|0\rangle$.

Right eigenstates of the number operators in a basis indexed by μ are formed as

$$
|\vec{n}\rangle \equiv \prod_{\mu=1}^{D} \frac{(a_{\mu}^{\dagger})^{n_{\mu}}}{\sqrt{n_{\mu}}}|0\rangle, \tag{A1}
$$

where \vec{n} denotes the vector of eigenvalues $[n_{\mu}]$. For a column vector $\xi = [\xi^\mu]$ of complex scalars, a general coherent state for the system may be constructed as

$$
|\xi\rangle \equiv e^{-(\xi^{\dagger}\cdot\xi)/2} \sum_{N=0}^{\infty} \frac{(a^{\dagger}\cdot\xi)^N}{N} |0\rangle.
$$
 (A2)

The coherent state is an eigenstate of the annihilation operators, with eigenvalue ξ^{μ} for each component a^{μ} .

The conjugate (bra) ground state is denoted $\langle 0|$. The conjugate number eigenstate $\langle \vec{n} \rangle$ also has eigenvalues n_{μ} , while the conjugate coherent state $\langle \xi^{\dagger} |$ is the left eigenvector of the creation operator with eigenvalues ξ_v^* for components a_v^{\dagger} . All these are normalized: $\langle 0 | 0 \rangle = \langle \vec{n} | \vec{n} \rangle = \langle \xi^{\dagger} | \xi \rangle = 1$.

The coherent states are overcomplete, and it is possible to construct from them a set of ensembles ρ which contain the Boltzmann equilibrium ensemble but which, as a set, are preserved under the unitary symmetry of the raising and lowering operator commutation relations. The *Gaussian* coherent ensembles of the form (9) (9) (9) in the main text are entropy maximizing $[18]$ $[18]$ $[18]$ subject to a constraint on Tr $(\rho \hat{n})$. The kernel *K* of the Gaussian must be positive definite and Hermitian for the inverse n from Eq. (10) (10) (10) to exist and to be Hermitian.

The densities (9) (9) (9) are readily shown $[18]$ $[18]$ $[18]$ to possess thermal occupation statistics when projected onto the number states of any single component μ (in any basis), and their exact entropies have the von Neumann form ([6](#page-5-0)) motivated on symmetry grounds in the text,

$$
S(\rho) \equiv -\operatorname{Tr}(\rho \ln \rho) = \operatorname{Tr}[(I+n)\ln(I+n) - n \ln n].
$$
\n(A3)

Here and in the main text parentheses will be used to denote traces with the quantum density matrix, and square brackets will denote the $D \times D$ scalar matrix trace. *I* is the $D \times D$ identity matrix.)

Rather than take the antique approach of "quantizing" a classical system, which would cast the Hilbert space as dependent on the Hamiltonian, we take the Hilbert space as primitive, and consider the set of all compatible Hamiltonians, each defined as $\hat{H} = Tr[E\hat{n}] = a_{\nu}^{\dagger} E_{\mu}^{\nu} a^{\mu}$, with respect to some $D \times D$ Hermitian matrix *E*. ρ becomes the equilibrium Bose density matrix when $K \equiv (e^{\beta E} - I)$.

In the simplest case of free evolution, effective action of the Hamiltonian on K can be evaluated by evolving ρ through a time δt to produce the distribution $\rho_{\delta t}$ as

$$
\rho_{\delta t} = e^{i\hat{H}\delta t} \rho e^{-i\hat{H}\delta t} = \int d\xi^{\dagger} d\xi \,\text{Det}\left(\frac{K}{\pi}\right) e^{-\xi^{\dagger} K \xi} |U\xi\rangle\langle\xi^{\dagger} U^{\dagger}|
$$

$$
= \int d\xi^{\dagger} d\xi \,\text{Det}\left(\frac{K}{\pi}\right) e^{-\xi^{\dagger} UKU^{\dagger} \xi} |\xi\rangle\langle\xi^{\dagger}|. \tag{A4}
$$

The notation $U = e^{iE\delta t}$ for this particular differential unitary evolution operator of vectors $\hat{\xi}$, and $U^{\dagger} \equiv e^{-iE\delta t}$ for its Hermitian conjugate, will be used below as a shorthand in the definition of free Green's functions. Between the first and second lines of Eq. ([A4](#page-13-0)), the joint change of variable ξ \rightarrow *U*[†] ξ , ξ [†] \rightarrow ξ [†] U has been performed. Hamiltonian evolution is unitary (acting by similarity transformation) on K and hence n , and so preserves the entropy $(A3)$ $(A3)$ $(A3)$. The more general Fokker-Planck equation (11) (11) (11) in the text is readily converted $[18]$ $[18]$ $[18]$ to the equation of motion (12) (12) (12) , by transformations similar to those in Eq. $(A4)$ $(A4)$ $(A4)$.

2. Generalizing Markov generating functions to respect unitary symmetry

The usual DP construction assumes a classical probability mass function *P* of integer arguments, which could be defined on the number basis of a particular CSCO of a *D*-dimensional quantum harmonic oscillator. At any single time, such a CSCO is selected by the diagonalizing basis of K , where Eq. (9) (9) (9) reduces to

$$
\rho = \sum_{\vec{n}} P(\vec{n}) |\vec{n}\rangle\langle\vec{n}|. \tag{A5}
$$

The usual Markovian moment-generating function Ψ for mass function *P* is obtained by introducing a vector $\vec{z} \equiv [z_i]$ of complex components, in terms of which

$$
\Psi(\vec{z}) = \sum_{\vec{n}} P(\vec{n}) \prod_{i=1}^{D} z_i^{n_i},\tag{A6}
$$

and subscript *i* has been used as a reminder that the diagonalizing basis depends instant by instant on K . Ψ can also be defined directly from the density ρ . If we construct a diagonal matrix *z* with eigenvalues $\{z_i\}$, we may write

QUANTUM-CLASSICAL CORRESPONDENCE PRINCIPLES...

$$
\Psi(\vec{z}) \equiv \text{Tr}\left(\rho \prod_{i=1}^{D} z_i^{\hat{n}_i}\right) = \text{Tr}(\rho e^{\text{Tr}[\hat{n} \ln z]},\tag{A7}
$$

in which the expression $Tr[\hat{n} \ln z]$ refers to the matrix trace and logarithm.

The generating function Ψ in Eq. ([A7](#page-14-1)) remains well defined for arbitrary Hermitian *z*, which we indicate with the notation $\Psi(z)$. Any linear transformation of the number matrix *nˆ* may be converted into an equivalent transformation on *z*, so the resulting class of generating functions is sufficient to represent arbitrary Fokker-Planck evolution of the form $(11).$ $(11).$ $(11).$

Some shorthand notation will be convenient below: If ln *z* and \hat{n} are written in the adjoint representation, $Tr[\hat{n} \ln z]$ is the inner product of their independent coefficients, which will therefore be denoted $\hat{n} \cdot \ln z$, where no confusion results. As a notational convenience, let $w = \ln z$, a quantity which will appear frequently.

3. Normal ordering and antinormal ordering

The action on ρ of the operators in the first two lines of Eq. (11) (11) (11) has a simple expression in terms of the generating function $(A7)$ $(A7)$ $(A7)$, but the action of the operators in the last line of Eq. (11) (11) (11) does not. The easiest way to derive a classical Liouville equation is actually to work with *two* generating functions, distinguished by the operator ordering of the number insertions that extract them from ρ .

Normal ordered (NO) products of operators, denoted : *:, are defined to have the index structure of *, but to place all creation operators to the left of any annihilation operator. Antinormal ordered (ANO) products of operators, denoted !*!, have the opposite prescription; all annihilation operators lie to the left of any creation operator. The lowest-order relation between NO and ANO operators, contracted with any matrix such as *w*, is thus

$$
a^{\dagger}wa = : a^{\dagger}wa : \equiv a^{\dagger}_{\nu}w^{ \nu}_{\mu}a^{\mu} = a^{\mu}w^{\nu}_{\mu}a^{\dagger}_{\nu} - w^{\mu}_{\mu}
$$
 (A8)

$$
\equiv ! \, a^{\dagger} w a \, ! - \text{Tr}[w]. \tag{A9}
$$

For this contraction it follows that

$$
e^{!a^{\dagger}wa!} = \text{Det}[z]e^{:a^{\dagger}wa!}.
$$
 (A10)

A little commutator algebra provides a relation between exponentiation and normal ordering. For the exponential of a NO number operator

$$
e^{\cdot a^{\dagger}wa} = :e^{a^{\dagger}(z-I)a} \equiv :e^{a^{\dagger}\epsilon a}; \qquad (A11)
$$

and for an ANO number operator

$$
e^{\mathrm{i}a^{\dagger}wa!} = ! e^{a^{\dagger}(I - z^{-1})a}!
$$
 $\equiv ! e^{a^{\dagger} \bar{\epsilon}a}!$ (A12)

At this point we have introduced the notations $\epsilon \equiv z - I$ and *¯I*−*z*−1—used also in the main text—for two combinations that will arise repeatedly.

Two generating functions, defined respectively by insertion of NO and ANO exponentials, are denoted

$$
\Psi \equiv \mathrm{Tr}[e^{\mathrm{i}a^{\dagger}wa}\rho] = \mathrm{Tr}[\mathrm{i}e^{a^{\dagger}\epsilon a}\!\cdot\!\rho],
$$

$$
\overline{\Psi} \equiv \text{Tr}[e^{l a^{\dagger} w a!} \rho] = \text{Tr}[! e^{a^{\dagger} \overline{\epsilon} a}! \rho] = \text{Det}[z] \Psi, \quad (A13)
$$

and the relation between them follows from Eq. $(A10)$ $(A10)$ $(A10)$. Explicit arguments of Ψ and $\overline{\Psi}$ will generally be suppressed. Their evaluations as analytic functions of *w*, *z*, ϵ , or $\bar{\epsilon}$ will be made clear by context.

From the form ([9](#page-6-1)) of ρ and the definitions ([A13](#page-14-0)), it is straightforward to compute that

$$
\Psi = \frac{1}{\text{Det}(I - K^{-1}\epsilon)},
$$
\n
$$
\overline{\Psi} = \frac{1}{\text{Det}[I - (I + K^{-1})\overline{\epsilon}]}. \tag{A14}
$$

Thus ϵ couples to K^{-1} , while $\bar{\epsilon}$ couples to $I + K^{-1}$.

4. From Fokker-Planck to Liouville equation

The bilinearity in *a* and a^{\dagger} of the Fokker-Planck equation (11) (11) (11) only translates to simple evolution of z if the operator ordering is the same as that employed in the generating function. Thus the function Ψ defined from NO insertions evolves simply under the first two lines of Eq. (11) (11) (11) , while the function $\overline{\Psi}$ evolves simply under the third line, in which all operators in the trace are ANO.

The interaction of bilinear operators with exponentiated operators can be organized according to operator ordering within each term, and relative ordering of the terms. For a general matrix *M*, the two possible products of NO operators reduce to

$$
:e^{a^{\dagger}\epsilon a}:a^{\dagger}Ma:=:e^{a^{\dagger}\epsilon a}(a^{\dagger}Ma):+:e^{a^{\dagger}\epsilon a}(a^{\dagger}\epsilon Ma);
$$

$$
:a^{\dagger}Ma::=e^{a^{\dagger}\epsilon a}:=(a^{\dagger}Ma)e^{a^{\dagger}\epsilon a}:+(a^{\dagger}Mea)e^{a^{\dagger}\epsilon a}:
$$

(A15)

while the two products for ANO operators reduce to

$$
!e^{a^{\dagger}\bar{\epsilon}a}!
$$

$$
!a^{\dagger}Ma! = !e^{a^{\dagger}\bar{\epsilon}a}(a^{\dagger}Ma)! - !e^{a^{\dagger}\bar{\epsilon}a}(a^{\dagger}M\bar{\epsilon}a)!,
$$

$$
!a^{\dagger}Ma! : !e^{a^{\dagger}\bar{\epsilon}a}! = !(a^{\dagger}Ma)e^{a^{\dagger}\bar{\epsilon}a}! - !(a^{\dagger}\bar{\epsilon}Ma)e^{a^{\dagger}\bar{\epsilon}a}!.
$$

(A16)

For the first line of Eq. (11) (11) (11) , the NO insertion and Eq. $(A15)$ $(A15)$ $(A15)$, with $M = E$, give

$$
\operatorname{Tr}[\cdot e^{a^{\dagger}\epsilon a} : i[a^{\dagger}Ea,\rho]] = -i \operatorname{Tr}[\cdot e^{a^{\dagger}\epsilon a}(a^{\dagger}[E,\epsilon]a) : \rho]
$$

$$
= -i \operatorname{Tr}\left[[E,\epsilon]\frac{\partial}{\partial \epsilon}\right] \operatorname{Tr}[\cdot e^{a^{\dagger}\epsilon a} : \rho]
$$

$$
= -i \operatorname{Tr}\left[[E,\epsilon]\frac{\partial}{\partial \epsilon}\right] \Psi. \tag{A17}
$$

For the second line, again using the NO insertion and this time $M = r + rn_R$, gives

$$
(r + rn_R)^{\nu}_{\mu} \operatorname{Tr} \left[:e^{a^{\dagger}\epsilon a} \cdot \left(a^{\mu} \rho a_{\nu}^{\dagger} - \frac{1}{2} \{ a_{\nu}^{\dagger} a^{\mu}, \rho \} \right) \right]
$$

\n
$$
= -\frac{1}{2} \operatorname{Tr} \left[:e^{a^{\dagger}\epsilon a} (a^{\dagger} \{ r + rn_R, \epsilon \} a) : \rho \right]
$$

\n
$$
= -\frac{1}{2} \operatorname{Tr} \left[\{ r + rn_R, \epsilon \} \frac{\partial}{\partial \epsilon} \right] \operatorname{Tr} \left[:e^{a^{\dagger}\epsilon a} : \rho \right]
$$

\n
$$
= -\frac{1}{2} \operatorname{Tr} \left[\{ r + rn_R, \epsilon \} \frac{\partial}{\partial \epsilon} \right] \Psi.
$$
 (A18)

The nonvanishing anticommutator $\{r + rn_R, I\}$ makes the offset of ϵ relative to *z* significant, where it is not in Eq. ([A17](#page-14-4)). For the last line in Eq. (11) (11) (11) , the ANO insertion gives a simple evolution equation, with $M = rn_R$ in Eq. ([A16](#page-14-5)) as follows:

$$
(rn_R)_{\mu}^{\nu} \operatorname{Tr} \left[e^{a^{\dagger} \bar{\epsilon} a} \cdot \left(a_{\nu}^{\dagger} \rho a^{\mu} - \frac{1}{2} \{ a^{\mu} a_{\nu}^{\dagger}, \rho \} \right) \right]
$$

\n
$$
= \frac{1}{2} \operatorname{Tr} \left[e^{a^{\dagger} \bar{\epsilon} a} (a^{\dagger} \{ r n_R, \bar{\epsilon} \} a) \cdot \rho \right]
$$

\n
$$
= \frac{1}{2} \operatorname{Tr} \left[\{ r n_R, \bar{\epsilon} \} \frac{\partial}{\partial \bar{\epsilon}} \right] \operatorname{Tr} \left[e^{a^{\dagger} \bar{\epsilon} a} \cdot \rho \right] = \frac{1}{2} \operatorname{Tr} \left[\{ r n_R, \bar{\epsilon} \} \frac{\partial}{\partial \bar{\epsilon}} \right] \overline{\Psi} .
$$

\n(A19)

To convert Eq. ([A19](#page-15-1)) into an equation on Ψ like Eqs. $(A17)$ $(A17)$ $(A17)$ and $(A18)$ $(A18)$ $(A18)$, we begin by converting the derivative operator on $\bar{\epsilon}$. Requiring that the identity for a general scalar function *f*,

$$
\operatorname{Tr}\left[\delta\overline{\epsilon}\frac{\partial}{\partial\overline{\epsilon}}\right]f = \operatorname{Tr}\left[\delta\overline{\epsilon}\frac{\partial f}{\partial\overline{\epsilon}}\right],\tag{A20}
$$

hold also in ζ or ϵ , and making use of cyclic rearrangement in the trace, yields the conversions

$$
\frac{1}{2} \operatorname{Tr} \left[\{rn_R, \vec{\epsilon} \} \frac{\partial}{\partial \vec{\epsilon}} \right] = \operatorname{Tr} \left[\left(zrn_R z - \frac{1}{2} \{rn_R, z \} \right) \frac{\partial}{\partial z} \right]
$$

$$
= \operatorname{Tr} \left[\left(\epsilon rn_R \epsilon + \frac{1}{2} \{ rn_R, \epsilon \} \right) \frac{\partial}{\partial \epsilon} \right].
$$
(A21)

The relation $\bar{\epsilon} = I - z^{-1}$ has created a quadratic perturbation in z or ϵ . With the relation ([A13](#page-14-0)) of $\overline{\Psi}$ to Ψ , Eq. ([A21](#page-15-3)) allows us to recast Eq. $(A19)$ $(A19)$ $(A19)$ as

$$
(rn_R)^{\nu}_{\mu} \operatorname{Tr} \left[:e^{a^{\dagger}\epsilon a} \cdot \left(a^{\dagger}_{\nu} \rho a^{\mu} - \frac{1}{2} \{ a^{\mu} a^{\dagger}_{\nu}, \rho \} \right) \right]
$$

\n
$$
= \frac{1}{\operatorname{Det}[z]} \operatorname{Tr} \left[\left(zrn_R z - \frac{1}{2} \{ rn_R z \} \right) \frac{\partial}{\partial z} \right] \operatorname{Det}[z] \Psi
$$

\n
$$
= \left\{ \operatorname{Tr}[rn_R \epsilon] + \operatorname{Tr} \left[\left(\epsilon rn_R \epsilon + \frac{1}{2} \{ rn_R, \epsilon \} \right) \frac{\partial}{\partial \epsilon} \right] \right\} \Psi.
$$

\n(A22)

Collecting terms from Eqs. $(A17)$ $(A17)$ $(A17)$ – $(A22)$ $(A22)$ $(A22)$, the differential equation on Ψ induced by Eq. ([11](#page-6-1)) for ρ becomes Eq. ([17](#page-8-1)) in the main text. Thus the Liouville operator is

$$
\mathcal{L} = \text{Tr}\left[\left(i[E, \epsilon] + \left\{ \frac{r}{2}, \epsilon \right\} - \epsilon r n_R \epsilon \right) \frac{\partial}{\partial \epsilon} \right] - \text{Tr}[r n_R \epsilon].
$$
\n(A23)

If Ψ is instantaneously defined by Eq. ([A14](#page-14-6)), the evaluation of Eq. (17) (17) (17) yields

$$
\frac{\partial \ln \Psi}{\partial t} = \text{Tr}[rn_R \epsilon] \n+ \text{Tr}\left[(I - K^{-1} \epsilon)^{-1} K^{-1} \left(-i[E, \epsilon] + \epsilon rn_R \epsilon - \left\{ \frac{r}{2}, \epsilon \right\} \right) \right] \n= \text{Tr}\left[(I - K^{-1} \epsilon)^{-1} \left(i[E, K^{-1}] + rn_R - \left\{ \frac{r}{2}, K^{-1} \right\} \right) \epsilon \right].
$$
\n(A24)

The second line in Eq. $(A24)$ $(A24)$ $(A24)$, obtained by cyclic rearrangement in the trace and cancellation of part of the *K*-independent surface term against the quadratic term in ϵ , verifies that the same evolution follows from keeping the argument ϵ invariant and allowing $K^{-1} = n$ to evolve under Eq. (12) (12) (12) . The fact that the entire consequence of the Fokker-Planck operator (11) (11) (11) can be absorbed in a classical equation of motion for *K* also verifies that the Gaussian coherent form (9) (9) (9) is stable under this most general bilinear form for quantum evolution.

APPENDIX B: THE TIME-LOOP PATH INTEGRAL

This Appendix treats the time-loop path integral, its relation to the Liouville operator, and the continuum limit, Keldysh rotation, and causal structure. We begin by defining the path integral as the quadrature of the evolution operator for the generating function Ψ . We then consider the alternative representation of $\Psi|_{z=I}$ (the trace of the evolved density matrix) as a generating functional, whenever matrices *iE*, *r*, and rn_R are taken to be not only time-varying parameters, but also sources to generate field insertions.

We begin with unitary evolution to define the discrete time-loop structure, and then add dissipative terms. From these it is possible to pass to the continuum limit, and to show how the Keldysh rotation manifests causal structure. The last subsection shows how the dissipative insertions are recovered from the free continuum integral when a trace is performed over a subset of the degrees of freedom in the density matrix.

1. Discrete time-loop integral

a. Free Hamiltonian evolution

The operator ρ , evolved through a time $T \equiv N \delta t$ with the free Hamiltonian \hat{H} , is converted into a pair of functional integrals by insertion of the coherent-state representation of unity

$$
1 = \int \frac{d\xi^{\dagger} d\xi}{\pi^D} |\xi\rangle\langle\xi^{\dagger}|
$$
 (B1)

in each interval δt on both bra and ket states. We use the field insertion protocol of Fig. [3](#page-16-2) to make contact with Kamenev

FIG. 3. Field insertion protocol for the time-loop path integral. As in Fig. [1,](#page-6-3) time advances to the right along links in increments δt . The solid nodes are positions of fields ξ_n^{\dagger} , ξ_n , and the hollow node is the original pair ξ^{\dagger} , ξ of ρ , which will be integrated out. Small arrows on links indicate direction along the time loop.

[26]. Though this convention creates a redundancy between the coherent states inserted on the bra side at time $t=0$ with the fields ξ, ξ^{\dagger} in ρ of Eq. ([9](#page-6-1)), it was adopted in Ref. [[26](#page-23-10)] to accommodate general density matrices, not necessarily diagonal in coherent states.

States $n \in (1, \ldots, N)$ are inserted at ascending times $(1, \ldots, N) \times \delta t$, and states $n \in (N+1, \ldots, 2N)$ are inserted at descending times $(N-1, \ldots, 0) \times \delta t$. The state insertions covering the first interval δt convert Eq. ([A4](#page-13-0)) into

$$
\rho_{\delta t} = \int \frac{d\xi_1^{\dagger} d\xi_1}{\pi^D} \int \frac{d\xi_{2N}^{\dagger} d\xi_{2N}}{\pi^D} \int \frac{d\xi_{2N-1}^{\dagger} d\xi_{2N-1}}{\pi^D} |\xi_1\rangle
$$

$$
\times \langle \xi_1^{\dagger} | e^{i\hat{H}\delta t} \rho | \xi_{2N} \rangle \langle \xi_{2N}^{\dagger} | e^{-i\hat{H}\delta t} | \xi_{2N-1} \rangle \langle \xi_{2N-1}^{\dagger} | \qquad (B2)
$$

Further time evolution proceeds by induction,

$$
\rho_{n\delta t} = \int \frac{d\xi_n^{\dagger} d\xi_n}{\pi^D} \int \frac{d\xi_{2N-n}^{\dagger} d\xi_{2N-n}}{\pi^D} |\xi_n\rangle
$$

$$
\times \langle \xi_n^{\dagger} | e^{i\hat{H}\delta t} \rho_{(n-1)\delta t} e^{-i\hat{H}\delta t} | \xi_{2N-n} \rangle \langle \xi_{2N-n}^{\dagger} |,
$$
 (B3)

up to time $(N-1)$ $(N-1)$ $(N-1)$ δt . These result in the time "legs" of Fig. 1 in the text.

The time-loop *S* matrix is produced from $\rho_{(N-1)\delta t}$, by insertion of $e^{\pm i\hat{H}\delta t}$, a *single* coherent-state insertion at *N* δt , and the taking of the trace, which formally yields unity as follows:

$$
1 = \operatorname{Tr}\left(\int \frac{d\xi_N^{\dagger} d\xi_N}{\pi^D} |\xi_N\rangle \langle \xi_N^{\dagger} | e^{i\hat{H}\delta t} \rho_{(N-1)\delta t} e^{-i\hat{H}\delta t} \right)
$$

$$
= \frac{1}{Z} \int \frac{d\xi_1^{\dagger} d\xi_1}{\pi^D} \dots \int \frac{d\xi_{2N}^{\dagger} d\xi_{2N}}{\pi^D} e^{-F}.
$$
(B4)

The inverse of the partition function Z in Eq. $(B4)$ $(B4)$ $(B4)$ results from integration over $d\xi^{\dagger}d\xi$ in the original ρ of Eq. ([9](#page-6-1)), and evaluates to

$$
\frac{1}{Z} = \frac{1}{\text{Det}(I + K^{-1})} = \Psi|_{z=0},\tag{B5}
$$

corresponding to argument $\epsilon = -I$ in Eq. ([A14](#page-14-6)). The quadratic form F in Eq. $(B4)$ $(B4)$ $(B4)$, involving only the numbered fields, evaluates to

$$
F = \begin{bmatrix} \xi_1^{\dagger} & \cdots & \xi_N^{\dagger} & \xi_{N+1}^{\dagger} & \cdots & \xi_{2N}^{\dagger} \end{bmatrix} \begin{bmatrix} I & & & & -Up \\ -U & \ddots & & & & \\ -U & I & & & & \\ & -U^{\dagger} & I & & & \\ & & -U^{\dagger} & \ddots & & \\ & & & -U^{\dagger} & I & \\ & & & & -U^{\dagger} & I \end{bmatrix} \begin{bmatrix} \xi_1 \\ \xi_1 \\ \xi_N \\ \xi_{N+1} \\ \vdots \\ \xi_{2N} \end{bmatrix} .
$$
 (B6)

It is expressed as a function of $p = (K+I)^{-1}$ rather than of *K* directly, as a result of the integration over $d\xi^{\dagger}d\xi$ used to produce the second line of Eq. ([B4](#page-16-1)). [p generalizes the Boltzmann factor for a single excitation in the equilibrium case where $K = e^{\beta E} - I$. The path integral itself evaluates to Det $(I - p)^{-1} = Det(I + K^{-1}) = Z$, and thus represents the partition function.] From the form *F* we readily obtain the free Green's function in the discrete representation

$$
\left\{\begin{bmatrix} \xi_1 \\ \vdots \\ \xi_N \\ \xi_{N+1} \\ \vdots \\ \xi_{2N} \end{bmatrix} \begin{bmatrix} \xi_1^{\dagger} & \cdots & \xi_N^{\dagger} & \xi_{N+1}^{\dagger} & \cdots & \xi_{2N}^{\dagger} \end{bmatrix} \right\} = \begin{bmatrix} U \\ \vdots \\ U_N \\ U_{N-1} \\ \vdots \\ U_{N-1} \\ \vdots \\ U^{N-1} \end{bmatrix} K^{-1} \begin{bmatrix} U^{\dagger} & \cdots & \cdots & \cdots & \vdots \\ U_N & U^{N-1} & \cdots & \cdots & \cdots & \vdots \\ U^{N} & U^{N-1} & \cdots & \cdots & \cdots & \vdots \\ U^{N-2} & \cdots & U^{N} & U^{N-1} & \cdots & \cdots \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ U^{N} & \cdots & U^{N} & U^{N-1} & \cdots & I \end{bmatrix},
$$
\n(B7)

consisting of a regular *K*−1-dependent dyadic, and a K^{-1} -independent lower-triangular form. The Green's function is more compact but less transparent in index form. Preparatory to performing the Keldysh rotation, it is convenient to use index $1 \le n \le N$ to indicate fields on the forward (ket) leg, and to rewrite $2N-n \rightarrow -n$, for $0 \le n \le N$, for fields on the backward (bra) leg. This convention is used in both Figs. 1 and 2 , and in Eq. (19) (19) (19) and Eq. (23) (23) (23) and afterward in the main text. (Thus both $\pm n$ denote fields at times $|n| \delta t$, and both $\pm N$ refer to the same field insertion at the apex of the time loop.) The four expectations involving forward and backward legs at $1 \le n \le N-1$ are then

$$
\langle \xi_{-n} \xi_{n'}^{\dagger} \rangle = U^{n} (K^{-1} + I) U^{\dagger n'},
$$

$$
\langle \xi_{n} \xi_{-n'}^{\dagger} \rangle = U^{n} (K^{-1}) U^{\dagger n'},
$$

$$
\langle \xi_{n} \xi_{n'}^{\dagger} \rangle = U^{n} [\theta_{n,n'}^{\dagger} (K^{-1} + I) + \theta_{n',n}^{\dagger} (K^{-1})] U^{\dagger n'},
$$

$$
\langle \xi_{-n} \xi_{-n'}^{\dagger} \rangle = U^{n} [\theta_{n,n'}^{\dagger} (K^{-1}) + \theta_{n',n}^{\dagger} (K^{-1} + I)] U^{\dagger n'}, \quad (B8)
$$

in which the $\theta_{n,n'}^{\pm}$ are Heaviside functions, both equal to *I* for $n>n'$ and 0 for $n \leq n'$. They differ at equal arguments, with $\theta_{n,n}^+ = I$ while $\theta_{n,n}^- = 0$. The corresponding index notation for the quadratic form $(B6)$ $(B6)$ $(B6)$ is

$$
F = \xi_1^{\dagger} U(I - p) \xi_0 + \sum_{n=1}^{N} \xi_n^{\dagger} (\xi_n - \xi_{n-1} - iE \delta t \xi_{n-1})
$$

+ $\xi_{-(n-1)}^{\dagger} [- (\xi_{-n} - \xi_{-(n-1)}) + iE \delta t \xi_{-n}].$ (B9)

b. Dissipative insertions

Interestingly, the easiest way to insert dissipative terms is through the generating function $(A13)$ $(A13)$ $(A13)$, and the associated quadrature of the Liouville equation

$$
\Psi_{n\delta t} \equiv e^{-\mathcal{L}(E_n, r_n, r_n, \delta t)} \Psi_{(n-1)\delta t}, \tag{B10}
$$

now allowing E , r , and rn_R to be arbitrary functions of time. Continuing to insert pairs of coherent states in the same positions as for free evolution, and working backward through the commutation relations $(A15)$ $(A15)$ $(A15)$ and $(A16)$ $(A16)$ $(A16)$ used to derive the Liouville operator, we generalize Eq. $(B9)$ $(B9)$ $(B9)$ to Eq. (23) (23) (23) of the main text.

2. Continuum limit and Keldysh rotation

The discrete formulation of the path integral has the virtue that all surface terms in it are explicit, making inversion to the (free) Green's function ([B7](#page-16-0)) straightforward. However, the continuum limit is the only practical basis for modeexpansion perturbation theory, for renormalization, or for tracing over unobserved "reservoir" degrees of freedom. This section concerns the encoding of boundary conditions from the discrete form, which become "implicit" in the continuum, in a set of *i* e prescriptions.

Times $t = n\delta t$ and $t' = n'\delta t$ are held fixed as $\delta t \rightarrow$, and fields are homogeneous of order zero: $\xi_n \rightarrow \xi_t$, $\delta_{n,n'}$

 $\rightarrow \delta t \delta(t-t')$, and the relevant Heaviside function $(\theta_{n,n'}^+)$ $+\theta_{n,n'}^-$ //2 $\rightarrow \theta(t-t')$, with the prescription that $\theta(0)=I/2$. In mode expansions the differences $\xi_n - \xi_{n-1} \equiv \partial t \partial_t \xi_{t-\delta t}$ and ξ_{-n} $-\xi_{-(n-1)} \equiv \delta t \partial_t \xi_{-t}$ define derivatives along the time loop, and the free quadratic form F of Eq. ([B9](#page-17-0)) is expressed as

$$
F = \xi_{\delta t}^{\dagger} U(I - p) \xi_0 + \delta t \sum_{n=1}^{N} \xi_t^{\dagger} (\partial_t - iE) \xi_{t - \delta t}
$$

+
$$
\xi_{-(t - \delta t)}^{\dagger} (-\partial_t + iE) \xi_{-t},
$$
 (B11)

in which the index ordering of ξ^{\dagger} relative to ξ reflects the time direction of causation on each leg, shown with arrows in Fig. [2.](#page-7-0) Passage from the sum to the integral gives the naïve free time-loop action

$$
F \to \xi_0^{\dagger} (I - p) \xi_0 + \int_0^T dt \Big[\xi_t^{\dagger} \quad \xi_{-t}^{\dagger} \Big] \Big[\begin{array}{c} \partial_t - iE \\ - \partial_t + iE \end{array} \Big] \Big[\begin{array}{c} \xi_t \\ \xi_{-t} \end{array} \Big], \tag{B12}
$$

in which field "ordering" is now implicit in both the integral and the surface term.

An *i* e prescription that recovers both the causal and correlation structures of Eq. $(B8)$ $(B8)$ $(B8)$ is neither obvious nor simple to use in the free time-loop representation $(B12)$ $(B12)$ $(B12)$. For this the Keldysh action and finite (rather than infinitesimal) dissipation terms are preferred. It turns out to be useful to derive the dissipation terms from a trace within the Keldysh causal structure, rather than taking them as primitive, because scalar corrections accompany the approximation of dissipative contact terms, which can be safely overlooked in the free action but must be kept in the dissipative action to correctly compute the partition function.

a. Keldysh fields, Green's functions, and action

The Keldysh fields are defined from time-loop fields, for $1 \le n \le N-1$, by the rotation ([24](#page-9-7)) in the main text. (This definition differs from the one in Ref. $\left[26\right]$ $\left[26\right]$ $\left[26\right]$ by a rescaling of the field ϕ_n to make the transformation unitary). The free Green's function obtained by transforming Eq. ([B8](#page-17-1)) under Eq. (24) (24) (24) has the considerably simpler structure

$$
\left\langle \begin{bmatrix} \phi_n \\ \psi_n \end{bmatrix} \begin{bmatrix} \phi_n^{\dagger} & \psi_n^{\dagger} \end{bmatrix} \right\rangle = U^n \left\{ \begin{bmatrix} \left(K^{-1} + \frac{I}{2} \right) & -\theta_{n,n'}^s \\ \theta_{n',n}^s & \\ \vdots & \\ \theta_{n,n'}^s \end{bmatrix} + \delta_{n,n'} \begin{bmatrix} I/4 \\ I \end{bmatrix} \right\} U^{\dagger n'}, \quad \text{(B13)}
$$

in which $\theta^s = (\theta^+ + \theta^-)/2$, and therefore $\theta^s_{n,n} = I/2$. $\delta_{n,n'}$ is the Kronecker delta. The continuum limit of Eq. $(B13)$ $(B13)$ $(B13)$ has the "tridiagonal" form (up to removable singularities at $t=t'$)

QUANTUM-CLASSICAL CORRESPONDENCE PRINCIPLES...

$$
\left\langle \begin{bmatrix} \phi_t \\ \psi_t \end{bmatrix} \begin{bmatrix} \phi_{t'}^{\dagger} & \psi_{t'}^{\dagger} \end{bmatrix} \right\rangle = e^{iEt} \begin{bmatrix} \left(K^{-1} + \frac{I}{2} \right) & -\theta(t - t') \\ \theta(t' - t) & \end{bmatrix} e^{-iEt'},
$$
\n(B14)

in which correlation and response functions are completely separated.

The block structure of Eq. $(B14)$ $(B14)$ $(B14)$ may be used to motivate an *i* e prescription and handling of the surface term in the action obtained by rotation of Eq. $(B12)$ $(B12)$ $(B12)$, written as

$$
F \rightarrow \left(\phi_{\delta t}^{\dagger} - \frac{1}{2}\psi_{\delta t}^{\dagger}\right)(I - p)\left(\phi_{0} + \frac{1}{2}\psi_{0}\right) + \int_{0}^{T} dt\left[\phi_{t}^{\dagger} \quad \psi_{t}^{\dagger}\right]
$$

$$
\times \left[\begin{matrix} -\partial_{t} + iE + \varepsilon \\ -\partial_{t} + iE - \varepsilon \end{matrix}\right] \left[\begin{matrix} \phi_{t} \\ \psi_{t} \end{matrix}\right].
$$
(B15)

The decomposition of the $t=0$ fields follows from their original placement as $\xi_{\delta t}^{\dagger}$ and $\xi_0 = \xi_{2N}$ in Eq. ([B11](#page-17-4)). The one explicitly implied expectation

$$
\langle \xi_0 \xi_{\delta t}^{\dagger} \rangle = (I - p)^{-1} = K^{-1} + I = \left\langle \left(\phi_0 + \frac{1}{2} \psi_0 \right) \left(\phi_{\delta t}^{\dagger} - \frac{1}{2} \psi_{\delta t}^{\dagger} \right) \right\rangle, \tag{B16}
$$

together with the block structure and (anti)symmetries of the Green's function $(B13)$ $(B13)$ $(B13)$, is sufficient to define the individual component expectations.

b. Dissipation in the Born approximation

The continuum action in Keldysh fields with finite dissipation (26) (26) (26) can be obtained directly from the discrete timeloop action (23) (23) (23) by taking the continuum limit on the time loop ([25](#page-9-5)), and then formally performing the Keldysh rotation. The formal rotation of the time-derivative terms is questionable, because the rotation in discrete fields produces other operator products besides those obtained by rotating the continuum, which must be shown to vanish in all contexts. Therefore it is in many respects preferable to perform the Keldysh rotation for unitary evolution, and then to derive finite dissipation by an explicit trace over a subset of degrees of freedom, and an explicitly defined Born approximation.

Suppose therefore that the closed-system degrees of freedom can be split into explicit *S*ystem and *R*eservoir component vectors, as

$$
\phi_t \equiv \begin{bmatrix} \phi_{St} \\ \phi_{Rt} \end{bmatrix},
$$

$$
\psi_t \equiv \begin{bmatrix} \psi_{St} \\ \psi_{Rt} \end{bmatrix}.
$$
(B17)

Suppose the (system \oplus reservoir) energy matrix decomposes as

$$
E = \begin{bmatrix} E_S & g \\ g^\dagger & E_R \end{bmatrix},
$$
 (B18)

in which *g* is a matrix of interaction terms and g^{\dagger} its Hermitian conjugate, and E_S and E_R are intrinsic energy matrices for system and reservoir. For simplicity set the "Boltzmann factor" matrix *p* block diagonal to define initial conditions as follows:

$$
p \equiv \begin{bmatrix} p_S \\ p_R \end{bmatrix} . \tag{B19}
$$

As a matter of notation let $p_R = (K_R + I)^{-1}$.

Expanding the (system \oplus reservoir) quadratic form *F* to second order in *g* and g^{\dagger} , from Eq. ([B15](#page-18-1)), gives the leading nonvanishing terms

$$
e^{-F} = e^{-(F_{S}+F_{R})} \left\{ 1 - \int_{0}^{T} dt \psi_{Si}^{\dagger} g \phi_{Rt} \int_{0}^{T} dt' \phi_{Rt'}^{\dagger} g^{\dagger} \psi_{St'} - \int_{0}^{T} dt \psi_{Si}^{\dagger} g \phi_{Rt} \int_{0}^{T} dt' \psi_{Rt'}^{\dagger} g^{\dagger} \phi_{St'} - \int_{0}^{T} dt \phi_{Si}^{\dagger} g \psi_{Rt} \int_{0}^{T} dt' \phi_{Rt'}^{\dagger} g^{\dagger} \psi_{St'} + O(gg^{\dagger})^{2} \right\}.
$$
\n(B20)

Tracing over the *R* fields converts the terms in curly braces in Eq. $(B20)$ $(B20)$ $(B20)$ to the reservoir expectations

$$
1 - \int_{0}^{T} dt \int_{0}^{T} dt' \Big[\phi_{St}^{\dagger} \phi_{St}^{\dagger} \Big] g \Big\langle \Big[\psi_{Rt} \Big] \Big[\psi_{Rt'}^{\dagger} \phi_{Rt'}^{\dagger} \Big] \Big\rangle g^{\dagger} \Big[\phi_{St'} \Big] \n= 1 - \int_{0}^{T} dt \int_{0}^{T} dt' \Big[\phi_{St}^{\dagger} \phi_{St}^{\dagger} \Big] g e^{iE_{R}t} \Big[-\theta(t - t') \Big(K_{R}^{-1} + I/2 \Big) \Big] e^{-iE_{R}t'} g^{\dagger} \Big[\phi_{St'} \Big] \n= 1 - \int_{0}^{T} dt \int_{0}^{T} dt' \Big[\phi_{St}^{\dagger} \phi_{St}^{\dagger} \phi_{St}^{\dagger} \Big] g e^{iE_{R}t} \Big[-I/2 \Big(K_{R}^{-1} + I/2 \Big) \Big] e^{-iE_{R}t'} g^{\dagger} \Big[\phi_{St'} \Big] \n- \int_{0}^{T} dt \int_{0}^{T} dt' \Big[\phi_{St}^{\dagger} \phi_{St}^{\dagger} \phi_{St}^{\dagger} \Big] g e^{iE_{R}t} \Big[-I/2 \Big(K_{R}^{-1} + I/2 \Big) \Big] e^{-iE_{R}t'} g^{\dagger} \Big[\phi_{St'} \Big] \n- \int_{0}^{T} dt \int_{0}^{T} dt' \Big[\phi_{St}^{\dagger} \phi_{St}^{\dagger} \phi_{St}^{\dagger} \Big] g e^{iE_{R}(t - t')} g^{\dagger} [\theta(t' - t) - \theta(t - t')] \Big[\Big[\phi_{St'} \Big] \Big[\phi_{St'} \Big],
$$
\n(B21)

in which the second and later lines assume that the reservoir density matrix is perturbed little enough by the system that we can replace $\langle \phi_{Rt} \phi_{Rt'}^{\dagger} \rangle$ by the freely evolving number density $e^{iE_R t} K_R^{-1} e^{-iE_R t'}$ within the decoherence time created by the oscillatory terms $e^{iE_R(t-t')}$. Back reaction of the system on the reservoir may be taken into account by allowing K_R^{-1} to depend on $(t+t')/2$.

If the reservoir dimension, coupling *g*, and spectrum of *ER* are such that the integrals over t and t' converge $[40]$ $[40]$ $[40]$, then for sufficiently low-frequency fields in the system, one may replace the oscillating kernels with time-local interactions denoted as

$$
ge^{iE_R(t-t')}g^{\dagger} \to r\delta(t-t'), \quad ge^{iE_Rt}K_R^{-1}e^{-iE_Rt'}g^{\dagger} \to (rn_R)\delta(t-t'),
$$

$$
ge^{iE_R(t-t')}g^{\dagger}[\theta(t'-t)-\theta(t-t')] \to i\delta E_S\delta(t-t').
$$
(B22)

 r , rn_R , and δE_S must be Hermitian, by the Hermiticity of the δ function and the reservoir energy matrix E_R . The correction δE_S to the system energy is of $O(gg^{\dagger})$, and will simply be absorbed into the effective system energy matrix E_S in what follows.

The local interaction approximation $(B22)$ $(B22)$ $(B22)$ slightly violates the causal structure of the theory. It can be checked that the expectations of the second and third lines in Eq. $(B20)$ $(B20)$ $(B20)$, over both reservoir and system degrees of freedom, are both zero, by the Green's functions $(B14)$ $(B14)$ $(B14)$. If the first line of Eq. $(B22)$ $(B22)$ $(B22)$ is inserted to produce a time-local action in Eq. $(B21)$ $(B21)$ $(B21)$, the resulting trace over system fields is nonzero, due to the evaluations $\theta(t-t) \equiv I/2$. We can correct this self-interaction, which leads to misevaluation of the system functional determinant but does not affect other correlations, by substituting

$$
\int dt' \phi_{Si}^{\dagger} g e^{iE_R(t-t')} g^{\dagger} \psi_{Si'} \rightarrow \phi_{Si}^{\dagger} r \psi_{St} - \text{Tr} \left[\frac{r}{2} \right],
$$

$$
\int dt' \psi_{Si}^{\dagger} g e^{iE_R(t-t')} g^{\dagger} \phi_{Si'} \rightarrow \psi_{Si}^{\dagger} r \phi_{St} - \text{Tr} \left[\frac{r}{2} \right].
$$
 (B23)

The other two lines of Eq. $(B22)$ $(B22)$ $(B22)$ do not require correction terms. (Alternatively a different regularization of the θ functions at equal argument could be used to absorb such surface terms.)

Absorbing the leading-order corrections from Eq. $(B21)$ $(B21)$ $(B21)$ into the effective system kernel converts the free system kernel F_S from the form $(B15)$ $(B15)$ $(B15)$ into the perturbed form

$$
F_S \rightarrow \left(\phi_{S\delta t}^{\dagger} - \frac{1}{2}\psi_{S\delta t}^{\dagger}\right)(I - p_S)\left(\phi_{S0} + \frac{1}{2}\psi_{S0}\right)
$$

+
$$
\int_0^T dt \left\{ \left[\phi_{St}^{\dagger} \quad \psi_{St}^{\dagger}\right] \left[\begin{matrix} -\partial_t + iE_S + r/2\\ -\partial_t + iE_S - r/2 \end{matrix} \right] \times \left[\begin{matrix} \phi_{St} \\ \psi_{St} \end{matrix} \right] - \text{Tr}\left[\begin{matrix} r\\ 2 \end{matrix} \right] \right\}, \tag{B24}
$$

from which Eq. (26) (26) (26) in the main text is taken. The large

dissipation terms $r/2$ validate the signs of the *i* ε 's in Eq. $(B15)$ $(B15)$ $(B15)$, and the field interactions also validate the formal rotation of the discrete action. Inverting the Keldysh transform ([24](#page-9-7)) gives the continuum time-loop action corresponding to the discrete dissipative action (23) (23) (23) as follows:

$$
F_S \rightarrow \xi_{S0}^{\dagger} (I - p_S) \xi_{S0} + \int_0^T dt \times \left\{ \left[\xi_{St}^{\dagger} \quad \xi_{S, -t}^{\dagger} \right] \times \left[\begin{array}{cc} \partial_t - iE_S + r/2 + rn_R & -rn_R \\ -(r + rn_R) & -\partial_t + iE_S + r/2 + rn_R \end{array} \right] \left[\begin{array}{c} \xi_{St} \\ \xi_{S, -t} \end{array} \right] - \text{Tr} \left[\frac{r}{2} \right] \right\}, \tag{B25}
$$

corresponding to Eq. (25) (25) (25) in the main text. The final term $Tr[r/2]$ in both equations, which does not affect Green's functions but does affect the partition function, is the term which would not have been obvious from the term $\text{Tr}[(rn_R)_n]$ in the discrete representation, because it depends on the regularization of field products at equal times.

This shift in the action by the term $-Tr[rn_R+r/2]$ is related to a constraint on the causal structure. Equation $(B14)$ $(B14)$ $(B14)$ requires $\langle \psi_{St} \psi_{St}^{\dagger} \rangle = 0$. The discrete counterpart in Eq. ([23](#page-9-5)), although differing nominally only by terms of $O(\delta t)$ in a mode expansion, has expectation

$$
\langle (\xi_{n-1} - \xi_{-n})(\xi_n^{\dagger} - \xi_{-(n-1)}^{\dagger}) \rangle = -I.
$$

Thus we must identify

$$
\psi_{St} \psi_{St}^{\dagger} \equiv (\xi_{St} - \xi_{S,-t}) (\xi_{St}^{\dagger} - \xi_{S,-t}^{\dagger})
$$

$$
\leftarrow (\xi_{n-1} - \xi_{-n}) (\xi_{n}^{\dagger} - \xi_{-(n-1)}^{\dagger}) + I, \qquad (B26)
$$

under which Eq. $(B25)$ $(B25)$ $(B25)$ also follows from Eq. (23) (23) (23) . The treatment of the Green's functions proceeds from the Keldysh action ([B24](#page-19-3)) as in the main text, with subscript *s* dropped.

c. Onsager-Machlup forms

By Eq. ([B3](#page-16-3)), the outer product $|\xi_n\rangle \langle \xi_{-n}^{\dagger}|$ is the counterpart at time *n* δt to the product $|\xi\rangle \langle \xi^{\dagger}|$ in the initial ρ of Eq. ([9](#page-6-1)). A path integral in which these fields are duals to one another follows from integrating out the $\{\xi_n^{\dagger}, \xi_{-n}\}\$, and has Onsager-Machlup form [[47](#page-23-30)].

One begins by introducing shifted time-loop fields

$$
\begin{aligned} \tilde{\xi}_{St}^{\dagger} &= \xi_{St}^{\dagger} - \left[(\partial_t - iE_S + r/2 + rn_R) \xi_{S,-t} \right]^{\dagger} (rn_R)^{-1}, \\ \tilde{\xi}_{S,-t} &= \xi_{S,-t} - (rn_R)^{-1} (\partial_t - iE_S + r/2 + rn_R) \xi_{St}, \end{aligned} \tag{B27}
$$

in terms of which F_S is expressed as

$$
F_S = \xi_{S0}^{\dagger} (I - p_S) \xi_{S0} + \int dt \tilde{\xi}_{S}^{\dagger} (-rn_R) \tilde{\xi}_{S,-t} - \text{Tr} \left[\frac{r}{2} \right]
$$

$$
+ \left[\left(\partial_t - iE_S + \frac{r}{2} \right) \xi_{S,-t} \right]^{\dagger} (rn_R)^{-1} \left(\partial_t - iE_S + \frac{r}{2} \right) \xi_{St}.
$$
(B28)

(A contour rotation is needed to integrate out $\tilde{\xi}_{St}^{\dagger}$ and $\tilde{\xi}_{S,-t}$

along a convergent contour.) The surface term and constant correction will, as before, change in discrete representations underlying this continuum limit. One such representation was derived in Eqs. (11) (11) (11) – (15) (15) (15) of Ref. $[18]$ $[18]$ $[18]$ and shown to lead to Eq. ([31](#page-9-4)) for K_S^{-1} . There the integral over $\tilde{\xi}_{St}^*$ and $\tilde{\xi}_{S_t-t}$, together with the $Tr[r/2]$, was absorbed in a discrete prefactor $\Pi_n 1 / \text{Det}[(rn_R)_n \delta t]$.

It is actually more natural to construct an Onsager-Machlup action by integrating out $\psi^{\dagger} \psi$, to exploit both the simpler Keldysh Green's function structure and the interpretation of $\psi \psi^{\dagger}$ as the classical noise field arising from quantum fluctuations. The appropriate shift of field variables is

$$
\tilde{\psi}_{St}^{\dagger} \equiv \psi_{St}^{\dagger} + \left[(\partial_t - iE_S + r/2) \phi_{St} \right]^{\dagger} (rn_R + r/2)^{-1},
$$

$$
\tilde{\psi}_{St} \equiv \psi_{St} - (rn_R + r/2)^{-1} (\partial_t - iE_S + r/2) \phi_{St}, \quad (B29)
$$

and the resulting action is

$$
F_S = \left(\phi_{S\delta t}^{\dagger} - \frac{1}{2}\psi_{S\delta t}^{\dagger}\right)(I - p_S)\left(\phi_{S0} + \frac{1}{2}\psi_{S0}\right)
$$

+
$$
\int dt \widetilde{\psi}_{St}^{\dagger} \left(r n_R + \frac{r}{2}\right) \widetilde{\psi}_{St} - \text{Tr}\left[\frac{r}{2}\right]
$$

+
$$
\left[\left(\partial_t - iE_S + \frac{r}{2}\right) \phi_{St}\right]^{\dagger} \left(r n_R + \frac{r}{2}\right)^{-1} \left(\partial_t - iE_S + \frac{r}{2}\right) \phi_{St}.
$$

(B30)

A discrete representation identical in structure to that for Eq. ([B28](#page-19-0)) is readily constructed, and the Gaussian kernel (rn_R) $+r/2$ ⁻¹ ensures that the resulting evolution equation for $K_S^{-1} + I/2$ reproduces Eq. ([31](#page-9-4)).

APPENDIX C: THE DOI-PELITI REPRESENTATION FOR NONCOMMUTING OBSERVABLES

As for the Schwinger-Keldysh time loop, the DP path integral may be used to represent either the original generating function $(A13)$ $(A13)$ $(A13)$ or a generating functional, depending on whether the complex argument or the source terms in the Liouville operator are varied. Here, as in Appendix B, the generating function will be used as the path to the generating functional.

1. Operator representation of general generating functions

To depart from the original Doi association of classical raising and lowering operators with eigenvalues in a quantum CSCO, we will work with the older representation of the classical generating function as a function of (matrix-valued) complex arguments. The assumption that the matrix logarithm can be expanded as an analytic polynomial in complex variables will then be used as the basis for the Doi construction. We begin, however, by noting the correspondence between analytic functions and Doi operators as an aid in organizing the later quadrature of the Liouville equation (17) (17) (17) .

a. Map between algebraic and analytic representations

The number 1 represents the Doi right "vacuum,"

$$
1 \leftrightarrow |0). \tag{C1}
$$

Complex scalar components of the matrix *z* are the raising operators

$$
z_j \leftrightarrow A_j^{\dagger}.
$$
 (C2)

Here *j* may be a vector index if *z* is diagonal with eigenvalues z_j , or a composite index such as μ_{ν} , or an index in the adjoint representation. Derivatives with respect to *z* are the lowering operators

$$
\frac{\partial}{\partial z_i} \leftrightarrow A^i,\tag{C3}
$$

hence

$$
[A^i, A_j^{\dagger}] = \delta_j^i. \tag{C4}
$$

A discrete number basis corresponds to a polynomial expansion for the generating function,

$$
\left(\prod_{j=1}^{D} z_j^{n_j}\right) \cdot 1 \leftrightarrow \prod_{j=1}^{D} (A_j^{\dagger})^{n_j}|0\rangle = |\vec{n}\rangle, \tag{C5}
$$

and lowering operators annihilate the right vacuum

$$
0 = \frac{\partial}{\partial z_i} 1 \leftrightarrow A^i | 0).
$$
 (C6)

The left vacuum evaluates the generating function at zero argument, and so is represented as

$$
\int Dz \,\delta(z) \leftrightarrow (0]. \tag{C7}
$$

The measure and Dirac δ function are over whatever components are assumed for *z*, defined so that acting on unity, they give $(0|0)=1$. Automatically the creation operators annihilate the left vacuum,

$$
0 = \int Dz \delta(z) z_i \leftrightarrow (0 | A^i, \tag{C8}
$$

and the inner product of the Glauber coherent state with all number states is unity,

$$
1 = \int Dz \delta(z) \exp \sum_{j} \partial/\partial z_{j} \left(\prod_{j=1}^{D} z_{j}^{n_{j}} \right) \cdot 1
$$

$$
\leftrightarrow (0 | \exp \sum_{j} A_{j} \prod_{j=1}^{D} (A_{j}^{\dagger})^{n_{j}} | 0). \tag{C9}
$$

The generating function Ψ of Eq. ([A13](#page-14-0)) thus represents the usual Doi state vector

$$
\Psi(z) \leftrightarrow |\Psi).
$$
 (C10)

b. Peliti field insertion

To construct the Peliti functional integral from an analytic representation of the generating function, it is convenient to drop the component index *j* from the matrix *z*. This is because the left Doi state makes *z* a dummy variable of integration, so that another such variable will be needed for each time in the path integral. Therefore index these matrixvalued variables z_n , for $n \in \{0, ..., N\}$ corresponding to times $(0, \ldots, N) \times \delta t$, as in the SK development.

The representation for a right coherent state follows from the usual algebraic form,

$$
(\zeta^{\dagger}) = (0|e^{-(\zeta^{\dagger}\zeta)/2} \sum_{N=0}^{\infty} \frac{(\zeta^{\dagger} \cdot A)^N}{N!}
$$

$$
\leftrightarrow \int Dz_0 \delta(z_0) e^{-(\zeta^{\dagger}\zeta)/2} \sum_{N=0}^{\infty} \frac{(\zeta^{\dagger} \cdot \partial/\partial z_0)^N}{N!}
$$

$$
= \int Dz_0 \delta(z_0) e^{-(\zeta^{\dagger}\zeta)/2} e^{\zeta^{\dagger} \cdot \partial/\partial z_0}.
$$
(C11)

(Note that again the inner product notation $\zeta^{\dagger} \cdot A$, or just $\zeta^{\dagger} \zeta$, is being used as shorthand for the $D \times D$ matrix trace where no ambiguity results.) The opening coherent state is obtained equivalently as follows:

$$
|\zeta| = e^{-(\zeta^{\dagger}\zeta)/2} \sum_{N=0}^{\infty} \frac{(A^{\dagger} \cdot \zeta)^N}{N!} |0\rangle \leftrightarrow e^{-(\zeta^{\dagger}\zeta)/2} \sum_{N=0}^{\infty} \frac{(z_1 \cdot \zeta)^N}{N!} \cdot 1
$$

$$
= e^{-(\zeta^{\dagger}\zeta)/2} e^{z_1 \cdot \zeta} \cdot 1. \tag{C12}
$$

The Peliti coherent-state insertion of unity,

$$
\int \frac{D\zeta^{\dagger}D\zeta}{\text{Det}(\pi)}|\zeta\rangle(\zeta^{\dagger}| \to \int \frac{D\zeta^{\dagger}D\zeta}{\text{Det}(\pi)} e^{-\zeta^{\dagger}\zeta} e^{z_1 \cdot \zeta} \int Dz_0 \delta(z_0) e^{\zeta^{\dagger} \cdot \partial/\partial z_0}
$$
\n
$$
= \int Dz_0 \delta(z_0) e^{z_1 \cdot \partial/\partial z_0}, \tag{C13}
$$

is then just the argument substitution operation $z_0 \mapsto z_1$. Corresponding to the measure Dz and Dirac δ , the notation Det(π) is shorthand for the determinant of π times the appropriate identity matrix for the representation of $z(\pi^D)$ if z is diagonal or π^{D^2} for general Hermitian *z*).

To initiate the path integral, use an insertion of unity to put the generating function at time zero, denoted $\Psi_0(z)$, into a standard coherent-state decomposition as follows:

$$
\int \frac{D\zeta_0^{\dagger} D\zeta_0}{\mathrm{Det}(\pi)} |\zeta_0\rangle(\zeta_0^{\dagger} |\Psi_0\rangle \leftrightarrow \int \frac{D\zeta_0^{\dagger} D\zeta_0}{\mathrm{Det}(\pi)} e^{(z_0 - \zeta_0^{\dagger}) \cdot \zeta_0} \Psi_0(\zeta_0^{\dagger}). \tag{C14}
$$

The generating function is then advanced in time through the recursion

$$
\Psi_{n\delta t}(z_n)
$$
\n
$$
= \int \frac{D\zeta_n^{\dagger} D\zeta_n}{\text{Det}(\pi)} e^{(z_n - \zeta_n^{\dagger})\zeta_n}
$$
\n
$$
\times \int Dz_{n-1} \delta(z_{n-1}) e^{\zeta_n^{\dagger} \cdot \partial/\partial z_{n-1} - \mathcal{L}_n(z_{n-1}, \partial/\partial z_{n-1}) \cdot \partial t} \Psi_{n-1}(z_{n-1}),
$$
\n(C15)

in which \mathcal{L}_n is the Liouville operator ([A23](#page-15-0)) parametrized by

 $(E, r/2, rn_R)$ ⁿ if these sources are time dependent, and expressed as a function of z_{n-1} and $\partial/\partial z_{n-1}$.

The DP generating function at time $N\delta t$ is therefore given by the path integral

$$
\Psi_{N\delta i}(z_N) = \int_0^N \mathcal{D}\zeta^{\dagger} \mathcal{D}\zeta \exp\left[(z_N - \zeta_N^{\dagger})\zeta_N + \sum_{n=1}^N L_n \delta t \right] \Psi_0(\zeta_0^{\dagger}), \tag{C16}
$$

from which Eq. (39) (39) (39) is drawn. The associated measure

$$
\int_0^N \mathcal{D}\zeta^{\dagger} \mathcal{D}\zeta \equiv \prod_{n=0}^N \int \frac{D\zeta_n^{\dagger} D\zeta_n}{\text{Det}(\pi)} \tag{C17}
$$

then defines the continuum limit (40) (40) (40) , and the action is given in Eq. (41) (41) (41) .

The generating functional is $\Psi_{N\delta t}$ evaluated at $z_N = I$, with $\{(E, r/2, rn_R)_n\}$ varied. (Strictly speaking, if we leave all of ${E, r/2, rn_R}$ Hermitian, the trace $\Psi_{N\delta f}(I) = 1$ is strictly preserved, so such variations generate only Ward identities of the theory. In constructing the DP-SK operator correspondence, we have thus implicitly considered more general variations.) The usual field shift $\zeta_n^{\dagger} \rightarrow \overline{\zeta}_n^{\dagger} \equiv \zeta_n^{\dagger} - I$ gives the discrete generating functional

$$
\Psi_{N\delta i}(I) = \int_0^N \mathcal{D}\tilde{\zeta}^{\dagger} \mathcal{D}\zeta \exp\left\{-\frac{\tilde{\zeta}_N^{\dagger}}{\tilde{\zeta}_N \tilde{\zeta}_N} + \sum_{n=1}^N L_n \delta t - \text{Tr}\ln[I - K_0^{-1}\tilde{\zeta}_0^{\dagger}]\right\}
$$
(C18)

of which the continuum limit defines Eq. (44) (44) (44) in the main text. It is perhaps worth remarking explicitly that in the discrete form, the Lagrangian is then written

$$
L_n \delta t \equiv (\tilde{\zeta}_n^{\dagger} - \tilde{\zeta}_{n-1}^{\dagger}) \cdot \zeta_{n-1} - \mathcal{L}_n(\tilde{\zeta}_n^{\dagger} + I, \zeta_{n-1}) \delta t. \quad (C19)
$$

Thus $\widetilde{\zeta}_n^{\dagger}$ has substituted for ϵ_{n-1} , and ζ_{n-1} for $\partial/\partial \epsilon_{n-1}$, in the Liouville operator $(A23)$ $(A23)$ $(A23)$ and Eq. (17) (17) (17) of the main text.

c. Stationary points and fluctuations

The discrete-form stationary points of the classical Lagrangian are

$$
(\widetilde{\xi}_n^{\dagger} - \widetilde{\xi}_{n-1}^{\dagger})/\delta t = [iE_n, \widetilde{\xi}_n^{\dagger}] + \left\{\frac{r_n}{2}, \widetilde{\xi}_n^{\dagger}\right\} - \widetilde{\xi}_n^{\dagger}(rn_R)_n \widetilde{\xi}_n^{\dagger},
$$

$$
(\zeta_n - \zeta_{n-1})/\delta t = [iE_n, \zeta_{n-1}] - \left\{\frac{r_n}{2}, \zeta_{n-1}\right\} + (rn_R)_n
$$

$$
+ (rn_R)_n \widetilde{\xi}_n^{\dagger} \zeta_{n-1} + \zeta_{n-1} \widetilde{\xi}_n^{\dagger}(rn_R)_n, \quad (C20)
$$

from which the continuum equation (45) (45) (45) follows as a regular limit.

Therefore we introduce the shifted field $\tilde{\zeta}_n = \zeta_n - K_{n\delta n}^{-1}$, where $K_{n\delta t}^{-1}$ is a solution to the stationary point condition ([45](#page-11-0)) for ζ_n and K_0^{-1} is the value appearing in the initial condition

[equal to K^{-1} of Eq. ([9](#page-6-1))]. The quadratic and higher dependence of the Liouville operator of shifted arguments is separated out by defining

$$
\mathcal{L}_n(\tilde{\zeta}_n^{\dagger} + I, \tilde{\zeta}_{n-1} + K_{(n-1)\delta t}^{-1}) \equiv \tilde{\zeta}_n^{\dagger} \cdot (K_{n\delta t}^{-1} - K_{(n-1)\delta t}^{-1}) + \tilde{\mathcal{L}}_n(\tilde{\zeta}_n^{\dagger}, \tilde{\zeta}_{n-1}).
$$
\n(C21)

The resulting kernel for the fluctuation matrices takes the form

$$
\widetilde{\mathcal{L}}_n(\widetilde{\zeta}_n^{\dagger}, \widetilde{\zeta}_{n-1}) = \operatorname{Tr} \left[\widetilde{\zeta}_{n-1} \left(iE + \frac{r}{2} \right)_{n} \widetilde{\zeta}_n^{\dagger} - \widetilde{\zeta}_n^{\dagger} \left(iE - \frac{r}{2} \right)_{n} \widetilde{\zeta}_{n-1} \right. \left. - (rn_R)_n \widetilde{\zeta}_n^{\dagger} \widetilde{\zeta}_{n-1} \widetilde{\zeta}_n^{\dagger} - (rn_R)_n \widetilde{\zeta}_n^{\dagger} \widetilde{\zeta}_{n-1} \widetilde{\zeta}_n^{\dagger} \right], \tag{C22}
$$

which serves as the basis for the continuum action (46) (46) (46) . As noted in the text, the fluctuation kernel $(C22)$ $(C22)$ $(C22)$ can be put into a standard tridiagonal form by accounting for the distinct matrix orderings between $\tilde{\zeta}$ and $\tilde{\zeta}^{\dagger}$.

2. Computation of the classical MSR response functions

To solve for the retarded and advanced Green's function components, note first that the absence of a $\tilde{\zeta}^2$ interaction in Eq. ([C22](#page-22-12)) makes the inversion of the $\tilde{\zeta}\tilde{\zeta}^{\dagger}$ interactions independent of the $\tilde{\zeta}^{\dagger 2}$ interaction, by the same arguments that relate Eqs. (27) (27) (27) and (28) (28) (28) for the Keldysh response functions in the main text. We may therefore collect terms in the exponent of Eq. $(C18)$ $(C18)$ $(C18)$ in either of the two equivalent forms

$$
\widetilde{\zeta}_{N}^{\dagger} \zeta_{N} - \sum_{n=0}^{N-1} L_{n} \delta t + \operatorname{Tr} \ln \left[I - \widetilde{\zeta}_{0}^{\dagger} K_{0}^{-1} \right]
$$
\n
$$
= \left[\widetilde{\zeta}_{0}^{\dagger} \cdots \widetilde{\zeta}_{N}^{\dagger} \right] \cdot \begin{bmatrix} 1 & & & \\ -u_{1} & \cdots & & \\ -u_{N} & 1 \end{bmatrix} \begin{bmatrix} \widetilde{\zeta}_{0} \\ \vdots \\ \widetilde{\zeta}_{N} \end{bmatrix} + O(\widetilde{\zeta}^{\dagger 2})
$$
\n
$$
= \left[\widetilde{\zeta}_{0} \cdots \widetilde{\zeta}_{N} \right] \cdot \begin{bmatrix} 1 & -u_{1}^{\dagger} & & \\ & \ddots & -u_{N}^{\dagger} & \\ & & 1 \end{bmatrix} \begin{bmatrix} \widetilde{\zeta}_{0}^{\dagger} \\ \vdots \\ \widetilde{\zeta}_{N}^{\dagger} \end{bmatrix} + O(\widetilde{\zeta}^{\dagger 2}), \tag{C23}
$$

where the inner product notation has been used for the trace

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and the operators u and u^{\dagger} (no longer unitary, but still conjugate) are defined in the adjoint representation by their action to the right on matrices as follows:

$$
u_n \widetilde{\zeta}_{n-1} = \widetilde{\zeta}_{n-1} + [iE_n, \widetilde{\zeta}_{n-1}] \delta t - \left\{ \frac{r_n}{2}, \widetilde{\zeta}_{n-1} \right\} \delta t,
$$

$$
u_n^{\dagger} \widetilde{\zeta}_n^{\dagger} = \widetilde{\zeta}_n^{\dagger} - [iE_n, \widetilde{\zeta}_n^{\dagger}] \delta t - \left\{ \frac{r_n}{2}, \widetilde{\zeta}_n^{\dagger} \right\} \delta t.
$$
 (C24)

In the simple case of E_n and r_n constant, the resulting Green's functions are the lower- and upper-triangular forms

$$
\left\langle \left| \begin{matrix} \tilde{\zeta}_{0} \\ \vdots \\ \tilde{\zeta}_{N} \end{matrix} \right| \begin{matrix} \tilde{\zeta}_{0}^{\dagger} \\ \tilde{\zeta}_{N} \end{matrix} \right\rangle = \begin{bmatrix} 1 \\ \vdots \\ u^{N} \cdots 1 \end{bmatrix},
$$
\n
$$
\left\langle \left| \begin{matrix} \tilde{\zeta}_{0}^{\dagger} \\ \vdots \\ \tilde{\zeta}_{N}^{\dagger} \end{matrix} \right| \begin{matrix} \tilde{\zeta}_{0}^{\dagger} \\ \tilde{\zeta}_{0}^{\dagger} \cdots \tilde{\zeta}_{N} \end{matrix} \right\rangle = \begin{bmatrix} 1 & \cdots & u^{\dagger N} \\ \vdots & \ddots & \vdots \\ & & 1 \end{bmatrix}. \qquad (C25)
$$

In discrete indices these are simply

$$
\langle \widetilde{\zeta}_n^{\dagger} \widetilde{\zeta}_n \cdot \rangle = u^{\dagger n' - n} \theta_{n',n}^+ = e^{-(iE + r/2)(n' - n)\delta t} \theta_{n',n}^+,
$$

$$
-\langle \widetilde{\zeta}_n \widetilde{\zeta}_n^{\dagger} \rangle = -u^{n-n'} \theta_{n,n'}^+ = -e^{(iE - r/2)(n-n')\delta t} \theta_{n,n'}^+, \quad (C26)
$$

and in the continuum limits they yield Eq. (47) (47) (47) in the main text.

The classical correlation function $\langle \tilde{\zeta}_n \tilde{\zeta}_{n'} \rangle$ is not pursued here, as it corresponds to a fourth-order moment in the SK representation, which has not been computed for comparison. It remains interesting that the response functions $(C26)$ $(C26)$ $(C26)$, also formally fourth-order moments, have as their only nonvanishing components the same Green's functions as the second-order SK response functions.

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