

Doi-Peliti methods for non-commuting observables

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The quantum-field methods derived by Doi and Peliti to treat reaction-diffusion problems were originally based on a classical probability description and on Markovian evolution. The fully-decoherent limit of an underlying quantum transport process, which these assumptions entail, restricts the classical description to the commuting observables of the quantum formulation, and coarse-grains the entropy to the equilibrium Boltzmann form. In this paper the Doi-Peliti formulation is generalized to describe driven quantum ensembles, for which the classical state variables arise as expectations of non-commuting quantum observables. The resulting classical description remains of Martin-Siggia-Rose form, but preserves the exact entropy of the quantum density matrix, including its symmetries under unitary transformation of the state variables and the resulting dependence on classical currents required by these symmetries. The Fokker-Planck equation defines the universality class of driven quantum ensembles, and within this class the classical state-variable field theory is invertible to the underlying Schwinger-Keldysh time-loop quantum formulation.

I. INTRODUCTION

Two field-doubling techniques for quantized systems, with similar formal structure but different physical interpretations, have found wide use for the study of time-dependent probabilistic processes. Schwinger's introduction of the time-loop S -matrix [21] made it possible to express time-dependent quantum correlations in both vacuum and finite-temperature systems as functions of initial data alone. Keldysh subsequently clarified the causal structure of the time-loop theory [13] by considering independent "classical" and "quantum" superpositions of fields on the forward and backward legs of the time loop. The Green's function for these fields has the now-familiar tri-diagonal form, whose blocks are the correlation function of classical components and the response functions of classical to quantum components.

Martin, Siggia, and Rose (MSR) later introduced a field homologous to Keldysh's quantum superposition of the time-loop fields [15], to create a tri-diagonal Green's function for the study of classical statistical field problems. 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 [4, 5] and Peliti [19, 20], for stochastic partial differential equations by Hochberg et. al. [10], and for conformally invariant operators by Cooper et. al. [3]. The stochastic formalism has been the subject of extensive reviews [16] and lecture notes [1], as has the homology between the Schwinger-Keldysh (SK) and Doi-Peliti (DP) field formalisms [12].

There is considerable overlap in the physical systems to which the two formalisms can be applied. The SK formalism provides a natural way to introduce dissipation into the treatment of quantum transport processes, a topic considered further below. Alternatively, if decoher-

ence is assumed to be so strong that the quantum density matrix and Hamiltonian evolution can be replaced altogether with a classical probability distribution evolving under a Markov process, the DP construction provides an independent pseudo-Hamiltonian description, and a prescription for perturbative renormalization of the diffusive field theory [10, 15, 16]. The MSR prescription also provides a systematic way to construct, for an arbitrary Markov process, the effective Hamiltonian [6] which is the basis for non-perturbative estimation of large-deviation probabilities [9, 14, 24].

Given the overlap in their domains of application, a topic that has received surprisingly little attention is the transformation back and forth between SK and DP representations for dissipative quantum systems. DP, and more generally MSR, formalisms are usually drawn directly from classical descriptions, which presume the existence of a probability distribution. If the distribution and its associated Markov process are effective representations of an underlying decoherent quantum system, they are defined on at most a complete set of commuting observables (CSCO) in the quantum formulation.

Sometimes the complete set of *classical state variables* needed to describe a dissipatively-evolving quantum density matrix cannot be captured by a CSCO in the quantum theory, and 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. 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 [8].

A related error – which is of conceptual importance whether or not it creates impediments to prediction – occurs in formulating a statistical mechanics for driven dissipative systems. The best approximation to the true entropy of a driven system that can be formed once its currents have been discarded is the Boltzmann entropy of

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its charges, treated as if they were equilibrium state variables. This equilibrium-*form* entropy measures the statistical uncertainty of an equilibrium distribution which is a *coarse-graining* of the actual driven distribution. As the actual distribution is not that of any equilibrium, the coarse-grained entropy is only a loose bound on the actual statistical uncertainty [22]. Coarse-graining is essential to entropy maximization principles [7], but the particular coarse-graining generated by the Markovian approximation removes the currents that are the distinguishing feature of the driven state, precluding any possible application of entropy maximization to account for these currents.

Onsager attempted to work around this problem by re-introducing currents as classical auxiliary fields, to be related to the gradients of the equilibrium state variables by means of classical dissipation coefficients [17]. 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. Exact treatment of driven quantum ensembles [22, 23], without the imposition of the Markovian approximation, shows that such phenomenological principles based on the coarse-grained entropy are sometimes unnecessary. Maximization of a true excess entropy, 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 [23].

This paper shows how DP methods can be applied to the classical description of driven, dissipative quantum systems which satisfy a maximum-entropy criterion, but for which the full complement of classical state variables cannot be represented within any CSCO of the underlying quantum theory. It will not be surprising that a DP construction can be performed for such systems; the DP field Hamiltonian simply represents the action of a Liouville operator on a generating function of the quantum theory, which we are free to specify. Perhaps more interesting will be the existence of the inverse construction; whenever the underlying quantum density is defined by maximum entropy, a complete classical description suffices to reconstruct the full quantum ensemble. The admission of state variables corresponding to non-commuting observables makes it possible to describe both charges and currents that are canonically conjugate under the quantum Hamiltonian, and thus to produce oscillating stationary states and other distributions incompatible with classical Markov processes.

A central feature of the paper will be the map between the probabilistic and quantum operators that relates the DP and SK levels of description. The homology of the formalisms, together with the difference in their interpretations, has so far obscured this relation. The interesting feature of the map will be the manner in which nonlinearities preserve both the classical equations of motion, and the fluctuation-dissipation theorem for stochastic driv-

ing.

All the main relations between quantum and classical representations can be found in Sec. II, which introduces the density matrices and generating functions considered here, and their connection through a Liouville equation. Sec. III then constructs the time-loop path integral for the SK representation, first for free evolution and then with dissipation introduced in various ways. Sec. IV converts the differential Liouville operator into the equivalent DP path integral, and compares the structural homology in the two representations to a few explicit operator maps (variants on the number operator in both theories) that can easily be constructed. Not surprisingly, the structural homology can be extended to a limited degree of identity in the free response functions of the two theories, even though the operator products with these Green’s functions do not represent equivalent observables. Finally Sec. V offers concluding remarks.

II. PRELIMINARIES: DENSITY MATRICES AND GENERATING FUNCTIONS

Two-field operator methods can be simply understood as a way to represent the action of differential Liouville operators on generating functions of complex arguments. Therefore we begin with the transformation between maximum-entropy quantum density matrices and their equivalent generating functions.

The DP path integral representation of the generating functional can further be understood as the time evolution of the generating function perturbed by time-dependent sources, and then evaluated at complex argument $z = 1$ where it is simply the trace of the density matrix. In order to identify the correspondence between classical sources and quantum operators on the density matrix, the basic transformation is derived in this section for a quantum density evolving with fully general dissipation terms. These terms will usually have the interpretation of dynamically generated operators in the most-general effective theory at leading order in perturbations. The following sections return to how such terms are generated by tracing over degrees of freedom within the quantum theory, starting from a free Hamiltonian.

A. Density matrices with structure in non-commuting observables

The problem of independent classical state variables arising from non-commuting charges and currents in quantum mechanics is readily captured in a class of maximum-entropy density matrices, which generalize the equilibrium density to reflect all of the symmetries in the underlying quantum kinematics. Much of the phenomenology of these density matrices was developed in Ref’s. [22, 23]. The dissipative dynamics of such densities has direct application in quantum optics [2]. They

may also be applied to the statistical description of driven chemical reactions, where the excitations describe particle number in a second-quantized field theory over nuclear positions, and the states correspond to distinct multi-electron occupancies of bond and transition-state orbitals. A field theory of this kind might serve as a foundation for deriving the effective transition-state Hamiltonian used by Eyring [9].

Consider a D -dimensional quantum simple harmonic oscillator, whose state space results from the action of D orthogonal creation and annihilation operators starting from a ground (ket) state $|0\rangle$. The operator commutation relations, $[a^\mu, a_\nu^\dagger] = \delta_\nu^\mu$, $\mu, \nu \in 1, \dots, D$, 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., $[\hat{n}_\nu^\mu] \equiv [a_\nu^\dagger a^\mu]$) 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

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

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

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

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, $\langle \vec{n}|$, is the left eigenvector of the number operator, also with eigenvalues n_μ . The conjugate coherent state, $\langle \xi^\dagger|$, is the left eigenvector of the creation operator with eigenvalues ξ_ν^* for components a_ν^\dagger . These are all normalized: $\langle 0|0\rangle = \langle \vec{n}|\vec{n}\rangle = \langle \xi^\dagger|\xi\rangle = 1$.

A set of density matrices that generalize the equilibrium density matrix, but retain a simple expression for the entropy and its maximization principle, are diagonal in the outer product of coherent states, with Gaussian weight:

$$\rho = \int d\xi^\dagger d\xi \text{Det}\left(\frac{K}{\pi}\right) e^{-\xi^\dagger K \xi} |\xi\rangle \langle \xi^\dagger|. \quad (3)$$

K is a $D \times D$ Hermitian matrix, assumed to have only positive eigenvalues. Its inverse is the classical expected excitation number

$$n \equiv \text{Tr}(\rho \hat{n}) = K^{-1}. \quad (4)$$

Whereas only D independent diagonal number operators can be formed, general Hermitian n have D^2 independent

parameters. Under any physical interpretation in which the $D(D+1)/2$ real, symmetric components of n correspond to time-reversal invariant (or ‘‘charge-valued’’) state variables, the $D(D-1)/2$ imaginary, antisymmetric components change sign under time reversal and have the interpretation of currents.

The densities (3) are readily shown [22] 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

$$S(\rho) \equiv -\text{Tr}(\rho \log \rho) \\ = \text{Tr}[(I + n) \log(I + n) - n \log n]. \quad (5)$$

(Here 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.) The matrix trace is invariant under similarity transform of n by unitary transformations, ensuring that the status of charge-valued and current-valued state variables is symmetric, and that the exact entropy cannot privilege one class over the other.

The Hamiltonian for such a simple-harmonic system is written (up to constants that do not affect the evolution of states) as $\hat{H} \equiv \text{Tr}[E \hat{n}] = a_\nu^\dagger E_\mu^\nu a^\mu$, for some $D \times D$ Hermitian matrix E . The equilibrium Bose density matrix results when $K \equiv (e^{\beta E} - I)$. The cases of interest here will be those in which $[E, K] \neq 0$. 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

$$\rho_{\delta t} = e^{i\hat{H}\delta t} \rho e^{-i\hat{H}\delta t} \\ = \int d\xi^\dagger d\xi \text{Det}\left(\frac{K}{\pi}\right) e^{-\xi^\dagger K \xi} |U\xi\rangle \langle \xi^\dagger U^\dagger| \\ = \int d\xi^\dagger d\xi \text{Det}\left(\frac{K}{\pi}\right) e^{-\xi^\dagger U K U^\dagger \xi} |\xi\rangle \langle \xi^\dagger|. \quad (6)$$

The notation $U \equiv e^{iE\delta t}$ has been introduced for the differential unitary evolution operator of vectors ξ , and $U^\dagger \equiv e^{-iE\delta t}$ for its Hermitian conjugate. To transform the second to the third line of Eq. (6), the joint change of variable $\xi \rightarrow U^\dagger \xi$, $\xi^\dagger \rightarrow \xi^\dagger U$ has been performed. It follows that the effect of Hamiltonian evolution is unitary on K and hence n , and so never changes the exact entropy (5).

The lowest-order dissipative generalization of unitary evolution that is linear in excitation number, n , generalizes the action on K in Eq. (6) to

$$\frac{dn}{dt} = i[E, n] + rn_R - \left\{\frac{r}{2}, n\right\}. \quad (7)$$

Here rn_R is a Hermitian source rate of excitations for n , and r is a positive-semidefinite Hermitian matrix of loss rates. The notation is chosen to simplify in the case of isotropic dissipation, in which r is a positive real number times I and n_R is the expectation of a Reservoir excitation number in diffusive exchange with n . Then the

particle-exchange term in Eq. (7) becomes $r(n_R - n)$. Linear dissipation is readily obtained when the system described by K is part of a larger simple-harmonic system also including the reservoir degrees of freedom, after averaging second-order system-reservoir interactions in the Born approximation [2]. For the purposes of this paper, r and rn_R need not have any particular relation.

Time evolution (7) exactly preserves the form (3) of the density matrix, and is obtained directly [23] by the operator Fokker-Planck evolution

$$\begin{aligned} \frac{\partial \rho}{\partial t} &= iE_\mu^\nu [a_\nu^\dagger a^\mu, \rho] \\ &+ (r + rn_R)_\mu^\nu \left(a^\mu \rho a_\nu^\dagger - \frac{1}{2} \{a_\nu^\dagger a^\mu, \rho\} \right) \\ &+ (rn_R)_\mu^\nu \left(a_\nu^\dagger \rho a^\mu - \frac{1}{2} \{a^\mu a_\nu^\dagger, \rho\} \right). \end{aligned} \quad (8)$$

Eq. (8) is the most general trace-preserving operator equation bilinear in a and a^\dagger , providing an alternative criterion to which Eq. (7) is the most general solution.

B. Probability distributions and generating functions

At any single time, it is always possible to diagonalize K , and with respect to the diagonalizing basis ρ is defined from a probability mass function P on the independent number components as

$$\rho = \sum_{\vec{n}} P(\vec{n}) |\vec{n}\rangle \langle \vec{n}|. \quad (9)$$

The 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

$$\Psi(\vec{z}) \equiv \sum_{\vec{n}} P(\vec{n}) \prod_{i=1}^D z_i^{n_i}, \quad (10)$$

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

$$\Psi(\vec{z}) \equiv \text{Tr} \left(\rho \prod_{i=1}^D z_i^{\hat{n}_i} \right) = \text{Tr} \left(\rho e^{\text{Tr}[\hat{n} \log z]} \right), \quad (11)$$

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

MSR and DP methods are conventionally defined for generating functions of the form (10) with D complex arguments, in which the mass function P evolves as a Markov process. For ρ as in Eq. (3) with $[E, K] \neq 0$, neither an invariant diagonalizing basis, nor a Markov process for the instantaneously-definable mass functions P ,

is possible. However, the second expression in Eq. (11), with z elevated to a general $D \times D$ complex matrix, provides an appropriate generalization of the classical generating function, while maintaining a decomposition to which MSR and DP methods can readily be applied. If $\log z$ and \hat{n} are written in the adjoint representation, $\text{Tr}[\hat{n} \log z]$ is the inner product of their independent coefficients, which will therefore be denoted in shorthand $\hat{n} \cdot \log z$ below where no confusion results. As a notational convenience, let $w \equiv \log z$, as this quantity will appear frequently

C. Normal-ordering and anti-normal ordering

The action on ρ of the operators in the first two lines of Eq. (8) has a simple expression in terms of the generating function (11), but the action of the operators in the last line of Eq. (8) does not. To expose the physical significance of this difference, it is convenient 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 whatever index structure appears in $*$, but to have all creation operators to the left of any annihilation operator. Anti-normal 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

$$a^\dagger w a =: a^\dagger w a : \equiv a_\nu^\dagger w_\mu^\nu a^\mu = a^\mu w_\mu^\nu a_\nu^\dagger - w_\mu^\mu \quad (12)$$

$$\equiv !a^\dagger w a! - \text{Tr}[w]. \quad (13)$$

For this contraction it follows that

$$e^{!a^\dagger w a!} = \text{Det}[z] e^{:a^\dagger w a:}. \quad (14)$$

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

$$e^{:a^\dagger w a:} =: e^{a^\dagger(z-I)a} :=: e^{a^\dagger \epsilon a} :, \quad (15)$$

and for an ANO number operator,

$$e^{!a^\dagger w a!} =!e^{a^\dagger(I-z^{-1})a}! \equiv!e^{a^\dagger \bar{\epsilon} a}!. \quad (16)$$

The notations $\epsilon \equiv z - I$ and $\bar{\epsilon} \equiv I - z^{-1}$ have been introduced for two combinations that will arise repeatedly.

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

$$\begin{aligned} \Psi &\equiv \text{Tr} \left[e^{:a^\dagger w a:} \rho \right] = \text{Tr} \left[: e^{a^\dagger \epsilon a} : \rho \right] \\ \bar{\Psi} &\equiv \text{Tr} \left[e^{!a^\dagger w a!} \rho \right] = \text{Tr} \left[!e^{a^\dagger \bar{\epsilon} a}! \rho \right] = \text{Det}[z] \Psi, \end{aligned} \quad (17)$$

and the relation between them follows from Eq. (14). Explicit arguments of Ψ and $\bar{\Psi}$ 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 (3) of ρ , the fact that coherent states are eigenstates of a or a^\dagger , the definitions (17) as traces, and the normalization of coherent states, it is straightforward to compute that

$$\begin{aligned}\Psi &= \frac{1}{\text{Det}(I - K^{-1}\epsilon)} \\ \bar{\Psi} &= \frac{1}{\text{Det}(I - (I + K^{-1})\bar{\epsilon})}.\end{aligned}\quad (18)$$

The first line in Eq. (18) follows from direct evaluation of the Gaussian integral, while the second line is most easily obtained from the first line and the relation (17) of $\bar{\Psi}$ to Ψ . The physically relevant observation is that ϵ couples to K^{-1} , while $\bar{\epsilon}$ couples to $I + K^{-1}$.

D. Time evolution of generating functions

Operator evolution (8) on ρ induces differential evolution of the argument z of the generating functions. Through their coupling to the number matrix in Eq. (18), this evolution can be converted to the equivalent evolution on K or n .

It might be expected, from the action of a and a^\dagger on coherent states, that a bilinear operator evolution equation should yield a simple harmonic oscillator Hamiltonian for z . This intuition is qualitatively correct as long as the operator ordering in the evolution equation corresponds to that in the generating function employed. (The simple harmonic Hamiltonian actually applies to ϵ or $\bar{\epsilon}$, whose

constant offsets relative to z are also important.) Thus the function Ψ defined from NO insertions evolves simply under the first two lines of Eq. (8), while the function $\bar{\Psi}$ 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

$$\begin{aligned}: e^{a^\dagger \epsilon a} :: a^\dagger M a : &= : e^{a^\dagger \epsilon a} (a^\dagger M a) : + : e^{a^\dagger \epsilon a} (a^\dagger \epsilon M a) : \\ : a^\dagger M a :: e^{a^\dagger \epsilon a} &= : (a^\dagger M a) e^{a^\dagger \epsilon a} : + : (a^\dagger M \epsilon a) e^{a^\dagger \epsilon a} :, \end{aligned}\quad (19)$$

while the two products for ANO operators reduce to

$$\begin{aligned}!e^{a^\dagger \bar{\epsilon} a} !a^\dagger M a! &= !e^{a^\dagger \bar{\epsilon} a} (a^\dagger M a)! - !e^{a^\dagger \bar{\epsilon} a} (a^\dagger M \bar{\epsilon} a)! \\ !a^\dagger M a !e^{a^\dagger \bar{\epsilon} a} &= !(a^\dagger M a) e^{a^\dagger \bar{\epsilon} a} ! - !(a^\dagger \bar{\epsilon} M a) e^{a^\dagger \bar{\epsilon} a} !. \end{aligned}\quad (20)$$

For the first line of Eq. (8), the NO insertion and Eq. (19), with $M = E$, give

$$\begin{aligned}\text{Tr} \left[: e^{a^\dagger \epsilon a} : i [a^\dagger E a, \rho] \right] &= -i \text{Tr} \left[: e^{a^\dagger \epsilon a} (a^\dagger [E, \epsilon] a) : \rho \right] \\ &= -i \text{Tr} \left[[E, \epsilon] \frac{\partial}{\partial \epsilon} \right] \text{Tr} \left[: e^{a^\dagger \epsilon a} : \rho \right] \\ &= -i \text{Tr} \left[[E, \epsilon] \frac{\partial}{\partial \epsilon} \right] \Psi. \end{aligned}\quad (21)$$

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

$$\begin{aligned}(r + r n_R)_\mu^\nu \text{Tr} \left[: e^{a^\dagger \epsilon a} : \left(a^\mu \rho a_\nu^\dagger - \frac{1}{2} \{a_\nu^\dagger a^\mu, \rho\} \right) \right] &= -\frac{1}{2} \text{Tr} \left[: e^{a^\dagger \epsilon a} (a^\dagger \{r + r n_R, \epsilon\} a) : \rho \right] \\ &= -\frac{1}{2} \text{Tr} \left[\{r + r n_R, \epsilon\} \frac{\partial}{\partial \epsilon} \right] \text{Tr} \left[: e^{a^\dagger \epsilon a} : \rho \right] \\ &= -\frac{1}{2} \text{Tr} \left[\{r + r n_R, \epsilon\} \frac{\partial}{\partial \epsilon} \right] \Psi. \end{aligned}\quad (22)$$

The non-vanishing anticommutator $\{r + r n_R, I\}$ makes the offset of ϵ relative to z significant, where it is not in Eq. (21). For the last line in Eq. (8), only the ANO insertion gives a correspondingly simple evolution equation, with $M = r n_R$ in Eq. (20):

$$\begin{aligned}(r n_R)_\mu^\nu \text{Tr} \left[!e^{a^\dagger \bar{\epsilon} a} ! \left(a_\nu^\dagger \rho a^\mu - \frac{1}{2} \{a^\mu a_\nu^\dagger, \rho\} \right) \right] &= \frac{1}{2} \text{Tr} \left[!e^{a^\dagger \bar{\epsilon} a} (a^\dagger \{r n_R, \bar{\epsilon}\} a) ! \rho \right] \\ &= \frac{1}{2} \text{Tr} \left[\{r n_R, \bar{\epsilon}\} \frac{\partial}{\partial \bar{\epsilon}} \right] \text{Tr} \left[!e^{a^\dagger \bar{\epsilon} a} ! \rho \right] \\ &= \frac{1}{2} \text{Tr} \left[\{r n_R, \bar{\epsilon}\} \frac{\partial}{\partial \bar{\epsilon}} \right] \bar{\Psi}. \end{aligned}\quad (23)$$

To convert Eq. (23) into an equation on Ψ like Equations (21,22), we begin by converting the derivative operator on $\bar{\epsilon}$. Requiring that the identity for a general scalar function f ,

$$\text{Tr} \left[\delta \bar{\epsilon} \frac{\partial}{\partial \bar{\epsilon}} \right] f = \text{Tr} \left[\delta \bar{\epsilon} \frac{\partial f}{\partial \bar{\epsilon}} \right], \quad (24)$$

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

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

$$= \text{Tr} \left[\left(\epsilon rn_R \epsilon + \frac{1}{2} \{rn_R, \epsilon\} \right) \frac{\partial}{\partial \epsilon} \right]. \quad (25)$$

The relation $\bar{\epsilon} \equiv I - z^{-1}$ has created a quadratic perturbation in z or ϵ , which will be essential for the correct implementation of a source term in the DP formulation. With the relation (17) of $\bar{\Psi}$ to Ψ , Eq. (25) allows us to recast Eq. (23) as

$$\begin{aligned} (rn_R)_\mu^\nu \text{Tr} \left[: e^{a^\dagger \epsilon a} : \left(a_\nu^\dagger \rho a^\mu - \frac{1}{2} \{a^\mu a_\nu^\dagger, \rho\} \right) \right] &= \frac{1}{\text{Det}[z]} \text{Tr} \left[\left(zrn_R z - \frac{1}{2} \{rn_R, z\} \right) \frac{\partial}{\partial z} \right] \text{Det}[z] \Psi \\ &= \left\{ \text{Tr}[rn_R \epsilon] + \text{Tr} \left[\left(\epsilon rn_R \epsilon + \frac{1}{2} \{rn_R, \epsilon\} \right) \frac{\partial}{\partial \epsilon} \right] \right\} \Psi. \end{aligned} \quad (26)$$

Collecting terms from Equations (21 - 26), the differential equation on Ψ induced by Eq. (8) for ρ is

$$\frac{\partial \Psi}{\partial t} = \left\{ \text{Tr}[rn_R \epsilon] + \text{Tr} \left[\left(-i[E, \epsilon] + \epsilon rn_R \epsilon - \left\{ \frac{r}{2}, \epsilon \right\} \right) \frac{\partial}{\partial \epsilon} \right] \right\} \Psi \equiv -\mathcal{L}\Psi, \quad (27)$$

identifying the Liouville operator as

$$\mathcal{L} = \text{Tr} \left[\left(i[E, \epsilon] + \left\{ \frac{r}{2}, \epsilon \right\} - \epsilon rn_R \epsilon \right) \frac{\partial}{\partial \epsilon} \right] - \text{Tr}[rn_R \epsilon]. \quad (28)$$

If Ψ is instantaneously defined by Eq. (18), the evaluation of Eq. (27) yields

$$\begin{aligned} \frac{\partial \log \Psi}{\partial t} &= \text{Tr}[rn_R \epsilon] + \text{Tr} \left[(I - K^{-1} \epsilon)^{-1} K^{-1} \left(-i[E, \epsilon] + \epsilon rn_R \epsilon - \left\{ \frac{r}{2}, \epsilon \right\} \right) \right] \\ &= \text{Tr} \left[(I - K^{-1} \epsilon)^{-1} \left(i[E, K^{-1}] + rn_R - \left\{ \frac{r}{2}, K^{-1} \right\} \right) \epsilon \right]. \end{aligned} \quad (29)$$

The second line in Eq. (29), obtained by cyclic rearrangement in the trace and cancellation of part of the K -independent surface term against the quadratic term in ϵ , shows that the same evolution follows from keeping the argument ϵ invariant and allowing $K^{-1} = n$ to evolve under Eq. (7).

We thus verify that the generating function evolution equation (27) recovers the entire content of the equation (7) for evolution of the state variables n , which in turn are sufficient to define the quantum density matrix ρ as a maximum-entropy distribution [23] with entropy (5). These equations admit oscillatory solutions at $r = 0$, $rn_R = 0$, which would be lost in a classical Markov equation, as well as more general growing and decaying solutions for n . Such solutions are possible because the components of n representing classical currents are explicitly present as degrees of freedom.

III. THE TIME LOOP PATH INTEGRAL

The two-field operator representations of time evolution in both the quantum and DP descriptions are converted into path integrals by insertions of coherent-state representations of unity. Initially these appear non-homologous, because number states and their Hermitian conjugates play a symmetric role in the quantum theory, whereas classical fields and their conjugate observables in the Glauber norm have asymmetric interpretations in the DP path integral. However, upon Keldysh rotation of the quantum fields, the formal homology is restored [12].

This section treats the time-loop path integral, its relation to the Liouville operator, and the continuum limit, Keldysh rotation, and causal structure. The path integral, with or without dissipative terms, may be constructed simply as a means to evolve the generating function via its underlying density matrix. Alternatively,

since the free Hamiltonian together with the loss and gain terms provides a complete set of trace-preserving insertions, these may be treated as time-dependent sources, in which case the generating function at argument $z = I$ becomes a generating functional of these sources.

We begin with the free, discrete-time time-loop S-matrix to define the protocol for coherent state insertions and to identify the structure of Green's functions. Dissipative terms are then added to the discrete-time integral. 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.

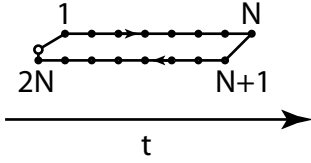


FIG. 1: Field insertion protocol for the time-loop path integral. Time advances to the right along links in increments δt . Solid nodes are positions of fields ξ_n^\dagger, ξ_n , and the hollow node is the original pair ξ^\dagger, ξ of ρ , which will be integrated out. Small arrows on links indicate direction along the time loop.

A. The discrete time-loop integral

1. 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

$$1 = \int \frac{d\xi^\dagger d\xi}{\pi^D} |\xi\rangle \langle \xi^\dagger| \quad (30)$$

in each interval δt on both bra and ket states. The time division structure used will be that shown in Fig. 1, so that states $n \in (1, \dots, N)$ are inserted at ascending times $(1, \dots, N) \times \delta t$, and states $n \in (N+1, \dots, 2N)$ are inserted at descending times $(N-1, \dots, 0) \times \delta t$. This particular state insertion converts Eq. (6) into

$$\rho_{\delta t} = \int \frac{d\xi_1^\dagger d\xi_1}{\pi^D} \int \frac{d\xi_{2N}^\dagger d\xi_{2N}}{\pi^D} \int \frac{d\xi_{2N-1}^\dagger d\xi_{2N-1}}{\pi^D} |\xi_1\rangle \langle \xi_1^\dagger| e^{i\hat{H}\delta t} \rho_{|\xi_{2N}\rangle} \langle \xi_{2N}^\dagger| e^{-i\hat{H}\delta t} |\xi_{2N-1}\rangle \langle \xi_{2N-1}^\dagger| \quad (31)$$

Further time evolution proceeds by induction,

$$\rho_{n\delta t} = \int \frac{d\xi_n^\dagger d\xi_n}{\pi^D} \int \frac{d\xi_{2N-n}^\dagger d\xi_{2N-n}}{\pi^D} |\xi_n\rangle \langle \xi_n^\dagger| e^{i\hat{H}\delta t} \rho_{(n-1)\delta t} e^{-i\hat{H}\delta t} |\xi_{2N-n}\rangle \langle \xi_{2N-n}^\dagger| \quad (32)$$

up to time $(N-1)\delta t$.

The time-loop S-matrix is produced from the bra and ket path integrals for $\rho_{(N-1)\delta t}$, by one final insertion of $e^{\pm i\hat{H}\delta t}$ on either side, followed by a *single* coherent-state insertion at $N\delta t$ and the taking of the trace, which formally yields unity:

$$\begin{aligned} 1 &= \text{Tr} \left(\int \frac{d\xi_N^\dagger d\xi_N}{\pi^D} |\xi_N\rangle \langle \xi_N^\dagger| e^{i\hat{H}\delta t} \rho_{(N-1)\delta t} e^{-i\hat{H}\delta t} \right) \\ &= \frac{1}{Z} \int \frac{d\xi_1^\dagger d\xi_1}{\pi^D} \dots \int \frac{d\xi_{2N}^\dagger d\xi_{2N}}{\pi^D} e^{-F}. \end{aligned} \quad (33)$$

The inverse of the partition function Z in Eq. (33) results from integration over $d\xi^\dagger d\xi$ in the original ρ of Eq. (3), and evaluates to

$$\frac{1}{Z} = \frac{1}{\text{Det}(I + K^{-1})} = \Psi|_{z=0}, \quad (34)$$

corresponding to argument $\epsilon = -I$ in Eq. (18). The quadratic form F in Eq. (33), involving only the numbered fields, evaluates to

$$F = \begin{bmatrix} \xi_1^\dagger & \cdots & \xi_N^\dagger & \xi_{N+1}^\dagger & \cdots & \xi_{2N}^\dagger \end{bmatrix} \begin{bmatrix} I & & & & & -Up \\ -U & \ddots & & & & \\ & -U & I & & & \\ & & -U^\dagger & I & & \\ & & & -U^\dagger & \ddots & \\ & & & & -U^\dagger & I \end{bmatrix} \begin{bmatrix} \xi_1 \\ \vdots \\ \xi_N \\ \xi_{N+1} \\ \vdots \\ \xi_{2N} \end{bmatrix}. \quad (35)$$

It is expressed as a function of $p \equiv (K + I)^{-1}$ 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. (33). (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 $\text{Det}(I - p)^{-1} = \text{Det}(I + K^{-1}) = Z$, and thus represents the partition function.)

From the form F we readily obtain the free Green's function in the discrete representation

$$\left\langle \begin{bmatrix} \xi_1 \\ \vdots \\ \xi_N \\ \xi_{N+1} \\ \vdots \\ \xi_{2N} \end{bmatrix} \begin{bmatrix} \xi_1^\dagger & \cdots & \xi_N^\dagger & \xi_{N+1}^\dagger & \cdots & \xi_{2N}^\dagger \end{bmatrix} \right\rangle = \begin{bmatrix} U \\ \vdots \\ U_N \\ U_{N-1} \\ \vdots \\ I \end{bmatrix} K^{-1} \begin{bmatrix} U^\dagger & \cdots & U^{\dagger N} & U^{\dagger N-1} & \cdots & I \end{bmatrix} + \begin{bmatrix} I & & & & & \\ \vdots & \ddots & & & & \\ U^{N-1} & \cdots & I & & & \\ U^{N-2} & \cdots & U^\dagger & I & & \\ \vdots & & \vdots & \vdots & \ddots & \\ U^\dagger & \cdots & U^{\dagger N} & U^{\dagger N-1} & \cdots & I \end{bmatrix}, \quad (36)$$

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 $1 \leq n \leq N$ to indicate fields on the forward (ket) leg, and to rewrite $2N - n \rightarrow -n$, for $0 \leq n \leq N$, for fields on the backward (bra) leg. (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 $1 \leq n \leq N - 1$ are then

$$\begin{aligned} \langle \xi_{-n} \xi_{n'}^\dagger \rangle &= U^n (K^{-1} + I) U^{\dagger n'} \\ \langle \xi_n \xi_{-n'}^\dagger \rangle &= U^n (K^{-1}) U^{\dagger n'} \\ \langle \xi_n \xi_{n'}^\dagger \rangle &= U^n \left[\theta_{n,n'}^+ (K^{-1} + I) + \theta_{n',n}^- (K^{-1}) \right] U^{\dagger n'} \\ \langle \xi_{-n} \xi_{-n'}^\dagger \rangle &= U^n \left[\theta_{n,n'}^- (K^{-1}) + \theta_{n',n}^+ (K^{-1} + I) \right] U^{\dagger n'}, \end{aligned} \quad (37)$$

in which the $\theta_{n,n'}^\pm$ are heaviside functions, both equal to I for $n > n'$ and 0 for $n < n'$. They differ at equal arguments, with $\theta_{n,n}^+ = I$ while $\theta_{n,n}^- = 0$. The corresponding

index notation for the quadratic form (35) is

$$\begin{aligned} F &= \xi_1^\dagger U (I - p) \xi_0 \\ &+ \sum_{n=1}^N \xi_n^\dagger (\xi_n - \xi_{n-1} - iE\delta t \xi_{n-1}) \\ &+ \xi_{-(n-1)}^\dagger (- (\xi_{-n} - \xi_{-(n-1)}) + iE\delta t \xi_{-n}) \end{aligned} \quad (38)$$

2. Dissipative insertions

More generally we can evolve ρ implicitly by defining Ψ at each time through the standard form (17). We replace the recursive relation (32) with the quadrature of the Liouville equation

$$\Psi_{n\delta t} \equiv e^{-\mathcal{L}(E_n, r_n, rn_{Rn})\delta t} \Psi_{(n-1)\delta t}, \quad (39)$$

now allowing E , r , and rn_R to be arbitrary functions of time, and continuing to insert pairs of coherent states in the same positions as for free evolution. Working backward through the commutation relations (19,20) used to derive the Liouville operator, we generalize Eq. (38) to

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

$$\begin{aligned}
& + \sum_{n=1}^N \xi_n^\dagger \left(\xi_n - \xi_{n-1} - \left(iE - \frac{r}{2} - rn_R \right)_n \delta t \xi_{n-1} \right) \\
& + \xi_{-(n-1)}^\dagger \left(\xi_{-(n-1)} - \xi_{-n} + \left(iE + \frac{r}{2} + rn_R \right)_n \delta t \xi_{-n} \right) \\
& - \xi_{-(n-1)}^\dagger (r + rn_R)_n \delta t \xi_{n-1} - \xi_n^\dagger (rn_R)_n \delta t \xi_{-n} \\
& + \text{Tr}[(rn_R)_n] \delta t. \tag{40}
\end{aligned}$$

Whereas free evolution couples only adjacent fields on the time loop, dissipation creates interactions between fields on forward and backward legs, similarly to interleaving Hamiltonian evolution with repeated tracing. The Onsager-Machlup effective action [18] derived below will illustrate the difference between the effective trace implemented by the gain and loss terms rn_R and r .

B. The continuum limit and Keldysh rotation

The continuum limit is the only practical basis for mode-expansion perturbation theory, or for tracing over unobserved “reservoir” degrees of freedom. However, passage to the continuum leaves some terms implicit at the level of the action, which are essential to the specification of Green’s functions. These must be fixed by explicit constraints on causal structure, only some of which are encoded in $i\varepsilon$ prescriptions.

The basic scaling relations defining the continuum are, for times $t = n\delta t$ and $t' = n'\delta t$, that fields $\xi_n \rightarrow \xi_t$ with no rescalings. $\delta_{n,n'} \rightarrow \delta t \delta(t - t')$, 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 $\xi_n - \xi_{n-1} \equiv \delta t \partial_t \xi_{t-\delta t}$ and $\xi_{-n} - \xi_{-(n-1)} \equiv \delta t \partial_t \xi_{-t}$ define derivatives along the time loop, and the free quadratic form F of Eq. (38) is expressed as

$$\begin{aligned}
F & = \xi_{\delta t}^\dagger U (I - p) \xi_0 \\
& + \delta t \sum_{n=1}^N \xi_t^\dagger (\partial_t - iE) \xi_{t-\delta t} + \xi_{-(t-\delta t)}^\dagger (-\partial_t + iE) \xi_{-t}, \tag{41}
\end{aligned}$$

in which the index ordering of ξ^\dagger relative to ξ reflects the time-direction of causation on each leg. Passage from the sum to the integral gives the naïve free time-loop action

$$\begin{aligned}
F & \rightarrow \xi_0^\dagger (I - p) \xi_0 \\
& + \int_0^T dt \begin{bmatrix} \xi_t^\dagger & \xi_{-t}^\dagger \end{bmatrix} \begin{bmatrix} \partial_t - iE & \\ & -\partial_t + iE \end{bmatrix} \begin{bmatrix} \xi_t \\ \xi_{-t} \end{bmatrix}, \tag{42}
\end{aligned}$$

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

An $i\varepsilon$ prescription that recovers both the causal and correlation structures of Eq. (37) is neither obvious nor simple to use in the free time-loop representation (42). 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.

1. Keldysh fields, Green’s functions, and action

The Keldysh fields are defined from time-loop fields by a rotation (which may be combined with an overall scaling of one field to make the transformation unitary). In the discrete indexing, for $1 \leq n \leq N - 1$,

$$\begin{bmatrix} \phi_n \\ \psi_n \end{bmatrix} \equiv \begin{bmatrix} I/2 & I/2 \\ -I & I \end{bmatrix} \begin{bmatrix} \xi_n \\ \xi_{-n} \end{bmatrix}. \tag{43}$$

ϕ_n is referred to as the *classical* component and ψ_n as the *quantum component*. The free Green’s function obtained by transforming Eq. (37) under Eq. (43) has the considerably simpler structure

$$\left\langle \begin{bmatrix} \phi_n \\ \psi_n \end{bmatrix} \begin{bmatrix} \phi_{n'}^\dagger & \psi_{n'}^\dagger \end{bmatrix} \right\rangle = U^n \left\{ \begin{bmatrix} (K^{-1} + \frac{I}{2}) & -\theta_{n,n'}^s \\ \theta_{n',n}^s & \end{bmatrix} + \delta_{n,n'} \begin{bmatrix} I/4 & \\ & I \end{bmatrix} \right\} U^{\dagger n'}, \tag{44}$$

in which $\theta^s = (\theta^+ + \theta^-)/2$, and therefore $\theta_{n,n}^s = I/2$. $\delta_{n,n'}$ is the Kronecker delta. The continuum limit of Eq. (44) has the “tri-diagonal” form (up to removable singularities at $t = t'$)

$$\left\langle \begin{bmatrix} \phi_t \\ \psi_t \end{bmatrix} \begin{bmatrix} \phi_{t'}^\dagger & \psi_{t'}^\dagger \end{bmatrix} \right\rangle = e^{iEt} \begin{bmatrix} (K^{-1} + \frac{I}{2}) & -\theta(t - t') \\ \theta(t' - t) & \end{bmatrix} e^{-iEt'}, \tag{45}$$

in which correlation and response functions are completely separated.

The block structure of Eq. (45) is the fundamental Keldysh representation of causality, and may be used to motivate

an $i\varepsilon$ prescription and handling of the surface term in the action obtained by rotation of Eq. (42), written as

$$F \rightarrow \left(\phi_{\delta t}^\dagger - \frac{1}{2} \psi_{\delta t}^\dagger \right) (I - p) \left(\phi_0 + \frac{1}{2} \psi_0 \right) + \int_0^T dt \begin{bmatrix} \phi_t^\dagger & \psi_t^\dagger \end{bmatrix} \begin{bmatrix} -\partial_t + iE - \varepsilon & -\partial_t + iE + \varepsilon \\ -\partial_t + iE - \varepsilon & -\partial_t + iE + \varepsilon \end{bmatrix} \begin{bmatrix} \phi_t \\ \psi_t \end{bmatrix}. \quad (46)$$

The decomposition of the $t = 0$ fields follows from their original placement as $\xi_{\delta t}^\dagger$ and $\xi_0 \equiv \xi_{2N}$ in Eq. (41). The one explicitly implied expectation

$$\begin{aligned} \langle \xi_0 \xi_{\delta t}^\dagger \rangle &= (I - p)^{-1} = K^{-1} + I \\ &= \left\langle \left(\phi_0 + \frac{1}{2} \psi_0 \right) \left(\phi_{\delta t}^\dagger - \frac{1}{2} \psi_{\delta t}^\dagger \right) \right\rangle, \end{aligned} \quad (47)$$

together with the block structure and (anti)symmetries of the Green's function (44), is sufficient to define the individual component expectations.

2. Dissipation in the Born approximation

To produce non-infinitesimal dissipation from the causal structure of the free theory, suppose that the closed-system degrees of freedom can be split into explicit System and Reservoir component vectors, as

$$\begin{aligned} \phi_t &\equiv \begin{bmatrix} \phi_{St} \\ \phi_{Rt} \end{bmatrix} \\ \psi_t &\equiv \begin{bmatrix} \psi_{St} \\ \psi_{Rt} \end{bmatrix}. \end{aligned} \quad (48)$$

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

$$E \equiv \begin{bmatrix} E_S & g \\ g^\dagger & E_R \end{bmatrix}, \quad (49)$$

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:

$$p \equiv \begin{bmatrix} p_S & \\ & p_R \end{bmatrix}. \quad (50)$$

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. (46), gives the leading nonvanishing terms

$$\begin{aligned} e^{-F} &= e^{-(F_S + F_R)} \left\{ 1 - \int_0^T dt \psi_{St}^\dagger g \phi_{Rt} \int_0^T dt' \phi_{Rt'}^\dagger g^\dagger \psi_{St'} \right. \\ &\quad - \int_0^T dt \psi_{St}^\dagger g \phi_{Rt} \int_0^T dt' \psi_{Rt'}^\dagger g^\dagger \phi_{St'} \\ &\quad \left. - \int_0^T dt \phi_{St}^\dagger g \psi_{Rt} \int_0^T dt' \phi_{Rt'}^\dagger g^\dagger \psi_{St'} + \mathcal{O}(gg^\dagger)^2 \right\}. \end{aligned} \quad (51)$$

Tracing over the R fields converts the terms in curly braces in Eq. (51) to the reservoir expectations

$$\begin{aligned} &1 - \int_0^T dt \int_0^T dt' \begin{bmatrix} \phi_{St}^\dagger & \psi_{St}^\dagger \end{bmatrix} g \left\langle \begin{bmatrix} \psi_{Rt} \\ \phi_{Rt} \end{bmatrix} \begin{bmatrix} \psi_{Rt'}^\dagger & \phi_{Rt'}^\dagger \end{bmatrix} \right\rangle g^\dagger \begin{bmatrix} \phi_{St'} \\ \psi_{St'} \end{bmatrix} \\ &= 1 - \int_0^T dt \int_0^T dt' \begin{bmatrix} \phi_{St}^\dagger & \psi_{St}^\dagger \end{bmatrix} g e^{iE_R t} \begin{bmatrix} \theta(t' - t) & \\ -\theta(t - t') & (K_R^{-1} + I/2) \end{bmatrix} e^{-iE_R t'} g^\dagger \begin{bmatrix} \phi_{St'} \\ \psi_{St'} \end{bmatrix} \\ &= 1 - \int_0^T dt \int_0^T dt' \begin{bmatrix} \phi_{St}^\dagger & \psi_{St}^\dagger \end{bmatrix} g e^{iE_R t} \begin{bmatrix} I/2 & \\ -I/2 & (K_R^{-1} + I/2) \end{bmatrix} e^{-iE_R t'} g^\dagger \begin{bmatrix} \phi_{St'} \\ \psi_{St'} \end{bmatrix} \\ &\quad - \int_0^T dt \int_0^T dt' \begin{bmatrix} \phi_{St}^\dagger & \psi_{St}^\dagger \end{bmatrix} g e^{iE_R(t-t')} g^\dagger [\theta(t' - t) - \theta(t - t')] \begin{bmatrix} I/2 & \\ I/2 & \end{bmatrix} \begin{bmatrix} \phi_{St'} \\ \psi_{St'} \end{bmatrix}, \end{aligned} \quad (52)$$

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 E_R are such that the integrals over t and t' converge [2], then for sufficiently low-frequency fields in the system, one may replace the oscillating kernels with time-local interactions denoted as

$$\begin{aligned} g e^{iE_R(t-t')} g^\dagger &\rightarrow r \delta(t-t') \\ g e^{iE_R t} K_R^{-1} e^{-iE_R t'} g^\dagger &\rightarrow (r n_R) \delta(t-t') \\ g e^{iE_R(t-t')} g^\dagger [\theta(t'-t) - \theta(t-t')] &\rightarrow i \delta E_S \delta(t-t'). \end{aligned} \quad (53)$$

r , $r n_R$, 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 $\mathcal{O}(g g^\dagger)$, and will simply be absorbed into the effective system energy matrix E_S in what follows.

The local interaction approximation (53) slightly violates the causal structure of the theory. It can be checked that the expectations of the second and third lines in Eq. (51), over both reservoir and system degrees of freedom, are both zero, by the Green's functions (45). If

the first line of Eq. (53) is inserted to produce a time-local action in Eq. (52), 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 mis-evaluation of the system functional determinant but does not affect other correlations, by substituting

$$\begin{aligned} \int dt' \phi_{S t'}^\dagger g e^{iE_R(t-t')} g^\dagger \psi_{S t'} &\rightarrow \phi_{S t}^\dagger r \psi_{S t} - \text{Tr} \left[\frac{r}{2} \right] \\ \int dt' \psi_{S t}^\dagger g e^{iE_R(t-t')} g^\dagger \phi_{S t'} &\rightarrow \psi_{S t}^\dagger r \phi_{S t} - \text{Tr} \left[\frac{r}{2} \right]. \end{aligned} \quad (54)$$

The other two lines of Eq. (53) 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. (52) into the effective system kernel converts the free system kernel F_S from the form (46) into the perturbed form

$$\begin{aligned} F_S &\rightarrow \left(\phi_{S \delta t}^\dagger - \frac{1}{2} \psi_{S \delta t}^\dagger \right) (I - p_S) \left(\phi_{S 0} + \frac{1}{2} \psi_{S 0} \right) \\ &+ \int_0^T dt \left\{ \begin{bmatrix} \phi_{S t}^\dagger & \psi_{S t}^\dagger \end{bmatrix} \begin{bmatrix} -\partial_t + iE_S - r/2 & -\partial_t + iE_S + r/2 \\ (r n_R + r/2) & (r n_R + r/2) \end{bmatrix} \begin{bmatrix} \phi_{S t} \\ \psi_{S t} \end{bmatrix} - \text{Tr} \left[\frac{r}{2} \right] \right\}. \end{aligned} \quad (55)$$

The large dissipation terms $r/2$ automatically appear with the same signs as the $i\varepsilon_S$ in Eq. (46), but in addition there is a new $\psi_S^\dagger \psi_S$ interaction. Inverting the Keldysh transform (43) gives the continuum time-loop action corresponding to the discrete dissipative action (40):

$$F_S \rightarrow \xi_{S 0}^\dagger (I - p_S) \xi_{S 0} + \int_0^T dt \left\{ \begin{bmatrix} \xi_{S t}^\dagger & \xi_{S, -t}^\dagger \end{bmatrix} \begin{bmatrix} \partial_t - iE_S + r/2 + r n_R & -r n_R \\ -(r + r n_R) & -\partial_t + iE_S + r/2 + r n_R \end{bmatrix} \begin{bmatrix} \xi_{S t} \\ \xi_{S, -t} \end{bmatrix} - \text{Tr} \left[\frac{r}{2} \right] \right\}, \quad (56)$$

from which the free action (42) can be regulated by taking $r/2 \rightarrow \varepsilon$ and $r n_R \rightarrow 0$.

The scalar correction term $\text{Tr}[r/2]$ in Eq. (56) differs from the correction $\text{Tr}[r n_R]$ in Eq. (40), due to a related constraint on the causal structure. Eq. (45) requires $\langle \psi_{S t} \psi_{S t}^\dagger \rangle \equiv 0$. The discrete counterpart in Eq. (40), although differing nominally only by terms of $\mathcal{O}(\delta t)$ 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

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

$$\leftarrow (\xi_{n-1} - \xi_{-n}) (\xi_n^\dagger - \xi_{-(n-1)}^\dagger) + I \quad (57)$$

under which Eq. (56) also follows from Eq. (40)

3. Keldysh Green's functions with dissipation terms

The dissipative Green's functions follow from the causal structure by inversion [12] of the Kernel matrix in Eq. (55), whose general structure is

$$\delta(t-t') \begin{bmatrix} -\partial_{t'} + iE_S + r/2 & \\ -\partial_{t'} + iE_S - r/2 & (rn_R + r/2) \end{bmatrix} = \begin{bmatrix} [D^A]^{-1} & \\ [D^R]^{-1} & [D^{-1}]^K \end{bmatrix}_{t,t'}, \quad (58)$$

while that of the Green's function (45) is

$$\left\langle \begin{bmatrix} \phi_{St} \\ \psi_{St} \end{bmatrix} \begin{bmatrix} \phi_{St'}^\dagger & \psi_{St'}^\dagger \end{bmatrix} \right\rangle = \begin{bmatrix} D^K & D^R \\ D^A & \end{bmatrix}_{t,t'}. \quad (59)$$

In the case that one can write

$$[D^{-1}]^K = M[D^A]^{-1} - [D^R]^{-1}M \quad (60)$$

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

$$D^K = MD^A - D^R M. \quad (61)$$

For the kernel (58), in which all of $[D^A]^{-1}$, $[D^R]^{-1}$, and $[D^{-1}]^K$ are time-local, we may choose $M_{t,t'} = (K_S^{-1} + I/2)_t \delta(t-t')$, for which Eq. (60) translates to

$$rn_R = \partial_t K_S^{-1} - [iE_S, K_S^{-1}] + \left\{ \frac{r}{2}, K_S^{-1} \right\} \quad (62)$$

at each time. Eq. (62) is of course the equation (7) applied to K_S^{-1} .

The Advanced and Retarded response Green's functions are readily evaluated to

$$\begin{aligned} D_{t,t'}^A &= e^{-(iE_S+r/2)(t'-t)} \theta(t'-t) \\ D_{t,t'}^R &= -e^{(iE_S-r/2)(t-t')} \theta(t-t'). \end{aligned} \quad (63)$$

To evaluate the Keldysh correlation function, note that Eq. (62) is solved from initial value K_{S0}^{-1} by

$$K_{St}^{-1} = e^{(iE_S-r/2)t} \mathcal{K}_t^{-1} e^{-(iE_S+r/2)t}, \quad (64)$$

in which

$$\mathcal{K}_t^{-1} \equiv K_{S0}^{-1} + \int_0^t dt' e^{-(iE_S-r/2)t'} (rn_R)_{t'} e^{(iE_S+r/2)t'}. \quad (65)$$

Also in terms of \mathcal{K}_t^{-1} , the Keldysh correlator is

$$D_{t,t'}^K = e^{(iE_S-r/2)t} [\theta(t-t') \mathcal{K}_{t'}^{-1} + \theta(t'-t) \mathcal{K}_t^{-1}] e^{-(iE_S+r/2)t'} + \frac{1}{2} (D_{t,t'}^A - D_{t,t'}^R). \quad (66)$$

At equal times,

$$\begin{aligned} D_{t,t}^K &= e^{(iE_S-r/2)t} \mathcal{K}_t^{-1} e^{-(iE_S+r/2)t} + \frac{I}{2} \\ &= K_{St}^{-1} + \frac{I}{2} \end{aligned} \quad (67)$$

agrees with the free correlator (45) in form, simply generalizing the evolution equation for K_{St}^{-1} to Eq. (62).

It may be worth noting that, upon transforming back from Keldysh to time-loop fields, the correlator that from Eq. (32) we would expect to generalize $\langle \xi \xi^\dagger \rangle$ in the original ρ of Eq. (3) is

$$\left\langle \xi_{St} \xi_{S,-t'}^\dagger \right\rangle = e^{(iE_S-r/2)t} [\theta(t-t') \mathcal{K}_{t'}^{-1} + \theta(t'-t) \mathcal{K}_t^{-1}] e^{-(iE_S+r/2)t'}. \quad (68)$$

Thus at equal times $\left\langle \xi_{St} \xi_{S,-t}^\dagger \right\rangle = K_{St}^{-1}$ as in Eq. (37).

4. Onsager-Machlup forms

By Eq. (32), the outer product $|\xi_n\rangle \left\langle \xi_{-n}^\dagger \right|$ is the counterpart at time $n\delta t$ to the product $|\xi\rangle \left\langle \xi^\dagger \right|$ in the initial ρ of Eq. (3). 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 [18].

One begins by introducing shifted time-loop fields

$$\begin{aligned}\tilde{\xi}_{St}^\dagger &\equiv \xi_{St}^\dagger - [(\partial_t - iE_S + r/2 + rn_R) \xi_{S,-t}]^\dagger (rn_R)^{-1} \\ \tilde{\xi}_{S,-t} &\equiv \xi_{S,-t} - (rn_R)^{-1} (\partial_t - iE_S + r/2 + rn_R) \xi_{St},\end{aligned}\quad (69)$$

in terms of which F_S is expressed as

$$\begin{aligned}F_S &= \xi_{S0}^\dagger (I - p_S) \xi_{S0} + \int dt \tilde{\xi}_{St}^\dagger (-rn_R) \tilde{\xi}_{S,-t} - \text{Tr} \left[\frac{r}{2} \right] \\ &+ \left[\left(\partial_t - iE_S + \frac{r}{2} \right) \xi_{S,-t} \right]^\dagger (rn_R)^{-1} \left(\partial_t - iE_S + \frac{r}{2} \right) \xi_{St}.\end{aligned}\quad (70)$$

(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 equations (11-15) of Ref. [23] and shown to lead to Eq. (62) for K_S^{-1} . There the integral over $\tilde{\xi}_{St}^\dagger$ and $\tilde{\xi}_{S,-t}$, together with the $\text{Tr}[r/2]$, was absorbed in a discrete prefactor $\prod_n 1/\text{Det}[(rn_R)_n \delta t]$.

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

$$\begin{aligned}\tilde{\psi}_{St}^\dagger &\equiv \psi_{St}^\dagger + [(\partial_t - iE_S + r/2) \phi_{St}]^\dagger (rn_R + r/2)^{-1} \\ \tilde{\psi}_{St} &\equiv \psi_{St} - (rn_R + r/2)^{-1} (\partial_t - iE_S + r/2) \phi_{St},\end{aligned}\quad (71)$$

and the resulting action is

$$\begin{aligned}F_S &= \left(\phi_{S\delta t}^\dagger - \frac{1}{2} \psi_{S\delta t}^\dagger \right) (I - p_S) \left(\phi_{S0} + \frac{1}{2} \psi_{S0} \right) + \int dt \tilde{\psi}_{St}^\dagger \left(rn_R + \frac{r}{2} \right) \tilde{\psi}_{St} - \text{Tr} \left[\frac{r}{2} \right] \\ &+ \left[\left(\partial_t - iE_S + \frac{r}{2} \right) \phi_{St} \right]^\dagger \left(rn_R + \frac{r}{2} \right)^{-1} \left(\partial_t - iE_S + \frac{r}{2} \right) \phi_{St}.\end{aligned}\quad (72)$$

A discrete representation identical in structure to that for Eq. (70) 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. (62).

IV. THE DOI-PELITI REPRESENTATION

As for the Schwinger-Keldysh time loop, the DP path integral may be used to represent either the original generating function (17) or a generating functional, depending on whether the complex argument or the source terms in the Liouville operator are varied. The generating function will be used here as the path to the generating functional.

A. The DP path integral

Rather than perform the DP construction with formal algebraic operators, I will use here the explicit representation of analytic functions and differential operators, to maintain the generating-function interpretation, and to clarify the inequivalent algebraic character [6] of left and right DP states, which is obscured in the formal representation. We begin with the representation, and then construct the path integral.

1. Analytic function representation

The number 1 represents the DP right “vacuum”,

$$1 \leftrightarrow |0\rangle. \quad (73)$$

Complex scalar components of the matrix z are the raising operators (denoted with capitals to distinguish them from the quantum operators)

$$z_j \leftrightarrow A_j^\dagger. \quad (74)$$

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

$$\frac{\partial}{\partial z_i} \leftrightarrow A^i, \quad (75)$$

hence

$$\left[A^i, A_j^\dagger \right] = \delta_j^i. \quad (76)$$

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

$$\left(\prod_{j=1}^D z_j^{n_j} \right) \cdot 1 \leftrightarrow \prod_{j=1}^D \left(A_j^\dagger \right)^{n_j} |0\rangle = |\vec{n}\rangle, \quad (77)$$

and lowering operators annihilate the right vacuum

$$0 = \frac{\partial}{\partial z_i} 1 \leftrightarrow A^i |0\rangle. \quad (78)$$

The left vacuum evaluates the generating function at zero argument, so its proper representation is

$$\int Dz \delta(z) \leftrightarrow |0\rangle. \quad (79)$$

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

$$0 = \int Dz \delta(z) z_i \leftrightarrow \langle 0 | A^i, \quad (80)$$

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

$$\begin{aligned} 1 &= \int Dz \delta(z) e^{\sum_j \partial/\partial z_j} \left(\prod_{j=1}^D z_j^{n_j} \right) \cdot 1 \\ &\leftrightarrow \langle 0 | e^{\sum_j A_j} \prod_{j=1}^D (A_j^\dagger)^{n_j} |0\rangle. \end{aligned} \quad (81)$$

The generating function Ψ of Eq. (17) thus represents the usual DP state vector

$$\Psi(z) \leftrightarrow |\Psi\rangle. \quad (82)$$

2. Field functional integrals

From this point on it is necessary to drop the component index j and simply refer to the whole matrix,

because in the complex-function representation, a single argument z will not suffice under time evolution. The right DP states make z s dummy variables of integration, and one will be needed for each time in the path integral. Therefore index these matrix-valued variables z_n , for $n \in 0, \dots, N$ corresponding to times $(0, \dots, N) \times \delta t$, as in the SK development.

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

$$\begin{aligned} \langle \zeta^\dagger | &= \langle 0 | e^{-(\zeta^\dagger \zeta)/2} \sum_{N=0}^{\infty} \frac{(\zeta^\dagger \cdot A)^N}{N!} \\ &\leftrightarrow \int Dz_0 \delta(z_0) e^{-(\zeta^\dagger \zeta)/2} \sum_{N=0}^{\infty} \frac{(\zeta^\dagger \cdot \partial/\partial z_0)^N}{N!} \\ &= \int Dz_0 \delta(z_0) e^{-(\zeta^\dagger \zeta)/2} e^{\zeta^\dagger \cdot \partial/\partial z_0}. \end{aligned} \quad (83)$$

(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

$$\begin{aligned} |\zeta\rangle &= e^{-(\zeta^\dagger \zeta)/2} \sum_{N=0}^{\infty} \frac{(A^\dagger \cdot \zeta)^N}{N!} |0\rangle \\ &\leftrightarrow e^{-(\zeta^\dagger \zeta)/2} \sum_{N=0}^{\infty} \frac{(z_1 \cdot \zeta)^N}{N!} \cdot 1 \\ &= e^{-(\zeta^\dagger \zeta)/2} e^{z_1 \cdot \zeta} \cdot 1. \end{aligned} \quad (84)$$

The DP coherent-state insertion of unity,

$$\begin{aligned} \int \frac{D\zeta^\dagger D\zeta}{\text{Det}(\pi)} |\zeta\rangle \langle \zeta^\dagger | &\rightarrow \int \frac{D\zeta^\dagger D\zeta}{\text{Det}(\pi)} e^{-\zeta^\dagger \zeta} e^{z_1 \cdot \zeta} \int Dz_0 \delta(z_0) e^{\zeta^\dagger \cdot \partial/\partial z_0} \\ &= \int Dz_0 \delta(z_0) e^{z_1 \cdot \partial/\partial z_0}, \end{aligned} \quad (85)$$

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

$$\int \frac{D\zeta_0^\dagger D\zeta_0}{\text{Det}(\pi)} |\zeta_0\rangle \langle \zeta_0^\dagger | \Psi_0 \leftrightarrow \int \frac{D\zeta_0^\dagger D\zeta_0}{\text{Det}(\pi)} e^{(z_0 - \zeta_0^\dagger) \cdot \zeta_0} \Psi_0(\zeta_0^\dagger). \quad (86)$$

The generating function is then advanced in time through the recursion

$$\Psi_{N\delta t}(z_n) = \int \frac{D\zeta_n^\dagger D\zeta_n}{\text{Det}(\pi)} e^{(z_n - \zeta_n^\dagger)\zeta_n} \int Dz_{n-1} \delta(z_{n-1}) e^{\zeta_n^\dagger \cdot \partial / \partial z_{n-1} - \mathcal{L}_n(z_{n-1}, \partial / \partial z_{n-1}) \delta t} \Psi_{n-1}(z_{n-1}), \quad (87)$$

in which \mathcal{L}_n is the Liouville operator (28) 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

$$\Psi_{N\delta t}(z_N) = \int_0^N \mathcal{D}\zeta^\dagger \mathcal{D}\zeta e^{(z_N - \zeta_N^\dagger)\zeta_N + \sum_{n=1}^N L_n \delta t} \Psi_0(\zeta_0^\dagger), \quad (88)$$

in which the measure

$$\int_0^N \mathcal{D}\zeta^\dagger \mathcal{D}\zeta \equiv \prod_{n=0}^N \int \frac{D\zeta_n^\dagger D\zeta_n}{\text{Det}(\pi)}, \quad (89)$$

and the Lagrangian

$$L_n \delta t \equiv (\zeta_n^\dagger - \zeta_{n-1}^\dagger) \cdot \zeta_{n-1} - \mathcal{L}_n(\zeta_n^\dagger, \zeta_{n-1}) \delta t, \quad (90)$$

so that ζ_n^\dagger substitutes for z_{n-1} , and ζ_{n-1} for $\partial / \partial z_{n-1}$ in \mathcal{L}_n .

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 $\Psi_{N\delta t}(I) = 1$ is strictly preserved, so such variations generate only Ward identities of the theory. In constructing the DP-SK operator correspondence, we will consider more general variations.)

Introducing the usual field shift $\zeta_n^\dagger \rightarrow \tilde{\zeta}_n^\dagger \equiv \zeta_n^\dagger - I$, corresponding to commuting the Glauber annihilation operators through the evolution kernel [1], one can write

$$\Psi_{N\delta t}(I) = \int_0^N \mathcal{D}\tilde{\zeta}^\dagger \mathcal{D}\zeta e^{-\tilde{\zeta}_N^\dagger \zeta_N + \sum_{n=1}^N L_n \delta t} \Psi_0(\tilde{\zeta}_0^\dagger + I), \quad (91)$$

in which the same Lagrangian is alternatively written

$$L_n \delta t \equiv (\tilde{\zeta}_n^\dagger - \tilde{\zeta}_{n-1}^\dagger) \cdot \zeta_{n-1} - \mathcal{L}_n(\tilde{\zeta}_n^\dagger + I, \zeta_{n-1}) \delta t. \quad (92)$$

Note that as ζ_n^\dagger has substituted for z_{n-1} , $\tilde{\zeta}_n^\dagger$ corresponds to the variable ϵ_{n-1} in Eq. (17). As $\partial / \partial z = \partial / \partial \epsilon$, we may equivalently regard ζ_{n-1} as $\partial / \partial \epsilon_{n-1}$. Thus the Liouville operator in Eq. (92) is simply the functional form (28), evaluated at $\epsilon \rightarrow \tilde{\zeta}_n^\dagger$ and $\partial / \partial \epsilon \rightarrow \zeta_{n-1}$. Similarly, the initial density has the form of Eq. (17) with $\epsilon \rightarrow \tilde{\zeta}_0^\dagger$. Thus the generating functional may be written

$$\Psi_{N\delta t}(I) = \int_0^N \mathcal{D}\tilde{\zeta}^\dagger \mathcal{D}\zeta e^{-\tilde{\zeta}_N^\dagger \zeta_N + \sum_{n=1}^N L_n \delta t - \text{Tr} \log[I - K_0^{-1} \tilde{\zeta}_0^\dagger]}. \quad (93)$$

Note that the generating-function expression for the inverse of the partition function is very similar,

$$\begin{aligned} \Psi_{N\delta t}(0) &= \frac{1}{\text{Det}(I + K_{N\delta t}^{-1})} = \frac{1}{Z_{N\delta t}}, \\ &= \int_0^N \mathcal{D}\zeta^\dagger \mathcal{D}\zeta e^{-\zeta_N^\dagger \zeta_N + \sum_{n=1}^N L_n \delta t - \text{Tr} \log[I + K_0^{-1}(I - \zeta_0^\dagger)]}, \end{aligned} \quad (94)$$

with the Lagrangian and initial determinant now taking their forms as functions of $z \rightarrow \zeta^\dagger$.

3. Stationary points and fluctuations

The compensation for the extra complexity of matrix-valued fields and a non-Gaussian Lagrangian in the DP representation is that the leading behavior of Green's functions can be separated in a nontrivial classical stationary point of Eq. (92). The conditions from varying ζ_{n-1} and $\tilde{\zeta}_n^\dagger$, respectively, are

$$\begin{aligned} (\tilde{\zeta}_n^\dagger - \tilde{\zeta}_{n-1}^\dagger) / \delta t &= [iE_n, \tilde{\zeta}_n^\dagger] + \left\{ \frac{r_n}{2}, \tilde{\zeta}_n^\dagger \right\} - \tilde{\zeta}_n^\dagger (rn_R)_n \tilde{\zeta}_n^\dagger \\ (\zeta_n - \zeta_{n-1}) / \delta t &= [iE_n, \zeta_{n-1}] - \left\{ \frac{r_n}{2}, \zeta_{n-1} \right\} + (rn_R)_n \\ &\quad + (rn_R)_n \tilde{\zeta}_n^\dagger \zeta_{n-1} + \zeta_{n-1} \tilde{\zeta}_n^\dagger (rn_R)_n. \end{aligned} \quad (95)$$

Stationary $\tilde{\zeta}_n^\dagger$ solves exactly the evolution equation for a kernel K , even though its classical value is $\tilde{\zeta}_n^\dagger \equiv 0$, and it evolves backward in time. Meanwhile, ζ_{n-1} evolves forward in time and solves the evolution equation for K^{-1} (as we would expect), perturbed by an additive noise field whose classical expectation is zero.

Therefore introduce the shifted field $\tilde{\zeta}_n \equiv \zeta_n - K_{n\delta t}^{-1}$, where $K_{n\delta t}^{-1}$ is a solution to the stationary point condition (95) for ζ_n and K_0^{-1} is the value appearing in the initial condition. Separate out the quadratic and higher dependence of the Liouville operator of shifted arguments by defining

$$\mathcal{L}_n \left(\tilde{\zeta}_n^\dagger + I, \tilde{\zeta}_{n-1} + K_{(n-1)\delta t}^{-1} \right) \equiv \tilde{\zeta}_n^\dagger \left(K_{n\delta t}^{-1} - K_{(n-1)\delta t}^{-1} \right) + \tilde{\mathcal{L}}_n \left(\tilde{\zeta}_n^\dagger, \tilde{\zeta}_{n-1} \right). \quad (96)$$

The resulting kernel for the fluctuation matrices takes on a form at quadratic order similar to the Keldysh kernel for dyadics [3, 12],

$$\tilde{\mathcal{L}}_n \left(\tilde{\zeta}_n^\dagger, \tilde{\zeta}_{n-1} \right) = \text{Tr} \left[\tilde{\zeta}_{n-1} \left(iE + \frac{r}{2} \right)_n \tilde{\zeta}_n^\dagger - \tilde{\zeta}_n^\dagger \left(iE - \frac{r}{2} \right)_n \tilde{\zeta}_{n-1} - (rn_R)_n \tilde{\zeta}_n^\dagger K_{n-1}^{-1} \tilde{\zeta}_n^\dagger - (rn_R)_n \tilde{\zeta}_n^\dagger \tilde{\zeta}_{n-1} \tilde{\zeta}_n^\dagger \right], \quad (97)$$

except that in Eq. (97) each field occupies the place of two *independent* Keldysh fields, with $\tilde{\zeta}$ standing in for both ϕ^\dagger and ϕ , and $-\tilde{\zeta}^\dagger$ taking the place of ψ^\dagger while $\tilde{\zeta}^\dagger$ takes the place of ψ . The symmetric form of the Keldysh Hamiltonian can 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 $-\tilde{\zeta}^\dagger$ becomes its Hermitian conjugate.

B. Structural homology versus operator mappings

The structural homology manifest in Eq. (97) results in some elements of identity between matrix and dyad Green's functions, without indicating an underlying operator correspondence as in Ref. [3]. To solve for the retarded and advanced Green's function components, note first that the absence of a $\tilde{\zeta}^2$ interaction in Eq. (97) makes the inversion of the $\tilde{\zeta}\tilde{\zeta}^\dagger$ interactions independent of the $\tilde{\zeta}^{\dagger 2}$ interaction. We may therefore collect terms in the exponent of Eq. (93) in either of the two equivalent forms

$$\begin{aligned} \tilde{\zeta}_N^\dagger \zeta_N - \sum_{n=0}^{N-1} L_n \delta t + \text{Tr} \log \left[I - \tilde{\zeta}_0^\dagger K_0^{-1} \right] &= \left[\tilde{\zeta}_0^\dagger \cdots \tilde{\zeta}_N^\dagger \right] \cdot \begin{bmatrix} 1 & & \\ -u_1 & \ddots & \\ & -u_N & 1 \end{bmatrix} \begin{bmatrix} \tilde{\zeta}_0 \\ \vdots \\ \tilde{\zeta}_N \end{bmatrix} + \mathcal{O}(\tilde{\zeta}^{\dagger 2}) \\ &= \left[\tilde{\zeta}_0 \cdots \tilde{\zeta}_N \right] \cdot \begin{bmatrix} 1 & -u_1^\dagger & \\ & \ddots & -u_N^\dagger \\ & & 1 \end{bmatrix} \begin{bmatrix} \tilde{\zeta}_0^\dagger \\ \vdots \\ \tilde{\zeta}_N^\dagger \end{bmatrix} + \mathcal{O}(\tilde{\zeta}^{\dagger 2}), \end{aligned} \quad (98)$$

where the inner product notation has been used for the trace 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:

$$\begin{aligned} u_n \tilde{\zeta}_{n-1} &\equiv \tilde{\zeta}_{n-1} + \left[iE_n, \tilde{\zeta}_{n-1} \right] \delta t - \left\{ \frac{r_n}{2}, \tilde{\zeta}_{n-1} \right\} \delta t \\ u_n^\dagger \tilde{\zeta}_n &\equiv \tilde{\zeta}_n - \left[iE_n, \tilde{\zeta}_n^\dagger \right] \delta t - \left\{ \frac{r_n}{2}, \tilde{\zeta}_n^\dagger \right\} \delta t. \end{aligned} \quad (99)$$

In the simple case of E_n and r_n constant, the resulting Green's functions are

$$\begin{aligned} \left\langle \begin{bmatrix} \tilde{\zeta}_0 \\ \vdots \\ \tilde{\zeta}_N \end{bmatrix} \begin{bmatrix} \tilde{\zeta}_0^\dagger \cdots \tilde{\zeta}_N^\dagger \end{bmatrix} \right\rangle &= \begin{bmatrix} 1 & & \\ \vdots & \ddots & \\ u^N & \cdots & 1 \end{bmatrix} \\ \left\langle \begin{bmatrix} \tilde{\zeta}_0^\dagger \\ \vdots \\ \tilde{\zeta}_N^\dagger \end{bmatrix} \begin{bmatrix} \tilde{\zeta}_0 \cdots \tilde{\zeta}_N \end{bmatrix} \right\rangle &= \begin{bmatrix} 1 & \cdots & u^{\dagger N} \\ & \ddots & \vdots \\ & & 1 \end{bmatrix}, \end{aligned} \quad (100)$$

or in indices,

$$\left\langle \tilde{\zeta}_n^\dagger \tilde{\zeta}_{n'} \right\rangle = u^{\dagger n' - n} \theta_{n', n}^+ = e^{-(iE+r/2)(n'-n)\delta t} \theta_{n', n}^+.$$

$$-\left\langle \tilde{\zeta}_n \tilde{\zeta}_{n'}^\dagger \right\rangle = -u^{n-n'} \theta_{n, n'}^+ = -e^{(iE-r/2)(n-n')\delta t} \theta_{n, n'}^+. \quad (101)$$

Here the formal operation of u and u^\dagger on the identity in the adjoint representation is given its explicit matrix representation in the second expression on each line. The signs are as suggested by Eq. (97), and the two Green's functions equal those in Eq. (63) for the Keldysh dyads that are their formal homologues.

To construct a limited but explicit operator correspondence, we may use its equivalent representation through field insertions in the SK and DP path integrals. The two bilinear NO insertions of Eq. (19), and the trace-preserving $a^\mu \rho a_\nu^\dagger$, considered independently, give the three mappings that couple to iE or r . These can then be used to simplify the remaining independent term that couples to rn_R . The four time-local insertions appearing in Eq. (8) lead to the mappings

$$\begin{aligned} \zeta_n^\dagger \zeta_{n-1} &\leftrightarrow \xi_{-n} \xi_{-(n-1)}^\dagger \\ \zeta_{n-1} \zeta_n^\dagger &\leftrightarrow \xi_{n-1} \xi_n^\dagger \\ \zeta_{n-1} &\leftrightarrow \xi_{n-1} \xi_{-(n-1)}^\dagger \end{aligned}$$

$$\zeta_n^\dagger + \zeta_n^\dagger \zeta_{n-1} \zeta_n^\dagger \leftrightarrow \xi_{-n} \xi_n^\dagger. \quad (102)$$

Both $\zeta_n^\dagger \zeta_{n-1}$ and $\zeta_{n-1} \zeta_n^\dagger$ arise from different matrix generalizations of $z\partial/\partial z \sim \partial/\partial w$, which we may have expected by Eq. (17) to lead to insertion of the quantum number operator. The matrix ordering in the DP representation is what determines whether the insertion goes into the forward or backward leg of the time loop.

Similarly, either by Eq. (37) (generalized to include dissipative terms), or directly from the Green's functions (101) and the stationary point evaluation, the first three products in Eq. (102) have expectation = $K_{n\delta t}^{-1} + \mathcal{O}(\delta t)$, in keeping with the usual observation that both A

and $A^\dagger A$ as isolated insertions yield the number operator in the DP formalism. We learn here, however, that the three operator combinations correspond to very different insertions in the time loop. The final line in Eq. (37) has expectation $K_{n\delta t}^{-1} + I$, by either evaluation. Away from equal times, however, the matrix and dyad green's functions do not coincide.

To see that the tilde fields with Green's functions (101) do not correspond to the Keldysh products with the same Green's functions, it is sufficient to write the Liouville operator in two forms, as

$$\begin{aligned} \mathcal{L}_n(\zeta_n^\dagger, \zeta_{n-1}) &= \text{Tr} \left[\left(iE + \frac{r}{2} + rn_R \right)_n \zeta_n^\dagger \zeta_{n-1} + \left(-iE + \frac{r}{2} + rn_R \right)_n \zeta_{n-1} \zeta_n^\dagger \right. \\ &\quad \left. - (r + rn_R)_n \zeta_{n-1} - (rn_R)_n (\zeta_n^\dagger + \zeta_n^\dagger \zeta_{n-1} \zeta_n^\dagger) + (rn_R)_n \right] \\ &= \text{Tr} \left[\left(iE + \frac{r}{2} \right)_n \left[\tilde{\zeta}_n^\dagger \zeta_{n-1} + \frac{1}{2} (\tilde{\zeta}_n^\dagger + \tilde{\zeta}_n^\dagger \zeta_{n-1} \tilde{\zeta}_n^\dagger + I) \right] - \left(iE - \frac{r}{2} \right)_n \left[\zeta_{n-1} \tilde{\zeta}_n^\dagger + \frac{1}{2} (\tilde{\zeta}_n^\dagger + \tilde{\zeta}_n^\dagger \zeta_{n-1} \tilde{\zeta}_n^\dagger + I) \right] \right. \\ &\quad \left. - \left(rn_R + \frac{r}{2} \right)_n (\tilde{\zeta}_n^\dagger + \tilde{\zeta}_n^\dagger \zeta_{n-1} \tilde{\zeta}_n^\dagger) - \frac{rn}{2} \right]. \end{aligned} \quad (103)$$

The first expression corresponds to the time-loop Hamiltonian (40) under the operator correspondence (102). The second is an approximation to its Keldysh transform using the indexing (102), which converges to the Hamiltonian in Eq. (55) in the continuum limit. The nonzero parts of the operator expectations $\langle \tilde{\zeta}_n^\dagger \tilde{\zeta}_{n'} \rangle = \langle \psi_n \phi_{n'}^\dagger \rangle$, $-\langle \tilde{\zeta}_n \tilde{\zeta}_{n'}^\dagger \rangle = \langle \phi_n \psi_{n'}^\dagger \rangle$ coincide, but the operators more generally do not.

C. The fluctuation-dissipation theorem

The value of the classical expression for time-loop quantities is summarized in the way it absorbs the leading relations of the fluctuation-dissipation theorem into the time-dependence of the classical stationary point, which as a deterministic relation is akin to a time-dependent equation of state. In a continuum limit, the stationary point Eq. (95) at $\tilde{\zeta}^\dagger \equiv 0$ may be arranged as

$$\partial_t K_t^{-1} + \left(\frac{r}{2} - iE \right) K_t^{-1} + K_t^{-1} \left(\frac{r}{2} + iE \right) = rn_R, \quad (104)$$

which is the standard solution for the covariance matrix of a linear Fokker-Planck equation [11] (p. 175, Eq. 5.166).

At the same time, for $rt \rightarrow \infty$, the solution (64,65) for K^{-1} goes to

$$K_t^{-1} \rightarrow \int_0^\infty du e^{-(r/2 - iE)u} (rn_R)_{t-u} e^{-(r/2 + iE)u}, \quad (105)$$

which is the covariance function $\langle \xi_t \xi_{-t}^\dagger \rangle$ by the correspondence (102). rn_R plays the role of a diffusion matrix in the Fokker-Planck equation, as was seen explicitly in the Glauber-Sudarshan “ \mathcal{P} -representation” in Eq. 8 of Ref. [23]. The covariance function is expressed through the response functions in terms of the diffusivity in Eq. (105), in the generalization of the standard fluctuation-dissipation theorem [11] (p. 179, Eq. 5.184) to a time-dependent source. The more general two-time covariance function is then given by Eq. (68).

V. CONCLUDING REMARKS

Much of this paper has been devoted to building machinery or checking consistency among different representations (with many correspondences still left unexplored). While these manipulations are necessary, it is important not to lose sight of the main conceptual results that underlie the derivation. Three are central.

First, it has been emphasized that a certain class of maximum-entropy driven ensembles is generic, in the Fokker-Planck sense that it arises as the stable class under the most general, second-order, trace-preserving evolution operator on a simple-harmonic oscillator density matrix (the calculations are not new [2, 23], although the point may not have been made this way before). The stable class is defined by Hamiltonian evolution together with linear diffusive transport, and the operators leading to dissipation are readily obtained through Born ap-

proximation of the coupling between subsystem components. The classical state variables for these ensembles are inevitably richer than the complete set of commuting observables in the quantum formulation, and the exact distribution entropy is a function of currents as well as charges.

Second, the form of the driven-state entropies follows from extending the equilibrium entropy function to respect the full symmetry group of the quantum *kinematics*. For the systems demonstrated, the kinematics are symmetric under unitary transformations in D dimensions. Different system Hamiltonians will mix charge-valued and current-valued state variables in different ways, but the most general set of possible Hamiltonians simply generates the symmetry group of the kinematics. Thus any entropy function required to coincide with the equilibrium entropy under one Hamiltonian, but to be invariant under reversible evolution as the Hamiltonian is arbitrarily varied, must have the form of Eq. (5).

Third, Martin-Siggia-Rose or Doi-Peliti methods for representing generating functions provide efficient means to identify classical stationary dynamics of the underlying Schwinger-Keldysh time loop, which cannot be expressed as shifts in the SK variables. Because it is based on the exact partition function, the DP representation automatically propagates the correct entropy through time, including its symmetries and current dependence. In turn, because the quantum density is defined by max-

imization of this entropy, the map from SK to DP representations is invertible. The resulting current-dependent classical equations of state provide a richer foundation for the statistical mechanics of dissipative driven processes, such as steady-state chemical reactions, than the cruder classical Markov description.

The somewhat surprising feature of the DP representation is the way in which it preserves time-loop correlations, despite having no time-loop structure itself. Although both the products $A^\dagger A$ and $a^\dagger a$ represent the “number operator”, and in some cases coincide, the same quantum number operator inserted at various positions maps to linear, quadratic, or cubic products of DP fields, and their ordering as matrices distinguishes legs on the time loop. Likewise, there is a structural homology between the DP representation and the Keldysh rotation – which also hides the explicit time loop – yet the DP operator products are not simply images of their Keldysh homologues.

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