Path-reversal, Doi-Peliti generating functionals, and dualities between dynamics and inference for stochastic processes

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(Dated: June 13, 2018)

A variety of fluctuation theorems, concerning probability ratios of rare versus common trajectories in stochastic processes, are defined in terms of reversed paths and driving protocols. A subset of these apply the measure of the original stochastic process to reversed paths, and have an interpretation in terms of time-reversed dynamics. More generally, the adjoint measure of the fluctuation theorems, constructed to reverse probability currents, may define a new stochastic process, which is not inherently dynamical and may even be incompatible with reverse-time dynamics. Here we develop a general interpretation of fluctuation theorems based on the adjoint process by considering the duality of the Kolmogorov-forward and backward equations that define the adjoint generator, as these equations apply asymmetrically to distributions and to observables. Kolmogorov-backward propagation of observables is related to problems of statistical inference, so we characterize the adjoint construction as a duality between dynamics and inference.

The adjoint process corresponds to the Kolmogorov backward equation in a generating functional that erases memory from the dynamics of its underlying distribution. We derive this result for general correlation functions by showing that fluctuation-theorem duality exchanges the roles of advanced and retarded Green’s functions. We work at the level of stochastic Chemical Reaction Networks, and show that dualization acts on the finite representation of the generating event-set, in a manner similar to the usual action of similarity transform on the (potentially infinite) set of state transitions. We use the Doi-Peliti functional integral representation of generating functionals, within which duality transformation takes a remarkably simple form as a change of integration variable. Our Green’s function analysis is used to recover the Extended Fluctuation-Dissipation Theorem of Seifert and Speck for non-equilibrium steady states, and to show that the causal structure responsible for it applies also to dualization about non-steady states.

I. INTRODUCTION: FLUCTUATION THEOREMS FROM DIFFERENT APPROACHES TO PATH REVERSAL

Given any two probability distributions $P$ and $P^*$ defined on a set of extended time trajectories for some system, it is a tautology that the average of $P^*/P$ in the distribution $P$ must be unity, because it is the same as the trace of the distribution $P^*$. In symbols, $E_P(P^*/P) \equiv 1$, where $E_P$ denotes expectation in measure $P$. At its simplest, the relation could be so little as the change of measure on the space of trajectories, and $P^*/P$ could be the Jacobean of the corresponding change of variables.

Starting in the early 1990s for dynamical systems [1–4], and a few years later for stochastic processes [5–11], a carefully chosen subset of these tautologies have been exploited to gain information about complex, potentially non-stationary non-equilibrium distributions in terms of simpler stationary or equilibrium distributions and functions along paths that can be measured mechanically or calorimetrically. What the family of tautologies have in common that have been put to this use, is that the probability $P^*$ is defined from $P$ in some way that involves reversing the direction in which each trajectory is traversed, generally along with the externally-imposed protocol of control parameters under which the distributions evolve.

When constructing a probability $P^*$ to study based on reversal, the most basic choice faced is whether to use the original measure $P$ while only reversing trajectories and protocols, or whether to construct a new measure that will reverse probability currents [12, 13, 14]. Relative to the process that generates $P$, the former choice results in what is conventionally termed the “backward” process, while the result of the latter choice is termed the “adjoint” process [15]. If the systems in question are Markovian stochastic processes, the backward and adjoint processes are the same precisely in the case that the transition probabilities satisfy a condition of detailed balance, in which case their steady states are true equilibrium distributions in the strict sense of Boltzmann/Gibbs thermodynamics.

The general class of theorems of the form $E_P(P^*/P) \equiv 1$ based on path reversal for stochastic processes are called Integral Fluctuation Theorems. Their refinements, in which the ratios $P^*/P$ are given a functional form for
individual trajectories, are called Detailed Fluctuation Theorems [14]. Integral and detailed fluctuation theorems have been derived to describe rare-event statistics in thermal ensembles [8 13], to estimate equilibrium free energy values by sampling mechanical work under non-equilibrium conditions, where they are known as Non-Equilibrium Work Relations (NEWRs) [5, 6, 9 11], to separate out the contributions to heat flows that maintain a non-equilibrium driven state from those that provide entropy to change the state [12, 13], and to derive generalized fluctuation-dissipation relations applicable to non-equilibrium steady states [13, 14, 24]. The literature on fluctuation theorems is now large; for reviews see [13, 17, 24, 26].

Markov processes with detailed balance are a very restricted class, about which a great deal is already known, and so much of the study of probabilities under path reversal aims at understanding more general cases. For these, different information is gained, and different limitations are faced, in the study of the backward versus the adjoint processes [17]. The backward process, requiring only a permutation of the probabilities defined in the original process, works directly from the original specification of dynamics, without reference to any particular solutions that they generate. The construction is limited, however, to cases in which every trajectory with a measure in the original system has a reverse which also has a measure in that system. Even when that is the case, the averages of $P^*/P$ produced for the backward process may not carry useful information about quite ordinary properties such as the Shannon entropy difference between non-equilibrium steady states connected by a slow parameter change [13].

Adjoint processes are more flexible than backward processes, but they are also more arbitrary. The adjoint process constructed from an underlying Markov process is essentially a new process; the trajectories to which it assigns probabilities are simply chosen to be the reverses of those in the original process, whether or not they themselves have probabilities in that process. However, the property of reversal of probability currents is not defined solely in terms of the transition probabilities of the original process: it must make reference to some state of the system from which those currents originate. Typically for non-stationary Markov chains, the reference distribution at any time is taken to be the stationary distribution that would result if the parameters in the Markov chain at that time were fixed. [70] This choice permits a definition of the adjoint that at least does not depend on extended-time solutions for probability distributions, but even the stationary distribution generally depends on probability flows among many or all system states, and as such is non-local in the state space [17]. In general it may also be difficult to construct explicitly. What is gained from the choice to study averages of $P^*/P$ for the adjoint process may be the ability to separate the maintenance-associated and change-associated costs of altering a non-equilibrium state [15, 18], as well as new identities among correlation functions and response functions in the non-equilibrium background [13, 14, 24, 27].

The great majority of work done in the emerging discipline of Stochastic Thermodynamics [26] involves path trajectories $P^*$ that can be somehow constructed from the backward process, seemingly for two reasons. One is that the backward process has an immediate interpretation in terms of events and their time-reverses in the original process, and thus can be used to understand the origin of thermodynamic arrows of time [20], even as these are manifested in quite complex systems [28, 29]. The second is that the major body of work in statistical physics since the 1930s [30, 34], to formulate a theory of non-equilibrium thermodynamics, has been based on the effort to derive constraints on non-equilibrium dynamics from changes in the equilibrium entropy. While not possible in general, and not as general as the pursuit of a full non-equilibrium large-deviation theory [35, 36], this strategy is highly successful for systems with a separation of timescales, in which a slow process with microscopically resolved discrete events evolves in the presence of a fast-relaxing thermal bath. For such systems the trajectory probabilities in the original and backward processes can be expressed in terms of changes in the bath’s thermodynamic entropy and the system’s Shannon entropy [14, 20], providing a conservative but still very productive extension of equilibrium thermodynamic methods to non-equilibrium systems.

Even cases in which $P^*$ was constructed as an adjoint process for an underlying system without detailed balance, such as the irreversible Langevin system studied by Hatano and Sasa [15], have been interpreted with respect to heat flows and entropy-production (with the equilibrium entropy state variable defining the entropy “produced” in the bath), and thus implicitly with reference to time reversal at least for the bath [57]. The very heavy dependence on time reversal for interpretations of fluctuation theorems or NEWRs has limited the study of adjoint processes. This is reflected in the caution given by Seifert [26] (p. 41) that, given only the Langevin equation itself without a further specification of context, the assignment of a quantity such as dissipated work based on analogy with physically reversible cases, may be “a purely formal one without real physical meaning.”

Adjoint fluctuation theorems, beyond time reversal

Often one wishes to study adjoint stochastic processes in which the transition probabilities for dynamics are not interpreted in terms of bath-entropy production, or they do not support detailed-balance equilibria, or where the reverses of allowed trajectories are not even allowed in the original process. Models of this form naturally arise in Chemical Reaction Network (CRN) theory [38, 39] for networks that produce steady states without detailed balance. While, for applications to chemistry, entropy-production interpretations may still be valid, this class...
of models equally well represents evolutionary population processes in which events of death and reproduction can reflect inputs of a completely different origin than physical thermodynamics. Even within chemistry, the choice to omit a reverse reaction from a CRN, which immediately precludes defining the backward process, is a commitment that the dynamics of the system is controlled by factors other than rare fluctuations against the likely directions of flow; it should be possible to understand these in their own terms as an effective theory.

For all cases it is desirable to assign a meaning to the adjoint process that follows directly from its construction from the original dynamics, without reference to time reversal and without dependence on additional framing outside the dynamical equations themselves. This is true even if the adjoint process may also have a case-dependent interpretation in terms of time reversal.

Our aim in this paper is to explain a natural semantics for fluctuation theorems based on the adjoint construction of $P^\ast$, which follows from the transposed representations of the underlying generator of the stochastic process. Introduced by Kolmogorov as the “forward” and “backward” evolution operators, these act respectively on probability distributions or on observables averaged in those distributions.

Transposing the action of a generator defines the sense of path- and protocol-reversal beneath the construction of the adjoint process, but by itself, this transposition is simply a regrouping of terms in a sum, with no new information. The nontrivial step in constructing the adjoint process is recognizing that the ratio $P^\ast / P$ constitutes a tilt that forms a generating functional on the evolving probability distribution of the underlying process. The adjoint processes that produce interesting fluctuation theorems are identified by going beyond the identity $E_P (P^\ast / P) \equiv 1$ to study the behavior of correlation functions in the presence of the tilt. The particular adjoint process produced by dualizing about the instantaneous steady states under the Markov generator is one that erases memory of the causal history of the distribution from correlation functions. Mathematically, this criterion is equivalent to interchanging the forms of the Kolmogorov forward and backward generators, in a sense we will make precise below. Other results known for the adjoint process, such as the extended Fluctuation-Dissipation Theorems (FDTs), follow from this memory-erasing property, not only for stationary nonequilibrium states, but also about non-stationary backgrounds.

If the natural interpretation of the backward process is physical, in terms of time-inverted sampling of dynamical paths, the natural interpretation of the adjoint process, suggested by the relation of Kolmogorov forward and backward equations, should be informational. The inverted time order by which operators depend on states under the Kolmogorov-backward equation has no relation to reversal of dynamics; it arises because in a causal process the expectations of operators depend on the conditions imprinted on states at earlier times. A generating functional alters the weight with which trajectories are sampled to produce average values, in a manner closely related to the procedure of importance sampling from statistical inference. Therefore we characterize the duality of fluctuation theorems using the adjoint process as being dualities between dynamics and inference for a stochastic process.

**Green’s functions from generating functionals, and the Doi-Peliti 2-field representation**

The tools to efficiently study the propagation of disturbances either forward or backward in time are the Green’s functions of the stochastic process. Familiar as the Green-Kubo relations for linear response to small perturbations, these are typically discussed in the context of perturbations near equilibrium. Within a generating functional, however, it is possible to compute fluctuation-response relations for perturbations about any background that the tilt of the generating functional makes into a saddle point. In cases where a perturbative expansion in higher-order moments of the fluctuation converges, the Green’s functions form a basis for higher orders of nonlinear response, while continuing to express the causal structure in the underlying process.

Our preferred system for working with Green’s functions is the Doi-Peliti (DP) functional integral framework for the representation of arbitrary generating functionals. The DP formalism is one of a larger family of 2-field functional integral (2FFI) methods that include the Martin-Siggia-Rose formalism for stochastic differential equations and the Schwinger-Keldysh time-loop for quantum systems with decoherence. The Doi operator representation abstracts the linear algebra of generating functions, and the Peliti construction then evaluates the time integrals of these on continuous basis sets derived from Poisson distributions, which become the field variables of functional integrals. This additional change of representation leads to very direct derivations of Green’s functions and fluctuation-dissipation relations, as well as very elegant routes to ray-theoretic or other semiclassical approximation methods.

The most important feature of the DP construction for us will be that the two fields of this 2FFI formalism directly represent the action of both the forward and backward generators. Time-dependent correlations can be computed either by propagating distributions forward in time with retarded Green’s functions which are causal, or by propagating observables backward in time with advanced Green’s function which are anti-causal. The relations between these and the equal-time correlation function is the basis for non-equilibrium fluctuation-dissipation relations. The anti-causality of the advanced Green’s function, in the context of saddle-point approximations, provides our connection be-
tween the backward equation and methods of importance sampling [54].

The elements we believe are new in this paper include the DP construction of fluctuation theorems for general discrete-state stochastic processes, which is a straightforward extension from the study of Langevin systems (equivalent to Gaussian-order fluctuations) in [10]. The elegant form of the DP generator for CRNs (Eq. (28) below) and the significance of its modular structure, although introduced previously [52, 56], will play a new role in the context of fluctuation theorems. It was recognized earlier by Baish [57] that the construction of the adjoint process corresponds in the DP functional integral to a simple change of the dummy variable of integration. We will show that this change of variable produces a similarity transformation of the adjacency matrix of the CRN, exactly reflecting on a finite generator set the similarity transform that defines the adjoint process on the matrix of transition probabilities which has the dimension of the state space. Although the extended FDT that we derive was chosen to recover the result of [20] for non-equilibrium steady states, our Green’s function derivation makes contact between two different notions of FDT, and also shows that the results extend to non-stationary backgrounds and non-linear fluctuations.

The presentation is organized as follows. Sec. III provides basic notation for discrete-state stochastic processes, and reviews the standard construction for fluctuation theorems using the adjoint process. We then review Kolmogorov forward/backward duality, and introduce the concepts and notations for the DP generating functional construction, emphasizing the particularly simple form it takes for stochastic CRNs.

Sec. III develops a very simple class of examples that can be solved exactly, to illustrate the meaning and roles of the conjugate fields in 2-field functional integrals, their connection to concepts from importance sampling, the way duality appears as a change of variables in the integral representation, and how tilting to form generating functionals interacts with dynamics, particularly for NEWRs.

Sec. IV extends the results of Sec. III from the stationary-point approximation to the Green’s functions for response and fluctuation, and to general CRNs for which a second-order expansion of the rate equations is defined. Here we introduce the versions of FDTs that emerge in functional integrals as a consequence of internal symmetries, and relate them to the more familiar forms used in [21, 58]. We provide explicit solution forms for the simple models of Sec. III in order to show the subtle manner in which path weights, by exchanging the roles of distributions and observables, harness causal and anticausal response functions that were already present as a reflection of the Kolmogorov transpose relation.

Sec. V derives the appropriate generalization of NEWRs in the CRN framework, emphasizing the connection between the required form of the path-weight function to produce anti-causal dynamics, and the original duality between the forward and backward equations with which we began the discussion.

II. BACKGROUND: DISCRETE-STATE STOCHASTIC PROCESSES, DUALIZATION, AND GENERATING FUNCTIONALS

We begin by defining the class of stochastic processes to be considered and introducing notation for the master equation and generator.

A. Discrete-state stochastic processes and generator

Let a state be given by a vector \( n \equiv [n_p] \) with non-negative integer-valued components, for \( p \in \{1, \ldots, P\} \). We will refer to \( p \) as an index of the \( \text{species} \) in the system, and \( n_p \) as the count of species \( p \). Let \( \rho_n \) be a probability density indexed on \( n \). Dynamics for \( \rho \) are governed by a continuous-time master equation of the form

\[
\frac{d \rho}{d \tau} = T \rho
\]

shorthand for

\[
\frac{d \rho_n}{d \tau} = \sum_{n'} T_{nn'} \rho_{n'}.
\]

\( T \equiv [T_{nn'}] \), called the \textit{transition rate matrix} of the stochastic process, is a representation of its generator. In general we regard \( T \) as having a fixed form — for instance reflecting a fixed set of reactions in a CRN — but adjustable parameters such as rate constants representing controls or interactions with an environment. Sometimes it is convenient to re-express the control parameters in terms of quantities such as mean values of the steady state they would produce; when we do so we denote those values with underbars, to distinguish them from mean values of dynamical states actually produced. Following [15], denote these parameters \( \varphi \); in general they may vary with time as the process runs.

B. Fluctuation theorems based on the adjoint process

The construction of the adjoint process to some underlying system follows from a relation between a path-weight that can be used to modify the measure on paths, and a dual generator constructed from the underlying Kolmogorov backward operator by absorption of the weighting terms. The path weight is derived from the stationary distribution at the instantaneous parameter values \( \varphi \). For systems with detailed balance evolving under a Hamiltonian, the logarithm is proportional to the energy. To review the construction as given in Equations (5–9) of [15], with minimal notation, we reduce the stochastic process to a discrete-time process by evolving
for finite time intervals, and treating the parameters in the generator as fixed within any short interval.

Let $\delta \tau$ be a small enough time interval that the parameters in $T$ are effectively constant over that interval, and introduce the matrix of one-step transition probabilities

$$W \equiv e^{\delta \tau T}$$

Let $\rho$ denote the steady-state distribution annihilated by $T$ at parameters $\alpha$. The one-step transition matrix satisfies

$$\sum_n W_{n'n} \rho_n = \rho_{n'} \quad \sum_n' W_{n'n} = 1 \quad \forall n,$$

where the second line states that $W$ is a stochastic matrix.

Denote a discrete-time trajectory in the lattice of species counts by $[n]$, which is a sequence of states $n_0, n_1, \ldots, n_K$ over a real-time interval of length $K \delta \tau \equiv T$. Let $[\alpha]$ likewise denote a protocol, a sequence of values of the control parameters $\alpha_0, \alpha_1, \ldots, \alpha_K$. Write $W_{n_k+1:n_k}^{(k)} = W_{n_k+1,n_k}(\alpha_k)$ for the matrix element in the one-step matrix at step $k$, between the $k$th and $(k+1)$th state in trajectory $[n]$, and likewise denote by $\rho_{(k)}(\alpha_k)$ the density at any $n$ in the steady state under $W^{(k)}$.

The expectation of any function $g_{[n]}$ on trajectories, starting from the steady-state density at step $k = 0$, is defined in the measure

$$\langle g \rangle \equiv \sum_{[n]} g_{[n]} \left( \prod_{k=0}^{K-1} W_{n_k+1:n_k}^{(k)} \right) \rho_{(0)}^{(0)}.$$  \hspace{1cm} (4)

By Eq. (3), at each step $k$

$$\sum_{n_k} W_{n_k+1:n_k}^{(k)} \rho_{n_k}^{(k)} = \rho_{n_k+1}^{(k)},$$

from which it follows that

$$\left( \prod_{k=0}^{K-1} \frac{\rho_{n_k+1}^{(k+1)}}{\rho_{n_k+1}^{(k)}} \right) = \left( \exp \left( \sum_{k=0}^{K-1} \log \frac{\rho_{n_k+1}^{(k+1)}}{\rho_{n_k+1}^{(k)}} \right) \right) = 1.$$  \hspace{1cm} (6)

$- \log \rho^{(k)}$ plays the role of a non-equilibrium generalization of the free energy in Eq. (3). Although in general we may not be able to express $\rho_{n_k}^{(k)}$ as a function of $n_k$ and $\alpha_k$, if we take the difference $\log \rho_{n_k+1}^{(k+1)} - \log \rho_{n_k+1}^{(k)}$ to define $d \tau (d \alpha_k / d \tau) \partial g(n; \alpha) / \partial \alpha$ in the limit $\delta \tau \to 0$, we may write Eq. (6) as

$$\left\langle \exp \int_0^T d \tau \left( \frac{d \alpha_k}{d \tau} \right) \frac{\partial \rho(n; \alpha)}{\partial \alpha} \right\rangle = 1.$$  \hspace{1cm} (7)

holding $T$ fixed as $\delta \tau \to 0$.

Re-grouping terms in the products in Eq. (6), the same path sum may be written

$$\left( \prod_{k=0}^{K-1} \frac{\rho_{n_k+1}^{(k+1)}}{\rho_{n_k+1}^{(k)}} \right) = \sum_{[\alpha]} \rho_{\alpha}^{(K)} \left( \prod_{k=0}^{K-1} \frac{1}{W_{n_k+1:n_k}^{(k)}} \right) \rho_{n_k}^{(k)}.$$  \hspace{1cm} (8)

The chain of sums produces a sequence of normalized distributions when evaluated from left to right in Eq. (6), whereas in Eq. (4) normalized distributions result from summing from right to left. Hence we identify the transpose of a new one-step operator $W^T$ as

$$\left( W^T \right)_{n'n} = \frac{1}{\rho_{n'}} W_{n'n} \rho_n \quad \text{or} \quad \hat{W}_{nn'} = \rho_n (W^T)_{nn'} \frac{1}{\rho_{n'}}.$$  \hspace{1cm} (9)

From Eq. (6) for $W$, it follows that

$$\sum_{n'} W_{n'n} \rho_{n'} = \rho_n \quad \sum_n W_{nn'} = 1 \quad \forall n'$$

In the limit $\delta \tau \to 0$, Eq. (6) is the one-step matrix for a transformed rate-matrix or generator

$$\hat{T}_{nn'} = \rho_n (T^T)_{nn'} \frac{1}{\rho_{n'}}.$$  \hspace{1cm} (11)

with the properties that

$$\sum_{n'} \hat{T}_{nn'} \rho_{n'} = 0 \quad \sum_n \hat{T}_{nn'} = 0 \quad \forall n'$$

The adjoint stochastic process, generated by $\hat{T}$, has the same steady states as the process defined by $T$, and it has nonzero probabilities on each trajectory that is the time-reverse of some trajectory for which $T$ produces non-zero probabilities.

Combining terms across the two lines in Eq. (9), the adjoint process could alternatively have been defined as the one that reverses probability flow between any two states in the stationary distribution $\rho_n$,

$$\hat{W}_{nn'} \rho_{n'} = W_{n'n} \rho_n.$$  \hspace{1cm} (13)

It is immediate that the condition of detailed balance is the statement that $W = W^T$ in which case $\rho_{n}$ is an equilibrium distribution at parameters $\alpha$. Clearly there is no implication of reversed dynamics in this construction; the index $k$ on $n$ and $\alpha$ is simply read in the reverse order from the original process to define the “forward” direction for $W$. 
C. Interpreting the adjoint process in terms of Kolmogorov forward-backward duality and memory erasure

To understand what the adjoint process means, accepting that part of its definition was our arbitrary choice of the stationary $\rho$ as the reference for reversal of currents, we consider the use of a similar transpose to relate the Kolmogorov-forward and backward equations for any stochastic process. In particular, we make explicit not only the role of distributions, but also that of observables which may be averaged to produce moments or correlation functions.

Consider the expectation of an arbitrary observable $\mathcal{O}$ at a single time in a distribution $\rho$, given by

$$\langle \mathcal{O} \rangle \equiv \sum_n \mathcal{O}_n \rho_n. \quad (14)$$

The $\mathcal{O}_n$ are chosen not to be explicit functions of time, so all time dependence in $\langle \mathcal{O} \rangle$ results from the evolution of $\rho$. This evolution can be expressed in two ways, as

$$\frac{d}{d\tau} \langle \mathcal{O} \rangle = \sum_n \mathcal{O}_n (T\rho)_n$$

$$= \sum_n (T^\dagger \mathcal{O})_n \rho_n. \quad (15)$$

The first line, in which $T$ acts on $\rho$, is called the forward equation, and the second line where $T^\dagger$ acts on $\mathcal{O}$ — also formally an adjoint when written this way, but we will think of it in terms of a matrix transpose to avoid confusion with the fluctuation-theorem adjoint — is called the backward equation [81], [82]. If these equations are integrated over a finite interval separating an initial condition $\rho(0)$ from $\mathcal{O}$ evaluated at a later time $\tau$, the forward equation evolves the distribution up to $\tau$, whereas the backward equation evolves the dependence of $\mathcal{O}$ (metaphorically, a “shadow cast by $\mathcal{O}$” on earlier times) down to the initial distribution.

The Kolmogorov-backward generator $T^\dagger$ is not yet the generator of the adjoint process; it is a stochastic matrix on the “wrong” index. The rescaling of Eq. (9) has the effect of exchanging the behavior of the indices that contract with distributions and with observables. To show how the the path weight [3] responsible for the rescaling is constructed as a tilt of a dynamically evolving distribution $\rho$ that is not generally equal to $\rho$, we begin by reviewing the use of generating functions and functionals to study the time evolution of distributions and correlation functions, and show how it is instantiated in the DP functional integral formalism.

D. Generating functions, and the Doi-Peliti framework

The Doi Hilbert space

It is often more convenient than working directly with the density $\rho$, to work with the moment-generating function. Historically, the generating function was introduced as a Laplace transform of the density

$$\Phi(z) \equiv \sum_n \left( \prod_p z^n_{p} \right) \rho_n, \quad (16)$$

in which $z = [z_p]$ is a vector of complex-valued arguments to $\Phi[81, 82]$. In this representation, The moment-generating function evolves in time under a Liouville equation induced by the master equation [11], of the form

$$\frac{\partial}{\partial \tau} \Phi(z) = -\mathcal{L} \left( z, \frac{\partial}{\partial z} \right) \Phi(z), \quad (17)$$

in which $\mathcal{L}(z, \partial/\partial z)$ is termed the Liouville operator.

For many uses it is not necessary to evaluate $\Phi$ as an analytic function of argument $z$; only the linear algebra induced by its formal power series is required. Here we adopt a representation due to Doi [42, 43] that replaces complex (analytic) variables and their derivatives by abstract raising and lowering operators, under the mapping

$$z_p \rightarrow a_p^\dagger; \quad \frac{\partial}{\partial z_p} \rightarrow a_p. \quad (18)$$

The algebra of these operators, induced by the action of partial derivatives on analytic functions, is given by

$$[a_p, a_q^\dagger] = \delta_{pq}. \quad (19)$$

The Doi construction of a Hilbert space of generating functions, with inner product corresponding to the trace of the underlying density, is a standard exercise [51], for which we provide a brief summary in App. A. The result is that the analytic generating function $\Phi(z)$ is replaced by a state vector $|\Phi\rangle$, on which time evolution under the Liouville operator [17] becomes

$$\frac{\partial}{\partial \tau} |\Phi\rangle = -\mathcal{L} (a^\dagger, a) |\Phi\rangle. \quad (20)$$

The evaluation of $\Phi(z)$ at $z = 1$, equivalent to tracing over the underlying density $\rho$, is accomplished with a projection operator that defines the inner product, given in Eq. (14). Crucially, the expectations of observables [14] are represented by operator insertions in the inner product, establishing a correspondence between distributions and observables on the index $n$, with states and operators in the Doi Hilbert space. One can invert the mapping [18] to restore the analytic structure of the generating function using its complex-variable argument in a modified version of the inner product, as

$$\langle 0 | e^{\sum_p z_p a_p^\dagger} |\Phi\rangle = \Phi(z). \quad (21)$$
This transformation will be useful in defining the functional-integral representation of generating functions next.

The Peliti 2-field functional integral

A functional-integral representation for the Hilbert space of time-dependent generating functions and functionals was introduced by Peliti [44, 45], building on the Doi algebra. It facilitates a variety of stationary-point approximations (related to the ray methods of Freidlin and Wentzel for diffusion equations [50]), and is one of a larger class of 2-field functional-integral (2FFI) methods including the Schwinger-Keldysh time-loop formalism [48, 49] for quantum systems, and the Martin-Siggia-Rose formalism for dissipative dynamical systems [47].

The Peliti method makes use of coherent states as basis elements for the expansion of arbitrary generating functions. For a vector \( \phi \equiv [\phi_p] \) of complex-valued coefficients, the coherent state

\[
|\phi\rangle \equiv e^{(t^\dagger - 1)\phi} |0\rangle
\]

is the generating function for a Poisson distribution with mean \( \phi \).

In the Doi algebra, dual to each right-hand coherent state is a projection operator, which is a function of the Hermitian conjugate vector \( \phi^\dagger \). Constructed from the left-hand ground state \( |0\rangle \) defined in Eq. (A1), it is given by

\[
(\phi) \equiv e^{(t - \phi^\dagger)} |0\rangle e^{\phi^\dagger a}.
\]

A representation of unity is obtained from the integral over coherent states and their conjugate projection operators, as

\[
\int \frac{d\phi^\dagger d\phi}{\pi^p} \left( \phi \right) \langle \phi | = I.
\]

When the representation (24) is inserted into an expression to provide an expansion in the basis \( (\phi^\dagger, \phi) \), these vectors become field variables of integration. The field \( \phi \) is termed the observable field, because it corresponds to the mean of a Poisson distribution, while \( \phi^\dagger \) is termed the response field, for reasons that will become clear when we study Greens functions in Sec. IV.

Evolution under the Liouville equation (20) can formally be reduced to quadrature and converted into a functional integral through repeated insertion of copies of the representation (24) of unity at small increments of time: more detail on this construction is provided in App. A2. If the inner product (21) is used at late time to re-establish a connection between the complex field variables, and the complex surface arguments \( z \) that can be used to probe \( \Phi \), the integral representation of the generating function for a distribution evolved from time \( \tau = 0 \) to \( \tau = T \) can be written

\[
\Phi_T(z) = \int_0^T D\phi^\dagger D\phi e^{(z - \phi^\dagger \phi)\phi} e^{-S\Phi} |\phi_0\rangle \langle\phi_0|.
\]

In Eq. (25) a new functional \( S \) with the form of a Lagrange-Hamilton action functional appears, which is defined in terms of the Liouville operator from Eq. (20) as

\[
S = \int_0^T d\tau \{ - (d_\tau \phi^\dagger) \phi + L(\phi^\dagger, \phi) \}.
\]

There are many reasons to adopt an extended-time, functional-integral representation for a function such as \( \Phi_T(z) \) evaluated at a single time, beyond simply extracting the moments of an underlying evolved density \( \rho_T \). The integral offers a way to insert operators at times \( \tau < T \) to study the dependence of late-time observables on regions in the distribution at earlier times, giving a representation of the backward equation. The density can also be given incremental weights in continuous time, making Eq. (26) an extended-time generating functional. We will use all these below to understand the origin of reverse-time evolution and anti-causality in NEWRs and their generalizations.

E. Nonlinear rate laws and concurrency: forms of the generators for Chemical Reaction Networks

A very general class of discrete-state stochastic processes are those for which each elementary event can remove a set of members from one or more species, and then introduce another set. The removal of all members in the removed set happens concurrently, and if a state has too few members of some species to populate the removed set, the event cannot occur. Processes in this class are of mathematical interest because the condition of concurrency makes the graphical representation of the process model a directed multi-hypergraph [53, 60], on which problems of constraint satisfaction are often computationally complex [61], and because the rate laws are generally nonlinear. They are of practical interest because they include models of Chemical Reaction Networks (CRNs) [39, 38, 62], though the class is rich enough to include a wide variety of other population processes as well. We will develop them here because removal and addition, performed respectively by lowering and raising operators, in the Doi-Peliti formalism stand in the relation of projection operators and states.

We will adopt a set of concepts and terms from the CRN literature, which are reviewed in App. B. Elementary events are termed reactions, and the input and output sets in each reaction are termed complexes. The representation of reactions in the transition rate matrix is decomposed into three components:

- **A stoichiometric matrix** denoted \( Y \) that gives the numbers of each species in any input or output complex;
an adjacency/rate matrix denoted $A_k$ ($k$ are the rate constants), which acts as the equivalent of a graph Laplacian between complexes; and

an activity function in two forms, denoted $\Psi_Y$ and $\psi_Y$. $\Psi_Y$, typically representing a sampling process, expresses the probability to form a complex in terms of the numbers of species $n$, and $\psi_Y$ is a corresponding function defined on shift operators or the arguments of the generating function.

In terms of these quantities, for a simple CRN where complexes are formed by sampling without replacement from the pools of species (the rule underpinning the usual mass-action rate law), the matrix $T$ that generates the forward equation can be written

$$T = \psi_Y \left( e^{-\partial/\partial n} \right) A_k \left[ \psi_Y \left( e^{\partial/\partial n} \right) \cdot \Psi_Y(n) \right] = \sum_{i,j} \left[ \psi_Y^{(2)}(j) - \psi_Y^{(1)}(j) \right] k_{ji} \psi_Y^{(1)(j)} \left( e^{\partial/\partial n} \right) \Psi_Y^{(i)}(n)$$

(27)

Here sub/superscripts $i$ and $j$ index complexes, the ordered pair $(i, j)$ indexes a reaction from complex $i$ to complex $j$ with associated rate constant $k_{ji}$, and $\Psi_Y^{(i)}$ is the count of ways in which the set in $i$ can be sampled from a state $n$. We indicate shift operators on functions indexed by $n$ with $e^{\partial/\partial n}$; the activity functions $\psi_Y^{(i)}$, defined in Eq. (15), are simply those that, with argument $e^{\partial/\partial n}$, shift the indices of all functions to their right upward in $n_p$ by the stoichiometric coefficient $y_{pi}$ of species $p$ in complex $i$.

The Liouville operator in the Doi representation, corresponding to the generating matrix (27), takes the strikingly simple form

$$-\mathcal{L}(a^i, a) = \psi_Y^{(2)}(a) A_k \psi_Y(a).$$

(28)

We have developed several consequences of the symmetric form (28) for the solution of moment hierarchies in 53, 58. The fact that such a formal symmetry exists between raising and lowering operators – or between states and projectors – will give the adjoint construction of the generator a comparably simple form whether or not the dynamics comes from a Hamiltonian.

The “form” of transition matrices and their adjoints

Eq. (27) shows the typical form of generators of the forward equation: shift operators act on the distribution and also on functions such as combinatorial factors that determine reaction rates (here $\Psi_Y(n)$). The backward generator $T^*$ may be formed by shifting indices in the sum (11); for this class of processes, it amounts to changing $\partial/\partial n \to -\partial/\partial n$, and having shift operators act to the left, where they no longer transform $\Psi_Y(n)$.

The surprising result of the NEWRs and their generalizations is that by adding a generating-functional weight to an evolving distribution, the characteristic forms of $T$ and $T^*$ can be interchanged. Although the inner product (11) for stochastic processes is inherently asymmetric between states and projection operators, the formal asymmetry in the Doi-Peliti functional integral is (up to a choice of boundary conditions) all contained within the kernel matrix $A_k$ in the Liouville operator (28). A suitable generalization of the transpose of this kernel can thus exchange the behavior of states and operators.

We show below in Eq. (9) that dualization of $A_k$ is carried out by a rescaling similarity transformation of the same form as the adjoint relation in Eq. (9), but instead of using probabilities $p_n$ indexed on states, it uses complex-activities $\psi_Y$ related to average particle number. The important feature of the 3-factor symmetric product form (28) is to encapsulate the network topology (a simple graph) within the factor $A_k$, allowing the activities $\psi_Y$ and $\psi_Y^T$ to act symmetrically on observable and response fields.

III. DUALITY BETWEEN STATES AND OPERATORS IN THE DOI-PELITI FORMALISM

We have shown how in the DP formalism distributions take the form of states, and observables correspond to operators. We show now how states and operators are represented respectively by the observable and response fields of the DP representation. In the context of a simple 2-state model, for which many expectations can be obtained exactly by stationary-point methods, we then demonstrate how the similarity transform of Eq. (9) may be effected by a simple change of variables, which has then the effect of exchanging the response and observable fields.

The change of variables also results in an extra term, which is a functional weight added to $\mathcal{L}$. This term corresponds to what has been called the excess heat in Langevin approximation 15, 18 (though here no Gaussian limit of fluctuations is required), and reduces to the total entropy production in the integral fluctuation theorem for systems with detailed balance 14, 20. Though forward and reverse dynamics are always present in a generating function, simply as a consequence of the duality between the forward and backward actions of the generator, the adjoint construction of the fluctuation theorems exchanges the forms of the forward and reverse generators as mentioned earlier. We show in the next section that the forward and reverse dynamics derived here for stationary paths extends to causality and anticausality of more general Green’s functions. We also point out connections of this procedure to the tilting transformation performed in Importance Sampling, which exchanges a weight function between a distribution and an observable while preserving expectation values.
A. States, operators, and duality: a single-time generating function in the DP representation

We begin not with dynamics, but simply with the construction of a generating function for a static distribution, in the DP representation. This will introduce the idea of a nominal distribution, for which the mean is reported by the expectations of bilinear forms $\phi^\dagger \phi$ in the Peltiti field integral, and will show how it differs from the distribution reported by the stationary point $\phi$ of the observable field alone. The nominal distribution will correspond to the tilted density in the generating function, while the state associated with $\phi$ and the operator associated with the stationary point $\phi^\dagger$ of the response field can vary depending on how the tilting is performed. Ideas and terminology associated with Importance Sampling are reviewed in App. C.

Our example will be a class of binomial distributions for a 2-state system, which can be written

$$\rho(n_a, n_b) \equiv \nu_a^{n_a} \nu_b^{n_b} \frac{N!}{n_a! n_b!}.$$  \hspace{1cm} (29)

$n_a$ and $n_b$ range over non-negative values with $N = n_a + n_b$ fixed, and we take $\nu_a + \nu_b = 1$. $\nu_a$ and $\nu_b$ are respectively the mean values of $n_a/N$ and $n_b/N$ under $\rho$.

The one degree of freedom in such distributions is a variable we denote $x$, with

$$\nu_a = \frac{1}{2} (1 - x); \quad \nu_b = \frac{1}{2} (1 + x).$$  \hspace{1cm} (30)

Two other quantities $\mu$ and $\xi$ that, in the case where $\rho$ is an equilibrium Gibbs distribution, have the interpretations respectively of a chemical potential and a free energy, are related to $x$ as

$$\frac{\nu_a}{\nu_b} \equiv e^{\beta \mu} \quad x = -\text{th} \frac{\beta \mu}{2} \quad \beta \xi \equiv \log \text{ch} \frac{\beta \mu}{2},$$  \hspace{1cm} (31)

where $\beta$ is inverse temperature.

We consider a starting distribution $\rho_0$ with parameters $\nu_{0a}$ and $\nu_{0b}$, and its generating function, constructed as in Eq. (16).

$$\Phi_0(z_a, z_b) \equiv \sum_{n_a = 0}^{N} z_a^{n_a} z_b^{n_b} \rho_0(n_a, n_b) = [\nu_{0a} z_a + \nu_{0b} z_b]^N.$$  \hspace{1cm} (32)

We will look only at contours for $z_a$ and $z_b$ which leave $\Phi_0$ normalized; these can be written

$$z_a = \frac{1 - x_T}{1 - x_0} \equiv \frac{\nu_a T}{\nu_{0a}}; \quad z_b = \frac{1 + x_T}{1 + x_0} \equiv \frac{\nu_b T}{\nu_{0b}},$$  \hspace{1cm} (33)

for some parameter $x_T$. The density $z_a^{n_a} z_b^{n_b} \rho_0(n_a, n_b)$ determines the mean values of $n_a$ and $n_b$ under $\Phi_0$, and will serve as the nominal distribution for the rest of the discussion of this static generating function.

The generating function can be formed from $\rho_0$ by one discrete tilt as in Eq. (32), or the tilt can be accumulated incrementally along a contour. Introduce an interval $[0, T]$, an increment $\delta \tau$, and a sequence of values $\tau = k \delta \tau$ for $k = 0, \ldots, T/\delta \tau$. Then introduce a sequence of values $\nu_{\tau}$ with $\nu_{0} = x_0$ and $\nu_{T} = x_T$, which we will take to converge to a smooth function (except possibly in the final step) as $\delta \tau \to 0$. Then $z_a$ and $z_b$ can be factored as

$$z_a = \prod_{\tau = d\tau}^{T} \left( \frac{\nu_a \tau}{\nu_a \tau - d\tau} \right); \quad z_b = \prod_{\tau = d\tau}^{T} \left( \frac{\nu_b \tau}{\nu_b \tau - d\tau} \right).$$  \hspace{1cm} (34)

Denote the last term in the product. Eq. (34)

$$z_{aT} = \left( \frac{\nu_a T}{\nu_a T - \delta \tau} \right); \quad z_{bT} = \left( \frac{\nu_b T}{\nu_b T - \delta \tau} \right).$$  \hspace{1cm} (35)

We will use these as boundary terms in the conversion (21) from the Doi algebra back to analytic functions. We will consider the two cases where $z_{aT}, z_{bT} = 1 + O(\delta \tau)$ so that $\nu_{aT - \delta \tau} \to \nu_{aT}$ and $\nu_{bT - \delta \tau} \to \nu_{bT}$; or where $z_{aT}, z_{bT} \sim O(\delta \tau^0)$ to impose a finite shift at the final value $\tau = T$.

The generating function (32), if tilted incrementally using the factorization (34), can be decomposed at any intermediate value $\tau$ into factors

$$\Phi_{\tau}(z_a, z_b) = \sum_{n_a = 0}^{N} \prod_{\tau' = \tau + d\tau}^{T} \left( \frac{\nu_{a\tau'}}{\nu_{a\tau'} - d\tau} \right)^{n_a} \left( \frac{\nu_{b\tau'}}{\nu_{b\tau'} - d\tau} \right)^{n_b} \rho_0(n_a, n_b),$$  \hspace{1cm} (36)

where we have defined

$$\rho_{\tau}(n_a, n_b) = \prod_{\tau' = \tau - d\tau}^{\tau} \left( \frac{\nu_{a\tau'}'}{\nu_{a\tau'}' - d\tau} \right)^{n_a} \left( \frac{\nu_{b\tau'}'}{\nu_{b\tau'}' - d\tau} \right)^{n_b} \rho_0(n_a, n_b).$$  \hspace{1cm} (37)

Referring to the review of Importance Sampling in App. C each of the distributions $\rho_{\tau}$ behaves as an importance distribution, and the residual factor in the second line of Eq. (36) behaves as its conjugate likelihood ratio, with respect to the nominal distribution in Eq. (32). We will show next how these factors are carried by observable and response fields in the functional integral.

In the limit $\delta \tau \to 0$, the intermediate density $\rho_{\tau}$ evolves along the parameter $\tau$ under the equation (making the state-index $n$ explicit and suppressing $\tau$ from the notation)

$$\frac{d\rho_{n}}{d\tau} = \frac{d\rho_{0}}{d\tau} \left( \frac{1 - x_0}{1 - x_{0}} \right) - n_a \left( \frac{1 + x_0}{1 - x_{0}} \right) \rho_{n} = -\frac{\beta \mu}{2} \left( n_b - n_a \right) - N x \rho_{n} \left( x \right),$$  \hspace{1cm} (38)
in which $\mathcal{Z}$ is the function with values $\mathcal{Z}_\tau$, introduced at the beginning of the section to define Eq. (34). (Here and below we use overdot `′ as a shorthand for $d/d\tau$.) We have introduced the “physical” variables $\Phi_\tau$ to make contact with the Hamiltonian construction of Crooks [8]. $[\mu (n_b - n_a) / 2 - N\xi]$ is the Hamiltonian that will produce the binomial distribution (29) at parameter $x$ as a Gibbs equilibrium, net of the instantaneous Gibbs free energy, and its $\tau$-derivative – a path “work” – acts as the generator of $\tau$-translation for $\rho$.

B. A functional integral representation for static generating functions

The parameter $\tau$ provides a coordinate along which a Doi-Peliti functional integral representation for $\Phi_0$ can be built. Depending on the contour $z_\tau$ assumed, the functional integral can represent either the one-shot tilt of Eq. (32), or a smooth incremental accumulation as in Eq. (36). Following the steps outlined in Sec. III D and App. A, the 2FFI representation is given by

$$\Phi_0(z_a, z_b) = \int \mathcal{D}\phi_a^\dagger \mathcal{D}\phi_a \mathcal{D}\phi_b^\dagger \mathcal{D}\phi_b e^{(z_{aT}-\phi_a^\dagger e^{(z_{aT}-\phi_a^\dagger)}+\phi_b^\dagger e^{-S}\Phi_0)} (\phi_{a\tau}, \phi_{b\tau}).$$

The action $S$ depends functionally on $x$ over the range $0 \leq \tau \leq T - \delta\tau$, with the last factors $z_{aT}$, $z_{bT}$ from Eq. (35) appearing in the boundary terms. We now compare two cases.

1. Identity map, followed by a discrete tilt

First consider the case $z_{aT} = z_a$, $z_{bT} = z_b$, $2\tau = \tau_0$ which we set equal to $x_0$ of the starting distribution. Because $\mu \equiv 0$, the action in Eq. (39) is given by

$$S_{null} = \int d\tau \left\{ - (d_\tau \phi_a^\dagger) \phi_a - (d_\tau \phi_b^\dagger) \phi_b \right\}.$$  

A functional integral with $S_{null}$ propagates $\rho_0$ through a sequence of identity maps (24), and the boundary terms apply the discrete tilt of Eq. (32) at $\tau = T$.

App. D D derives the stationary-point solutions for the observable and response fields. These, and the number field given in the stationary-point approximation by $\tilde{n}_a \approx \phi_a^\dagger \phi_a$, $\tilde{n}_b \approx \phi_b^\dagger \phi_b$, take values

$$\tilde{\phi}_a = \frac{N}{2} (1 - x_0) \quad \tilde{\phi}_b = \frac{N}{2} (1 + x_0),
\tilde{\phi}_{a\tau} = z_a \quad \tilde{\phi}_{b\tau} = z_b,
\tilde{n}_a = \frac{N}{2} z_a (1 - x_0) \quad \tilde{n}_b = \frac{N}{2} z_b (1 + x_0)
= \frac{N}{2} (1 - x_T) \quad = \frac{N}{2} (1 + x_T).$$

2. Static generating function, accumulated continuously

Next consider the complementary case where $z_{aT}$, $z_{bT} = 1 + \mathcal{O}(\delta\tau)$, and $\mathcal{Z}_\tau$ interpolates smoothly between $z_0 = x_0$ of the initial distribution, and $z_T \to x_T$ set by $z_a$, $z_b$ as $\tau \to T$. The action in Eq. (39) for this case is given by
where the term in \( \dot{\mu} \) implements the \( \tau \)-evolution of Eq. (33). The existence of \( \tau \)-derivatives in the “kinetic” term of \( S_{\text{ini}} \), which merely reflects the overlap \( \langle \phi_{\tau + \dot{\phi}_{\tau}} \mid \phi_{\tau} \rangle \) between adjacent representations of unity (24), suggests a way to remove the time-derivative term by a change of variable, which is the 2FFI expression of the duality transform of the NEWRs and their generalizations.

The change of variables that expresses duality in Doi-Peliti functional integrals is one already recognized by Baish [57]. From the original field variables \( (\phi^1, \phi) \), introduce two new variables \( (\bar{\phi}^1, \bar{\phi}) \) defined by

\[
\bar{\phi}^a = \frac{\varphi^a}{1 - x} \quad \bar{\phi}_a = (1 - x) \varphi_a \\
\bar{\phi}^b = \frac{\varphi^b}{1 + x} \quad \bar{\phi}_b = (1 + x) \varphi_b. \tag{43}
\]

In the dual variables the action (42) becomes

\[
S = \int d\tau \left\{ - (d_\tau \bar{\phi}^a) \bar{\varphi}_a - (d_\tau \bar{\phi}^b) \bar{\varphi}_b \right\}. \tag{44}
\]

We recover the form (40) of the null action, in a basis which is tilted to absorb the generating-functional weight in each interval \( d\tau \).

Stationary-point solutions in the original and dual variables are derived in App. (172) \( \bar{\varphi}^1 \) and \( \bar{\varphi} \) are constant as in the last example, though at different values because the change of variables alters their boundary conditions. The stationary-point solutions in the original fields are now non-trivial functions of \( \tau \):

\[
(\bar{\phi}_a)_{\tau} = \frac{N}{2} \left( 1 - x_{\tau} \right) \quad (\bar{\phi}_b)_{\tau} = \frac{N}{2} \left( 1 + x_{\tau} \right),
\]

\[
(\bar{\phi}^a)_{\tau} = \frac{1 - x_T}{1 - x_{\tau}} \quad (\bar{\phi}^b)_{\tau} = \frac{1 + x_T}{1 + x_{\tau}}.
\]

\[
\bar{n}_a = \frac{N}{2} \left( 1 - x_T \right) \quad \bar{n}_b = \frac{N}{2} \left( 1 + x_T \right). \tag{45}
\]

Note that \( \bar{n} \) continues to report the mean in the nominal distribution \( e^{\frac{\partial}{\partial n_a} - \frac{\partial}{\partial n_b}} \rho_{\tau}(n_a, n_b) \), while now \( \bar{\phi} \) is the mean in \( \rho_{\tau} \) from Eq. (37), and \( \bar{\phi}^a \) produces the conjugate \( \tau \)-dependent likelihood ratio in Eq. (36).

**C. Generating functions and functionals of dynamically evolving distributions**

The main result from Sec. (111A) and Sec. (111B) is that, for the generating function of a static distribution, the nominal distribution is determined, though it can be factored into importance distributions and likelihood ratios in a continuum of ways. The expression of this freedom in the functional integral is important for understanding the meaning and roles of the observable and response fields in the Doi-Peliti construction. In this section we will show that for the generating function or functional of an evolving state, the nominal distribution becomes dynamical. The new feature is that the nominal distribution itself, as well as the way it is factored into importance distributions and likelihood ratios, now depends on the way weights are accumulated along paths.

We will show that, in the static generating function of an evolved distribution, the nominal distribution is a simple sum of the sample distribution propagated with retarded dynamics, and the generating-function weight propagated (in a suitable measure) with advanced dynamics. However, if an incremental tilting protocol is matched to the dynamics, the evolution of the sample distribution can be made memoryless, while the nominal distribution evolves entirely with advanced dynamics. The required matching protocol defines the construction of the adjoint process, and it has the effect of transposing the forms of forward and backward generators.

To keep the example as simple as possible, we introduce the minimal non-trivial dynamics for the 2-state system, which preserves the binomial form (29) of distributions under arbitrary time-dependent rate parameters. A minimal transition rate matrix (27) is given by

\[
T = \nu_a \left( e^{\frac{\partial}{\partial n_a} - \frac{\partial}{\partial n_b}} - 1 \right) n_a + \nu_b \left( e^{\frac{\partial}{\partial n_b} - \frac{\partial}{\partial n_a}} - 1 \right) n_b, \tag{46}
\]

describing single-particle hops with per-particle rates \( \nu_a \) (for \( A \rightarrow B \)) and \( \nu_b \), and (for \( B \rightarrow A \)). We will take \( \nu_a \) and \( \nu_b \) to define the contour \( \mathcal{C}_T \), where \( \tau \) is now a time coordinate and not simply an arbitrary parameter. The 2-state system of course possesses detailed balance, making this a standard NEWR [0]. However, the tilting protocols, 2FFI variable changes, and causality arguments of this and the next section also go through more generally, in the same form except that a non-equilibrium steady state must be computed.

1. Generating function of an evolved distribution, formed discretely at the end of evolution

We first consider a single-time generating function, like Eq. (62), but applied to a distribution evolved to time \( \tau = T \) under the master equation (46). This illustrates a case where the observable field \( \bar{\phi} \) corresponds to the ex-
pected, time-dependent coherent state, but the nominal distribution differs from this state because it also reflects the existence of the late-time tilt in the generating function. Write this generating function from Eq. (39) now as \( \Phi_T(z_{aT}, z_{bT}) \). The arguments \( (z_{aT}, z_{bT}) \) will in general be different from \( (z_a, z_b) \) of Eq. (39), because they will shift the distribution from a time-dependent contour \( \tilde{x} \) different from the initial value \( x_0 \).

The action in the integral (25) for this case is

\[
S_{\text{dyn}} = \int d\tau \left\{ -(d_{\tau} \phi^\dagger_a) \phi_a - (d_{\tau} \phi^\dagger_b) \phi_b + \frac{1}{2} \left( \phi^\dagger_b - \phi^\dagger_a \right) \left[ (1 - \bar{z}) \phi_b - (1 + \bar{z}) \phi_a \right] \right\}. \tag{47}
\]

The terms including a factor \( \bar{z} \) come from the Liouville operator corresponding to \( T \) in Eq. (13).

Stationary-point solutions under the action \( S_{\text{dyn}} \) are given in App. D.3. We introduce a new function \( \tilde{x}_\tau \) with initial value \( x_0 \), and satisfying

\[
\frac{d\tilde{x}}{d\tau} = -(\bar{x} - \bar{z}). \tag{48}
\]

In terms of its solution,

\[
(\tilde{\phi}_a)_\tau = \frac{N}{2} (1 - \tilde{x}_\tau) \quad (\tilde{\phi}_b)_\tau = \frac{N}{2} (1 + \tilde{x}_\tau). \tag{49}
\]

Comparing this to the first line of Eq. (15), \( \bar{x} \) for \( S_{\text{tilt}} \) has been replaced with the retarded solution \( \tilde{x} \) for \( S_{\text{dyn}} \).

The stationary-path solutions for the response fields are more complicated, and are given in Eq. (D.12). The number fields, however, can be shown to satisfy

\[
\left( \bar{n}_b - \bar{n}_a \right) - \frac{N \tilde{x}}{1 - \bar{x}^2} = e^{-(T-\tau)} \left( \bar{n}_b - \bar{n}_a \right) - \frac{N \tilde{x}}{1 - \bar{x}^2} \Big|_T. \tag{50}
\]

If \( z_{aT} = z_{bT} = 1 \) in the generating function \( \Phi_T \), \( \bar{n} \) coincides with the coherent-state mean \( \tilde{\phi} \) from Eq. (13), as in the usual expositions \cite{62,64,65}. If \( z_{bT} - z_{aT} \neq 0 \) in the generating function, the left-hand side of Eq. (50) is nonzero, and the deviation of \( \left( \bar{n}_b - \bar{n}_a \right) \) from \( N \tilde{x} \) decays exponentially backward in time, with a measure \( (1 - \bar{x}^2) \) which gives the instantaneous variance in the coherent state at \( \tilde{\phi} \).

\[
S_{\text{Crooks}} = \int d\tau \left\{ -(d_{\tau} \phi^\dagger_a) \phi_a - (d_{\tau} \phi^\dagger_b) \phi_b + \frac{1}{2} \left( \phi^\dagger_b - \phi^\dagger_a \right) \left[ (1 - \bar{z}) \phi_b - (1 + \bar{z}) \phi_a \right] \right\}. \tag{52}
\]

Although the matrix \( T \) is invisible in Eq. (51) when acting on the instantaneous equilibrium distribution, the Liouville term remains in the action, and governs the evolution of more general distributions and correlation functions. We label this action \( S_{\text{Crooks}} \) because, as we noted following Eq. (38), \( \bar{\mu} \left[ (1 - \bar{z}) \phi^\dagger_b \phi_b - (1 + \bar{z}) \phi^\dagger_a \phi_a \right] /2 \) is the time derivative of the difference between a Hamiltonian and local free energy, which is the normalization convention of \cite{9}.

To solve this case, we observe that the transformation \( 43 \) removes the explicit time-derivative term from \( S_{\text{Crooks}} \) as it does for \( S_{\text{tilt}} \) (it is the same term), giving the form

\[
S_{\text{Crooks}} = \int d\tau \left\{ -(d_{\tau} \varphi^\dagger_a) \varphi_a - (d_{\tau} \varphi^\dagger_b) \varphi_b + \frac{1}{2} \left[ (1 - \bar{z}) \varphi^\dagger_b \varphi_b - (1 + \bar{z}) \varphi^\dagger_a \varphi_a \right] (\varphi_b - \varphi_a) \right\}. \tag{53}
\]

2. Cumulative generating functional matched to the time evolution

Finally we consider the interaction between dynamics and incremental tilting, so that we form a time-dependent generating functional and not simply a single-time generating function. Return to the argument decomposition \( z_{aT} = 1 + O(\delta \tau), z_{bT} = 1 + O(\delta \tau) \), and replace the generating function from Eq. (39) with one written \( \Phi_{\tau}(z_{aT}, z_{bT}) \), to indicate that the tilting protocol will depend functionally on a contour \( \tilde{x} \) that we have yet to specify.

To identify the appropriate contour for incrementally tilting an evolving distribution, note that for a binomial density advancing along a parameter \( \tau \) under Eq. (38), one can freely add a factor of the instantaneous generator \( T \) with the rate constants depending on \( \bar{x}_\tau \) without altering the result, because the tilted distribution is instantaneously annihilated by \( T \):

\[
\frac{d\rho}{d\tau} = \left\{ T - \beta \bar{x}_\tau \left( n - \frac{N}{2} \right) \right\} \rho. \tag{51}
\]

The action in Eq. (39), with \( \hat{\tau} \) set equal to \( \bar{x} \) as suggested by Eq. (51), becomes

\[
S_{\text{Crooks}} = \int d\tau \left\{ -(d_{\tau} \phi^\dagger_a) \phi_a - (d_{\tau} \phi^\dagger_b) \phi_b + \frac{1}{2} \left( \phi^\dagger_b - \phi^\dagger_a \right) \left[ (1 - \bar{z}) \phi_b - (1 + \bar{z}) \phi_a \right] \right\}. \tag{52}
\]
The new observation is what the duality transform does to the term originating from the Liouville operator: it interchanges the roles of $\phi$ and $\phi^\dagger$ with those of $\varphi^\dagger$ and $\varphi$, respectively. If the Liouville term is written as a bilinear form (first introduced by Keldysh \[46, 49\]), duality has the effect of transposing the matrix kernel of this form. We show in Sec. \[31\] how this result generalizes for non-linear and non-Hamiltonian systems.

Stationary-point solutions for $S_{\text{Crooks}}$ in the original and dual variables are derived in App. \[D.3\]. As for the static generating functional with continuous tilting, and as suggested by Eq. \[51\], fields $\phi$ again take the values in the first line of Eq. \[45\].

To describe the $\bar{n}$ fields and the behavior of the nominal distribution, we introduce a new mean field contour $\bar{x}$ with $\bar{x}_T = x_T$, evolving under the advanced dynamics

$$\frac{d\bar{x}}{d\tau} = (\bar{x} - \bar{x}) $$

this is contrasted with retarded dynamics under the un-weighted stochastic process shown in Eq. \[48\]. In terms of the solution $\bar{x}$ to Eq. \[54\], $\bar{n}_a + \bar{n}_b = N$ at all times, and

$$(\bar{n}_b - \bar{n}_a)_{\tau} = N\bar{x}_{\tau}. $$

Thus the nominal distribution evolves under time-reversed dynamics, but the exact form of the solution for $\tau < T$ depends on the fact that the generating functional has been continued to a time $\tau = T$ in the future. The shift from retarded to advanced dynamics reflects the reverse-time evolution that the backward equation produces for any operator, as applied to the particular case where the operator is a path weight chosen to erase memory from the instantaneous distribution given by the coherent state at $\phi$.

The surprising result is that this path-weighting protocol does not only time-reverse the dynamics of binomial distributions, but transposes the whole kernel in the Liouville operator. In the usual DP theory for unweighted distributions, the stationary values of response fields are fixed points of the backward equation. Under the transform \[13\], the stationary value for the dual observable field becomes a fixed point of the (dual) forward equation. The consequence is that the generator of the backward equation takes on the equivalent form to the generator of a forward equation, rather than the adjoint form. It implies, as we show next, a transposition of causal and anti-causal propagation in general correlation functions.

D. Dynamics, tilting, and duality working directly in number fields

Before studying fluctuations, however, we make a brief digression to introduce a change of variables from the coherent-state field variables $(\phi^\dagger, \phi)$, to a set $(n, \eta)$ that stand in the relation of action-angle variables \[14\] to the original fields. As explained elsewhere \[51\], this is a canonical transformation with respect to the functional integral \[52\] and is thus usable for the study of Green’s functions and FDTs. It allows us to work directly in the number field as an elementary (rather than composite) variable, with a conjugate field that has the interpretation of a chemical potential \[53\].

The transformation from coherent-state to number fields for the two-state system is given by

$$\begin{align*}
\phi_a^\dagger &\equiv e^{\eta_a} & \phi_a &\equiv e^{-\eta_a} n_a \\
\phi_b^\dagger &\equiv e^{\eta_b} & \phi_b &\equiv e^{-\eta_b} n_b.
\end{align*}$$

The combination $\eta_b + \eta_a$ does not appear in $\mathcal{L}$, because the stochastic process \[10\] conserves total particle number, so we perform a second shift to diagonal variables

$$\begin{align*}
h &\equiv \frac{1}{2} (\eta_b + \eta_a) & N &\equiv (n_b + n_a) \\
\eta &\equiv (\eta_b - \eta_a) & n &\equiv \frac{1}{2} (n_b - n_a).
\end{align*}$$

The un-tilted dynamical action \[17\] becomes, in these variables,

\[
S_{\text{dyn}} = \int d\tau \left\{ -N d_\tau h - n d_\tau \eta + \frac{1}{2} \left[ (1 + \varphi) (1 - e^\eta) \left( \frac{N}{2} - n \right) + (1 - \varphi) (1 - e^\eta) \left( \frac{N}{2} + n \right) \right] \right\}.
\]

The tilted action \[52\] is then

$$S_{\text{Crooks}} = \int d\tau \left\{ -N d_\tau (h - \beta \xi) - n d_\tau (\eta - \beta \mu) + \frac{1}{2} \left[ (1 + \varphi) (1 - e^\eta) \left( \frac{N}{2} - n \right) + (1 - \varphi) (1 - e^\eta) \left( \frac{N}{2} + n \right) \right] \right\},$$

where for the first time $\xi$ from Eq. \[31\] is written explicitly, showing its role \[3\] as a normalizing factor.

The duality transformation in action-angle variables is simpler than in coherent-state variables, and is suggested immediately by the removal of explicit time-dependence from the kinetic term in Eq. \[59\]; we simply shift the fields conjugate to the particle numbers:

$$\begin{align*}
h &\equiv h - \beta \xi \\
\eta &\equiv \eta - \beta \mu.
\end{align*}$$
Using the variable relations \(31\) to simplify terms, the dual representation of the action becomes

\[
S_{\text{Crooks}} = \int d\tau \left\{ -\left( d_\tau \hat{h} \right) N - (d_\tau \hat{\eta}) n + \frac{1}{2} \left[ \left( 1 + \varphi \right) - (1 - \varphi) e^\eta \right] \left( \frac{N}{2} - n \right) + \left[ (1 - \varphi) - (1 + \varphi) e^{-\eta} \right] \left( \frac{N}{2} + n \right) \right\}
\] \( (61) \)

\( \hat{h} \) and \( \hat{\eta} \) are the action-angle variables that would have been obtained from Eq. \(33\) by transforming directly in the dual \( \varphi^\dagger, \varphi \) variables. Note that \( n \) and \( N \) are not affected by the duality transformation at all, though their stationary-path equations of motion and Greens functions will be different when tilting leads to action \(61\), relative to the un-tilted action \(38\).

E. Connection of the field-integral approach to the similarity-transform derivation of Crooks

To close the section, we show how the transformation of the 2FFI action above is recovered directly from the similarity-transform construction as given by Crooks \(3\).

In that construction, final-time parameters \( \nu_a, \nu_b \) are imposed to create the desired reference state, and representations of unity are then inserted in the form of multiplication and division by Gibbs factors at intermediate times. The similarity transform over each segment of Liouville evolution converts the generator matrix \( T \) into its dual, while the incomplete cancellation of the Gibbs factors at different times generates an explicit time-dependence that can be canceled if an appropriate weight is multiplied onto the evolving density at each time-step.

For these binomial distributions, following Eq. \(38\), the Hamiltonian is

\[
H = \mu (n_b - n_a).
\] \( (62) \)

Initial distributions, which are assumed to be of Gibbs form with Hamiltonian \( H_0 \) at \( \tau = 0 \) are evolved with the quadrature of the master equation \(1\), which we write as the time-ordered product of one-step operators from Eq. \(2\), giving \( \prod_{\tau=0}^{T-\delta \tau} e^{\delta \tau T_\tau} e^{-\beta H_0} = e^{-\beta H_T} \prod_{\tau=0}^{T-\delta \tau} (e^{\beta H_\tau + \delta \tau} e^{\delta \tau T_\tau} e^{-\beta H_\tau}) \).

The relevant similarity transform, as in Eq. \(38\), is carried out with a matrix product that is the same for either plain or tilted Liouville evolution:

\[
\prod_{\tau=0}^{T-\delta \tau} e^{\delta \tau T_\tau} e^{-\beta H_0} = e^{-\beta H_T} \prod_{\tau=0}^{T-\delta \tau} (e^{\beta H_\tau + \delta \tau} e^{\delta \tau T_\tau} e^{-\beta H_\tau}).
\] \( (63) \)

We suppose that \( \delta \tau \) is sufficiently small to write

\[
e^{\beta H_\tau + \delta \tau} e^{\delta \tau T_\tau} e^{-\beta H_\tau} \approx 1 + \delta \tau \left[ e^{\beta H_\tau + \delta \tau} + d_\tau (\beta H_\tau) \right]
\approx 1 + \delta \tau \left[ \tilde{T}_\tau + d_\tau (\beta H_\tau) \right].
\] \( (64) \)

Here the notation \( \tilde{T} \) designates the generator matrix acted on through similarity transform with \( e^{\beta H} \).

Applied to the matrix product in Eq. \(38\), the similarity transform \(64\) produces

\[
\prod_{\tau=0}^{T-\delta \tau} e^{\delta \tau T_\tau} e^{-\beta H_0} = e^{-\beta H_T} \prod_{\tau=0}^{T-\delta \tau} e^{\delta \tau \tilde{T}_\tau}.
\] \( (65) \)

The similarity transform is equivalent to the change of integration variables \(33\) in the functional integral, and by itself has no affect on any computed quantities. If, however, the tilting factor \(-d_\tau (\beta H_\tau)\) from Eq. \(38\) had been introduced in the original evolution equation, that would then cancel the corresponding term from the similarity transform, leaving only \( \tilde{T} \), to give

\[
\prod_{\tau=0}^{T-\delta \tau} e^{\delta \tau \tilde{T}_\tau} (T - d_\tau (\beta H_\tau)) e^{-\beta H_0} = e^{-\beta H_T} \prod_{\tau=0}^{T-\delta \tau} e^{\delta \tau \tilde{T}_\tau}.
\] \( (66) \)

For the two-state model \( e^{\beta H} \) can be written

\[
e^{\beta H} = \left( \frac{\nu_a}{\nu_b} \right)^n = \left( \frac{1 - \varphi}{1 + \varphi} \right)^n,
\] \( (67) \)

in which case the similarity-transformed generator becomes

\[
e^{\beta H} T e^{-\beta H} = \left( e^{-\beta \partial n} \nu_a - \nu_b \right) n_a + \left( e^{\beta \partial n} \nu_b - \nu_a \right) n_b
\equiv \tilde{T}.
\] \( (68) \)

If we denote by \( \tilde{\mathcal{L}} \) the Liouville operator obtained by the usual construction using \( \tilde{T} \) rather than \( T \), that evaluation gives

\[
\tilde{\mathcal{L}} = (\nu_b - \nu_a e^\eta) n_a + (\nu_a - \nu_b e^{-\eta}) n_b
= \frac{1}{2} \left\{ \left[ (1 + \varphi) - (1 - \varphi) e^\eta \right] n_a + \left[ (1 - \varphi) - (1 + \varphi) e^{-\eta} \right] n_b \right\}.
\] \( (69) \)

Thus we correctly recover the Liouvillian term in the transformed \( S_{\text{Crooks}} \) of Eq. \(61\).

IV. BEYOND STATIONARY POINTS: TILTING FROM CAUSALITY TO ANTI-CAUSALITY IN THE FULL DISTRIBUTION

Sec. \(III\) used several simplifications from a 2-state example and a stationary-point analysis to show where the sense of time reversal in NEWRs originates in the duality between distributions and observables. In this section we show for general correlation functions and general
stochastic CRNs (as long as the effects of nonlinearity can be expanded in perturbation series for fluctuations), that the time-reversal illustrated above for stationary points extends to a full transposition in the roles of observable and response fields, and of causal with anti-causal response functions. We demonstrate this by studying the Green’s function expansion obtained from the second-order approximation to the action functional, which is also the source of fluctuation-dissipation relations both for unweighted evolving distributions and for their generating functionals. We show how these are derived from internal symmetries of 2-field integrals, and relate them to the Extended FDTs of Seifert and Speck [20]. The key step in all such constructions is the replacement of correlation functions derived from the dynamical action with others derived from the Hatano-Sasa tilt term, concisely reviewed and placed in context of related approaches to extended FDTs in [24].

A. Green’s function expansions, Ward identities, and Fluctuation-Dissipation Theorems

In a field theory, there may be relations among the expectations of different operator products in a time-dependent distribution implied by internal symmetries of the theory. These are known as the Ward identities of the field theory [60]. In 2FFI representations, some of these identities are produced by shifts of the dummy variables of integration. One important group are the Green’s functions, which describe the propagation of disturbances in response to idealized point-like perturbing events. Here we consider the free Green’s functions, which describe the propagation of disturbances at leading (Gaussian) order; more general response functions can often be constructed from these by common perturbative methods [60].

In the study of free Green’s functions, a condensed notation greatly simplifies the presentation. Regard $\phi$ as a column vector and $\phi^\dagger$ as its conjugate row vector, and likewise for dual fields $\varphi$ and $\varphi^\dagger$. Then for any field action [20] the quadratic-order expansion in fields which controls Gaussian fluctuations may be cast in the form [40]

$$S = \int d\tau \left\{ - (d_\tau \phi^\dagger) \phi + \phi^\dagger D_\tau \phi - \phi^\dagger \Delta_\tau \phi^\dagger T / 2 \right\}. \quad (70)$$

Here $D_\tau$ is the drift matrix for the hopping rates in the stochastic process – generally time-dependent through a varying parameter such as $x_\tau$ – and $\Delta_\tau$ is a possible source for stochastic fluctuations. For the free theories produced by the two-state example, the quadratic-order expansion is the whole action, and $\Delta \equiv 0$ in the coherent-state variables.

1. The free Green’s function arrived at as a variational identity, and the most basic FDT

Let $\langle \rangle$, when bracketing field variables, denote expectation in the functional integral [25]. Starting from the expectation

$$\langle \left[ \phi^\dagger \phi^T \right]_{\tau'} \rangle$$

at a time $\tau'$, consider the variation produced by the pair of shifts of dummy variable of integration at some (generally different) time $\tau$:

$$0 = \left[ \frac{\delta}{\delta \phi^\dagger} \right]_{\tau} \left\langle \left[ \phi^\dagger \phi^T \right]_{\tau'} \right\rangle$$

$$= I \delta_{\tau \tau'} - \left[ \begin{array}{cc} 0 & d_\tau + D_\tau \\ -d_\tau + D_\tau & 0 \end{array} \right] \left\langle \left[ \phi^\dagger T \phi \right]_{\tau} \left[ \phi^\dagger \phi^T \right]_{\tau'} \right\rangle. \quad (71)$$

Here $I$ stands for the $2P \times 2P$ identity matrix and $\delta_{\tau \tau'}$ is the Dirac $\delta$-function that results from the Kronecker $\delta$ scaled by $1/\delta \tau$ as $\delta \tau \to 0$ in the skeletonized measure [AS].

In the first line of Eq. (71), the variation is zero because a shift of a dummy variable of integration produces no change in the value of an integral. In the second line, the $\delta$-function variation comes from the direct action of the shift on the argument of the expectation value at $\tau'$, while the second term comes from functional variation of $S$ in the exponential of Eq. (25).

The causal structure of a stochastic process in forward time ensures [10] that the expectation has a form first propounded by Keldysh [19] for dissipative quantum field theories,

$$\left\langle \left[ \phi^\dagger T \phi \right]_{\tau} \left[ \phi^\dagger \phi^T \right]_{\tau'} \right\rangle = \left\langle 0 G^R G^K \right\rangle_{\tau \tau'}, \quad (72)$$

in which $G^R, G^A, \text{and} G^K$ are the retarded, advanced, and Keldysh Green’s functions of the theory. The retarded and advanced Green’s functions are solutions to the inhomogeneous differential equations

$$(d_\tau + D_\tau) G^R_{\tau \tau'} = I \delta_{\tau \tau'},$$

$$(d_\tau + D_\tau^T) G^A_{\tau \tau'} = I \delta_{\tau \tau'} \quad (73)$$

from the diagonal blocks of Eq. (71), (where $I$ now stands for the $P \times P$ identity matrix), while $G^K$ is the solution to the homogeneous differential equation

$$(d_\tau + D_\tau) G^K_{\tau \tau'} = 0 \quad (74)$$

from the upper-right off-diagonal block. The general form that is admitted [10] for such a homogeneous solution is

$$G^K_{\tau \tau'} = G^K_{\tau \tau'} M_{\tau \tau'} + M_{\tau \tau'} G^K_{\tau \tau'}, \quad (75)$$
where $M_\tau$ satisfies the differential equation
\[ d_\tau M_\tau + D_\tau M_\tau + M_\tau D_\tau^T = 0. \] (76)

Equations (76, 74) are the essential relations defining the Fluctuation-Dissipation Theorem (FDT). The retarded and advanced Green’s functions, which govern the response of fields to external perturbations, also determine the rate of decay of endogenous noise and thus the level of self-maintained fluctuations. For equilibrium states, these reduce to the familiar FDT. For non-equilibrium distributions, whether steady or time-dependent, they capture the essential relation between dissipative relaxation under the retarded and advanced Green’s functions, and the kernel $M_\tau$ which serves as the source of fluctuations.

For the action (75), the matrix $D_\tau$ is
\[ D_\tau = \begin{bmatrix} 0 & 0 \\ -\mathcal{L}_\tau & 1 \end{bmatrix} \] (77)

Because the stationary-path backgrounds $\bar{\phi}$ and $\bar{\phi}^\dagger$ are homogeneous solutions to the equations of motion, we may subtract them out, and the equations (76, 74) are satisfied for residual fluctuations $\phi' \equiv \phi - \bar{\phi}$ and $\phi'^\dagger \equiv \phi^\dagger - \bar{\phi}^\dagger$. The explicit forms for $G^R$ and $G^A$ in the convenient basis of even and odd symmetry are then
\[
\frac{1}{2} \left< \begin{bmatrix} \phi_b' + \phi_a' \\ \phi_b' - \phi_a' \end{bmatrix}_\tau \left( \begin{bmatrix} \phi_b' + \phi_a' \\ \phi_b' - \phi_a' \end{bmatrix}_\tau \right) \right> \equiv
G^{R}_{\tau > \tau'} = \Theta_{\tau > \tau'} \begin{bmatrix} 1 & 0 \\ \int^\tau_{\tau'} d\tau'' e^{-\tau'' - \tau'} & 1 \end{bmatrix},
\]
\[
\frac{1}{2} \left< \begin{bmatrix} \phi_b' + \phi_a' \\ \phi_b' - \phi_a' \end{bmatrix}_\tau \left( \begin{bmatrix} \phi_b' + \phi_a' \\ \phi_b' - \phi_a' \end{bmatrix}_\tau \right) \right> \equiv
G^{A}_{\tau > \tau} = \Theta_{\tau > \tau'} \begin{bmatrix} 1 & 0 \\ \int^\tau_{\tau'} d\tau'' e^{-\tau'' - \tau'} & 1 \end{bmatrix}.
\] (78)

The Keldysh Green’s function at equal time, which coincides with the value of $M_\tau$, is given by
\[
\frac{1}{2} \left< \begin{bmatrix} \phi_b' + \phi_a' \\ \phi_b' - \phi_a' \end{bmatrix}_\tau \left( \begin{bmatrix} \phi_b' + \phi_a' \\ \phi_b' - \phi_a' \end{bmatrix}_\tau \right) \right> \equiv
G^{K}_{\tau} = -\frac{N}{2} \left[ 1 \right] \left[ 1 \right] \mathcal{L}_\tau.
\] (79)

For a free theory, the expectations of general operators are obtained by combinatorial contractions with the above Green’s functions, by the usual Wick expansion [60]. Here we will evaluate one such expectation using a shift of the variables of integration to illustrate its relation to the simple FDT from the Green’s function alone.

2. The Green’s function expansion and Ward identities for general observables

Let $O_{\tau'}$ be some observable which is a function of the fields in the functional integral at a time $\tau'$. Consider the same symmetries as above, under shifts of the integration variables, but now for the quantity
\[
\left< O_{\tau'} \left[ \phi^\dagger \phi^T \right]_{\tau''} \right>.
\]

The Ward identity generalizing Eq. (71) for this composite observable is
\[
0 = \left[ \frac{\delta}{\delta \phi^\dagger} \right] \left< O_{\tau'} \left[ \phi^\dagger \phi^T \right]_{\tau''} \right> + \left[ \frac{\partial O_{\tau'}}{\partial \phi^\dagger} \right] \left[ \phi^\dagger \phi^T \right]_{\tau'} \delta_{\tau'\tau''} - \left[ \begin{bmatrix} 0 & d_\tau + D_\tau^T \end{bmatrix} \right] \left< O_{\tau'} \left[ \phi^T \phi \right]_{\tau} \right> \left[ \phi^\dagger \phi^T \right]_{\tau''}.
\] (80)
It follows, from the definition of the Green’s function as the inverse of the kernel for the equations of motion, that the expectation must have the form

\[
\left\langle O_{\tau'} \left[ \phi^T \right] \right\rangle _{\tau} = \left[ \begin{array}{cc} 0 & G^A \end{array} \right]_{\tau \tau'} \left\langle \left[ \partial O / \partial \phi^T \right]_{\tau'} \left[ \phi^T \right]_{\tau'} \right\rangle + \left( O_{\tau'} \right) \left[ \begin{array}{cc} 0 & G^A \end{array} \right]_{\tau \tau'}. \tag{81}
\]

This is the implementation of the Wick expansion of arbitrary observables in terms of contractions of their derivatives with the free Green’s function.

**B. Green’s functions and Ward identities in the dual process**

Because the duality transform \[13\] can be used to absorb the explicit time derivative from Eq. \[51\] or its generalizations, the generating functional possesses an equivalent field theory to the one for the underlying process. The observation made following Eq. \[53\] that duality transposes the structure of the dynamical equations from fields to their conjugates has the consequence that, for Green’s functions, the block-diagonal form \[72\] is likewise transposed, resulting in a transposition from causal to anti-causal response in the Green’s functions.

1. **Anti-Keldysh form and anti-causality**

In the tilted theory, after transformation to dual field variables, the second-order action becomes

\[
S = \int d\tau \left\{ - (d_{\tau} \phi^T) \phi + \phi^T D_{\tau} \phi - \phi^T \Delta_{\tau} \phi^T / 2 \right\}. \tag{82}
\]

For the two-state example, \[\tilde{D}_{\tau} = D^T_{\tau}\] though this need not be the case more generally. The variational condition has the same form as Eq. \[74\] with \[\tilde{D}\] replaced by \[\tilde{D}\] and \((\phi^T, \phi)\) replaced by \((\phi^T, \phi)\).

In order for the stationary-path backgrounds to vanish under the dual equations of motion, the expectation of the outer product of fields must take the transposed block-diagonal, or “anti-Keldysh” form

\[
\left\langle \left[ \phi^T \right] \left[ \phi^T \right] \right\rangle _{\tau} = \left[ \begin{array}{cc} \hat{G}^K & \hat{G}^A \end{array} \right]_{\tau \tau'}. \tag{83}
\]

The dual retarded and advanced Green’s functions are the transposes of those in the un-tilted theory, reflecting the fact that here \[\tilde{D}_{\tau} = D^T_{\tau}\].

These Green’s functions still have the same causal structure with respect to ordering of the time-indices as their counterparts \[73\], but as noted above, the dependence on \[\tilde{\phi}\] is shifted from the \[\phi\] fields to the counterpart \[\phi^T\] fields. As a result, the causal structure couples very differently to the expectations of operators, in the same way as the mean value \[\langle x^T \rangle\] switches from retarded dynamics \[75\] in the underlying stochastic process to advanced dynamics \[54\] in the tilted generating functional.

A Ward identity equivalent to Eq. \[80\] for an arbitrary arbitrary operator \(\langle O_{\tau'} \rangle\) in the dual variables is

\[
0 = \left[ \frac{\delta}{\delta \phi^T} \right]_{\tau} \left\langle O_{\tau'} \left[ \phi^T \right] \right\rangle _{\tau'} + \left\langle \left[ \partial O / \partial \phi^T \right]_{\tau'} \left[ \phi^T \right]_{\tau'} \right\rangle _{\tau} \delta_{\tau \tau'} - \left[ \begin{array}{cc} 0 & d_{\tau'} \end{array} \right]_{\tau \tau'} \left\langle O_{\tau'} \left[ \phi^T \right] \right\rangle _{\tau} = \left( O_{\tau'} \right) I \delta_{\tau \tau'} + \left\langle \left[ \partial O / \partial \phi^T \right]_{\tau'} \left[ \phi^T \right]_{\tau'} \right\rangle _{\tau} - \left[ \begin{array}{cc} 0 & d_{\tau} + \tilde{D}_{\tau} \end{array} \right]_{\tau \tau'} \left\langle O_{\tau'} \left[ \phi^T \right] \right\rangle _{\tau}, \tag{85}
\]

\[
= \left\langle O_{\tau'} \right\rangle I \delta_{\tau \tau'} + \left\langle \left[ \partial O / \partial \phi^T \right]_{\tau'} \left[ \phi^T \right]_{\tau'} \right\rangle _{\tau} \delta_{\tau \tau'} - \left[ \begin{array}{cc} 0 & d_{\tau} + \tilde{D}_{\tau} \end{array} \right]_{\tau \tau'} \left\langle O_{\tau'} \left[ \phi^T \right] \right\rangle _{\tau} + \left( O_{\tau'} \right) I \delta_{\tau \tau'} + \left\langle \left[ \partial O / \partial \phi^T \right]_{\tau'} \left[ \phi^T \right]_{\tau'} \right\rangle _{\tau} \delta_{\tau \tau'} - \left[ \begin{array}{cc} 0 & d_{\tau} + \tilde{D}_{\tau} \end{array} \right]_{\tau \tau'} \left\langle O_{\tau'} \left[ \phi^T \right] \right\rangle _{\tau}, \tag{85}
\]

\[
= \left\langle O_{\tau'} \right\rangle I \delta_{\tau \tau'} + \left\langle \left[ \partial O / \partial \phi^T \right]_{\tau'} \left[ \phi^T \right]_{\tau'} \right\rangle _{\tau} \delta_{\tau \tau'} - \left[ \begin{array}{cc} 0 & d_{\tau} + \tilde{D}_{\tau} \end{array} \right]_{\tau \tau'} \left\langle O_{\tau'} \left[ \phi^T \right] \right\rangle _{\tau} + \left( O_{\tau'} \right) I \delta_{\tau \tau'} + \left\langle \left[ \partial O / \partial \phi^T \right]_{\tau'} \left[ \phi^T \right]_{\tau'} \right\rangle _{\tau} \delta_{\tau \tau'} - \left[ \begin{array}{cc} 0 & d_{\tau} + \tilde{D}_{\tau} \end{array} \right]_{\tau \tau'} \left\langle O_{\tau'} \left[ \phi^T \right] \right\rangle _{\tau}, \tag{85}
\]
and its solution is
\[
\left\langle \mathcal{O}_{\tau'} \left[ \varphi^{\dagger \tau} \right] \right\rangle_{\tau} = \left[ \begin{array}{cc} \hat{G}^K & \hat{G}^A \\
 & \hat{G}^R \end{array} \right]_{\tau\tau'} \left\langle \left[ \frac{\partial \mathcal{O}}{\partial \phi^{\dagger \tau}} \right] \right\rangle_{\tau} + \left\langle \mathcal{O}_{\tau'} \right\rangle \left[ \begin{array}{cc} \hat{G}^K & \hat{G}^A \\
 & \hat{G}^R \end{array} \right]_{\tau\tau'}. \tag{86} \]

These Ward identities subsume all consequences of FDTs for 2-field functional integrals, and the solutions [78 84] demonstrating the shift from causality in the underlying process to anti-causality in the dual generating functional extends the results of Sec. III from stationary points to general correlations. However, formulations of FDTs may take many forms, and the “extended FDT” for non-equilibrium steady states derived in [20] appears quite different from the above formulae. We will return in Sec. V D to show how the Green’s function expansion can be used to evaluate the response to physical perturbation of the boundary conditions, and how the combination of the anticausality in the generating functional, with the Ward identities resulting from internal symmetry, can be used to produce another collection of operator equivalences which are the extended FDTs.

C. Causal and anti-causal Green’s functions in number fields

A derivation and comparison of the Green’s functions in the action-angle variables of Sec. III D for the un-weighted distribution and the dual generating functional, gives further insight into the coexistence of forward and reverse-time propagation in all these functional integrals, and the way it is harnessed under duality.

The number field corresponds to a bilinear operator in \( \phi^{\dagger} \) and \( \phi \), so it inherits both causal and anti-causal responses from their respective dynamics. The anticausality of the nominal distribution shown in equations [54 55] results from changing the way forward and backward responses couple to changes in the physical boundary conditions, within a block-diagonal matrix that retains overall Keldysh form.

Although the interpretation of the number fields is more direct than that of coherent-state fields, the non-linearity of the action-angle variable transformation [56] converts the bilinear coherent-state action for a free field theory into a more complicated form involving transcendental functions in the number fields, which is more difficult to work with algebraically. Therefore we will compute here only the set of terms directly responsible for fluctuations in the number field.

The shift of integration variable that defines Green’s functions for the number field is made in \( \eta \) (or respectively, \( \tilde{\eta} \)) in the plain or dual variables. The two Ward identities corresponding to the upper row in Eq. (86), from variation of the actions [59] and [61] respectively, are given by

\[
0 = \frac{\delta}{\delta \eta_{\tau'}} \left\langle \left[ \eta \ n \right]_{\tau'} \right\rangle = \left[ \begin{array}{cc} 1 & 0 \\
0 & \end{array} \right] \delta_{\tau\tau'} - \left\langle \left( d_{\tau'} + ch \eta + x sh \eta \right) n - (sh \eta + x ch \eta) \frac{N}{2} \tau \right\rangle_{\tau},
\]

\[
0 = \frac{\delta}{\delta \tilde{\eta}_{\tau'}} \left\langle \left[ \tilde{\eta} \ n \right]_{\tau'} \right\rangle = \left[ \begin{array}{cc} 1 & 0 \\
0 & \end{array} \right] \delta_{\tau\tau'} - \left\langle \left( d_{\tau'} + ch \tilde{\eta} - x sh \tilde{\eta} \right) n - (sh \tilde{\eta} - x ch \tilde{\eta}) \frac{N}{2} \tau \right\rangle_{\tau},
\]

In the second line of each expression several simplifications are made. Terms involving fluctuations of \( N \) are dropped, because \( N \) is constant. Stationary-path values, which are homogeneous solutions to the equations of motion, are subtracted out to leave expressions for remainders \( \eta' \equiv \eta - \bar{\eta}, \ n' \equiv n - \bar{n}, \) and \( \tilde{\eta}' \equiv \tilde{\eta} - \bar{\tilde{\eta}} \), and terms linear in fluctuations about the stationary paths are also removed because by construction these have zero mean. Finally, it can be checked to follow from the stationary-path equation of motion, that the fluctuation source term for \( \left( \eta' \right)^2 \) or \( \left( \tilde{\eta}' \right)^2 \) – this is the term from \( \Delta_{\tau} \) in the second-order expansion corresponding to Eq. (70), which would be zero in coherent-state fields [40] but is non-zero in action-angle variables [51] – takes the same form \( - (N - 2\bar{n})/2 \) in both the forward and reverse-time solutions, though the functional form \( \bar{n} \) appearing in this expression differs for the two solutions.

The formulae for the retarded and advanced Green’s functions in the \( (\eta,n) \) sector are as for the coherent-state system. The Keldysh Green’s functions for fluc-
uations in \( n \) in the two cases have the standard forms \( G^{K_n}_{\tau,\tau'} = G^{R}_{\tau,\tau'}M_{\tau} + M_{\tau}G^{A}_{\tau,\tau'} \), or \( G^{K}_{\tau,\tau'} = G^{R}_{\tau,\tau'}M_{\tau} + M_{\tau}G^{A}_{\tau,\tau'} \), only now the kernel functions \( M \) or \( \tilde{M} \) satisfy the homogeneous equations

\[
|d_{\tau} + 2 \left( ch \bar{\eta} + \frac{x}{2} e^{-\eta} \right)| M = \frac{1}{2} (N - 2n \bar{x}) ,
\]

\[
|d_{\tau} + 2 \left( ch \bar{\eta} - \frac{x}{2} e^{-\eta} \right)| \tilde{M} = \frac{1}{2} (N - 2n \bar{x}) \tag{88}
\]

(compare to Eq. (79) for coherent state fields).

Further solution details are worked out in App. [E]. The important result for understanding the nature of anticausality in the dual generating functional is the form of the Green’s functions in the dual theory,

\[
\left[
\begin{array}{cc}
0 & \hat{G}^A \\
\hat{G}^R & \hat{G}^K \\
\end{array}
\right]_{\tau,\tau'} = \Theta_{\tau'>\tau} e^{-(\tau'-\tau)} \left[
\begin{array}{cc}
0 & 1 \ \\
0 & 0 \\
\end{array}
\right]_{\tau,\tau'},
\]

\[
+ \Theta_{\tau'\tau} e^{-(\tau'-\tau)} \left[
\begin{array}{cc}
0 & 1 \ \\
0 & 0 \\
\end{array}
\right]_{\tau,\tau'},
\tag{89}
\]

in which \( \tilde{M} = N (1 - \bar{x}^2) / 4 \) from Eq. (E3), and \( \bar{x} \) satisfies Eq. (54). We return to use these forms in Eq. (91) below.

D. Extended FDTs from the anticausality and Ward identities of generating functionals

The term Fluctuation-Dissipation Theorem can refer to multiple concepts that are related but that differ in detailed form. In the original work of Einstein, and in the Extended FDTs of Seifert and Speck [20], the goal is to relate the response of a system to perturbations in its physical boundary conditions or control parameters, to the magnitude of its fluctuations in the absence of the perturbation, which define a measure of susceptibility.

In 2FFI representations, including the Schwinger-Keldysh time-loop for quantum mechanics and the DP construction for stochastic processes, the presence of the response fields places a layer of intermediate variables between the operator that represents an external disturbance and the measure of the system’s response. The advanced and retarded Green’s functions \( \tilde{G}_{\tau,\tau'} \), written as correlation functions between the observable and response fields, give the response to any perturbation, and these are related to the fluctuation spectrum through the Keldysh relations \( \tau > \tau' \). In 2FFI theories, these Ward-identity relations are known as FDTs [40]. In this section we relate them to the more familiar extended [20] and generalized [52] FDTs usually derived from state-space methods by working with the action \( S_{\text{Crooks}} \). Needless to say, the relations hold more generally beyond any specific form of the action.

Starting from the action \( S_{\text{Crooks}} \) of Eq. (52) in the original field variables \( \phi^\dagger, \phi \), we wish to compute the effect of a perturbation in \( \bar{x}_x \) on the expectation \( O_{\tau'} \), as in Sec. [IV A 2]. Although only the shift in the generating matrix \( \Xi \) is a “physical” perturbation in the boundary conditions on the stochastic process, we vary the generating functional along the contour where the path-weight factor remains matched to the generator, which means varying \( \bar{x}_x \) and \( \bar{x} \) in the second term in \( S_{\text{Crooks}} \) as well. The result is an expression for the variation of \( O_{\tau'} \) as a sum of two operator products, one with the variational term from the Liouville operator and the other from the path weight:

\[
\frac{\delta}{\delta \bar{x}_x} \langle O_{\tau'} \rangle = -\frac{1}{2} \left\{ \langle O_{\tau'} (\phi_b^\dagger - \phi_a^\dagger) (\phi_b + \phi_a) \rangle_{\tau} + \frac{d}{d\tau} \left\{ \frac{1}{1 - \bar{x}_x^2} \langle O_{\tau'} [\phi_b^\dagger \phi_b (1 - \bar{x}_x) - \phi_a^\dagger \phi_a (1 + \bar{x}_x)] \rangle_{\tau} \right\} \right\} . \tag{90}
\]

In the second term we have used an integration by parts to transfer the \( d/d\tau \) from its original argument \( \tau \) in Eq. (52) to the expectation value.

Variation of \( \bar{x}_x \) is not inherently a symmetry as the shift of a dummy integration variable is, so it is not apparent in the original variables \( (\phi^\dagger, \phi) \) that when \( \tau < \tau' \) the variation on the left-hand side of Eq. (90) is actually identically zero. This is true, however, as a consequence of anticausality of the Green’s functions in the generating functional, and this observation gives us a way to compute the first operator product on the right-hand side of Eq. (90) in terms of the second.

Although the variation leading to Eq. (90) was performed within a class of matched generating functionals, in the particular case where \( \bar{x}_x \) is constant, the background for \( \bar{x}_x \) in the action (52) is zero, so both of the expectation values on the right-hand side of Eq. (90) must also be those of the underlying stochastic process. Since we have chosen the initial state \( \rho_0 \) to be annihilated by the generator (40), these expectations are those of a (non-equilibrium or equilibrium) steady state. Relations of the form (90) are the extended FDTs for non-equilibrium steady states introduced by Seifert and Speck [20] (see also Verley et al. [22, 23]). They fit within the class of “generalized FDTs” defined by Polettini and Esposito [52].

In the more general case, with \( \bar{x}_x \) non-constant, the relation (90) still holds, though now the expectation values refer to those in the generating functional with \( \bar{x}_x \) nonzero. The total variation \( \delta \langle O_{\tau'} \rangle / \delta \bar{x}_x \) remains zero even in the
dynamical case – which is far from apparent in the original variables – as a consequence of the memory-erasing effect of the weighting term, and the anti-causal correlation structure that results.

The duality transformation \[ \text{(13)} \], together with the Green’s function evaluations of Sec. \[ \text{IV.B.1} \] provide a way to show vanishing of the variation \[ \text{(80)} \] and thus the extended FDT for steady states and its dynamical generalization. Variation with \( \delta \varphi \) in the action \[ \text{(13)} \] gives only one term:

\[
\frac{\delta}{\delta \varphi} \langle \mathcal{O} \rangle = -\frac{1}{2} \langle \mathcal{O} (\varphi^\dagger_b + \varphi^\dagger_a) (\varphi_b - \varphi_a) \rangle .
\] \[ \text{(91)} \]

after which the Ward identity from Eq. \[ \text{(80)} \] may be used to evaluate the expectation in terms of a Green’s function expansion,

\[
\langle \mathcal{O}_\tau (\varphi^\dagger_b + \varphi^\dagger_a) (\varphi_b - \varphi_a) \rangle = \Theta_{\tau > \tau'} e^{-(\tau - \tau')} \left. \frac{\partial \mathcal{O}}{\partial (\varphi_b - \varphi_a)} \right|_{\tau'} \langle \varphi^\dagger_b + \varphi^\dagger_a \rangle_{\tau'} + \Theta_{\tau' > \tau} \left. \frac{\partial \mathcal{O}}{\partial (\varphi_b + \varphi_a)} \right|_{\tau'} (\varphi_b - \varphi_a)_{\tau'}.
\] \[ \text{(92)} \]

There is the potential for coupling with either ordering of \( \tau \) and \( \tau' \), because both retarded and advanced Green’s functions make a contribution. However, if the second term on the right-hand side of Eq. \[ \text{(92)} \] is evaluated in a Green’s function expansion of \( \partial \mathcal{O} / \partial (\varphi_b + \varphi_a) \), there is no contribution for \( \tau < \tau' \) by Eq. \[ \text{(84)} \]. Therefore \( (\varphi_b - \varphi_a)_{\tau} \) is evaluated at its stationary-point value, which by Eq. \[ \text{(118)} \] and the initial conditions \[ \text{(18)} \] is zero. In this way the “anti-causality” of what we have termed the nominal distribution in Sec. \[ \text{III.C.2} \] is extended to correlation functions of arbitrary observables. Variation of the parameters in the Liouville operator (\( \xi \) in the examples) at times \( \tau \) earlier than the support \( \tau' \) of some observable \( \mathcal{O} \) cannot be propagated to \( \mathcal{O} \) because they are only carried on the \( \varphi^\dagger \) fields, which propagate only to times earlier than \( \tau \).

1. For free theories, short-cuts using the background fields

For a free theory, where the stationary path is also the exact mean, the result of a variation \( \delta \varphi \) can be computed directly by computing the dependence of \( \mathcal{O}_\tau \) on the shifted stationary path. In the dual generating functional in variables \( (\varphi^\dagger, \varphi) \), the result is

\[
\delta \langle \mathcal{O}_\tau \rangle = \frac{\partial \langle \mathcal{O}_\tau \rangle}{\partial (\varphi_b^\dagger - \varphi_a^\dagger)} \delta (\varphi_b^\dagger - \varphi_a^\dagger)_{\tau'} + \frac{\partial \langle \mathcal{O}_\tau \rangle}{\partial (\varphi_b + \varphi_a)} \delta (\varphi_b + \varphi_a)_{\tau'}
\]

\[
= \frac{\partial \langle \mathcal{O}_\tau \rangle}{\partial (\varphi_b^\dagger - \varphi_a^\dagger)} \Theta_{\tau > \tau'} e^{-(\tau - \tau')} \langle \varphi_b^\dagger + \varphi_a^\dagger \rangle_{\tau'} \delta \varphi + \frac{\partial \langle \mathcal{O}_\tau \rangle}{\partial (\varphi_b + \varphi_a)} \Theta_{\tau' > \tau} (\varphi_b - \varphi_a) \delta \varphi
\]

\[
= \frac{\partial \langle \mathcal{O}_\tau \rangle}{\partial (\varphi_b^\dagger - \varphi_a^\dagger)} \Theta_{\tau > \tau'} e^{-(\tau - \tau')} 2 \delta \varphi .
\] \[ \text{(93)} \]

The second and third lines use solutions for \( \varphi^\dagger \) and \( \varphi \) from App. \[ \text{D.4} \] recovering the advanced and retarded decay terms of Eq. \[ \text{(92)} \], including vanishing of the second term for \( \tau < \tau' \).

Writing out the extended FDT directly in number fields clarifies the way in which a shift from causality to anti-causality is accomplished by a change in the way terms couple to boundary conditions. The same steps that lead to
Eq. (93), starting from the action (61), lead to

\[
\frac{\delta}{\delta \tilde{\phi}_x} \langle O_{\tau'} \rangle = - \left\langle O_{\tau'} \left[ (1 + e^{\eta}) \left( \frac{N}{2} - n \right) - (1 + e^{-\eta}) \left( \frac{N}{2} + n \right) \right] \right\rangle \\
\approx 2 \left[ -\frac{N}{2} (1 + ch \tilde{\eta}_x) \right] \left\langle \left[ \tilde{\eta}' n' \right]_{\tau} \left[ \tilde{\eta}' n' \right]_{\tau'} \right\rangle \left[ \frac{\partial O/\partial \eta}{\partial O/\partial n} \right]_{\tau'} \\
= 2 \left[ -\frac{N}{2} \left( \frac{2}{1 - x^2_{\tau'}} \right) \right] \left\langle \left[ \tilde{\eta}' n' \right]_{\tau} \left[ \tilde{\eta}' n' \right]_{\tau'} \right\rangle \left[ \frac{\partial O/\partial \eta}{\partial O/\partial n} \right]_{\tau'} \\
= 2 \left[ -\frac{N}{2} \left( \frac{2}{1 - x^2_{\tau'}} \right) \right] \Theta_{\tau' > \tau} e^{-(\tau - \tau') \frac{1 - \bar{x}^2_{\tau}}{1 - \bar{x}^2_{\tau'}}} \left[ \begin{array}{cc} 0 & 0 \\ 0 & 1 \end{array} \right] + \Theta_{\tau' > \tau} e^{-(\tau' - \tau) \frac{1 - \bar{x}^2_{\tau}}{1 - \bar{x}^2_{\tau'}}} \left[ \begin{array}{cc} 0 & 1 \\ 0 & M_{\tau} \end{array} \right] \left[ \frac{\partial O/\partial \eta}{\partial O/\partial n} \right]_{\tau'}.
\]

(94)

In the first line, the stationary-path part of the term in square brackets is zero by the equations of motion, and \( \approx \) in the second line indicates the leading expansion to second order in fluctuations, the same order to which we have expanded Green’s functions in the action-angle variables.

The only nonzero term in the Green’s function at \( \tau' > \tau \) in the last line is orthogonal, by Eq. (93), to the vector \( \left[ -N/2 \ 2/(1 - \bar{x}_\tau^2) \right] \) in Eq. (94), ensuring that for \( \tau < \tau' \) \( \delta \langle O_{\tau'} \rangle/\delta \tilde{\phi}_x = 0 \). In the particular case that \( O = \left[ \tilde{\eta} \ n \right] \), Eq. (94) recovers the variation of the stationary path for \( \tau > \tau' \),

\[
\frac{\delta \tilde{\eta}_x}{\delta \tilde{\phi}_x} = \frac{2}{1 - \bar{x}^2_{\tau'}}, \\
\frac{\delta n_{\tau'}}{\delta \tilde{\phi}_x} = \frac{N}{2} e^{-(\tau - \tau')}. 
\]

(95)

The sensitivity of the response field in the first line includes the measure term \( 1 - \bar{x}^2_{\tau'} \) that we first saw in the backward propagation of final-time tilting weights in Eq. (60).

The anti-causality of correlation functions demonstrated in this section extends to more general non-linear rate laws, by using the Wick expansion of higher-order perturbations about the stationary-path background, wherever the perturbation series converges.

**V. DUALITY BEYOND TIME REVERSAL**

We now show how the constructions of the previous sections can be applied at the level of the CRN framework of Sec. II.E. The main new observation is the way duality transformation for systems with non-linear rate laws (corresponding to non-“free” field theories) generalizes the operation of transposing the kernel of the Liouville operator that was exhibited in Eq. (53).

**A. Dualizing about steady states under the transition matrix**

As we noted in Sec. II.E, the adjacency matrix \( A_k \) on the complex network defines the relevant concept of a graph Laplacian for stochastic processes on CRNs. Acting on this network with a suitable topology-preserving transformation exchanges the roles of observable and response fields in the DP functional integral.

Since we will define duality transforms about steady states of the generator (27) with strictly positive species counts, we mention first the conditions under which such solutions are ensured to exist. The Feinberg deficiency-zero criterion [39, 62] is a sufficient condition as long as all rate constants in \( A_k \) are nonzero. Steady states may exist for a much wider range of CRNs than these, but their existence can then depend quantitatively on the rate constants.

Let \( n^* \) denote the vector of steady-state numbers for \( n \) under the stochastic process with the topological adjacency matrix \( A_{\text{top}} \) from Eq. (32). By this choice of reference matrix, \( \psi_{Y^i}(n^*) = \text{const.} \) is always a right eigenvector of \( A_{\text{top}} \), so we may choose \( n^* \equiv 1 \Rightarrow \psi_{Y^i}(n^*) = 1; \forall i \leq 84 \).

Let \( \bar{n} \) denote the steady state under the stochastic process with matrix \( A_k \) from Eq. (31). Whenever all \( n_{\bar{p}} > 0 \), the appropriate generalization of Eq. (43) to the more general CRN is

\[
\phi_p \equiv \left( \frac{n_p}{n_{\bar{p}}} \right) \varphi_p, \\
\phi_{\bar{p}}^\dagger \equiv \left( \frac{n_{\bar{p}}}{n_p} \right) \varphi_{\bar{p}}^\dagger.
\]

(96)

The evaluation of the Liouville operator (28) in dual fields gives
\[
\psi^T_i(\phi^i) A_k \psi_Y(\phi)
= \psi^T_i(\phi^i) \sum_{(i,j)} (w_j - w_i) k_{ji} w_j^T \psi_Y(\phi)
= \psi^T_i(\phi^i) \left[ \text{diag} (\psi_Y(n^*) / \psi_Y(n)) \right] \sum_{(i,j)} (w_j - w_i) k_{ji} w_j^T \left[ \text{diag} (\psi_Y(n) / \psi_Y(n^*)) \right] \psi_Y(\varphi)
\equiv \psi^T_i(\phi^i) \sum_{(i,j)} w_i \hat{k}_{ij} \left( w_j^T - w_i^T \right) \psi_Y(\varphi)
\equiv \psi^T_i(\phi^i) \hat{A}_k \psi_Y(\varphi).
\] (97)

Here \([\text{diag} (v)]\), for a vector \(v \equiv [v_i]\), denotes the diagonal matrix with \(i\)th entry \(v_i\). In passing from the third to the fourth line of Eq. (97), we have used the fact that
\[
\sum_{(j|i)} \hat{k}_{ji} = \sum_{(j|i)} \hat{k}_{ij}
\] (98)

implied by \(\psi_Y(n^*) = 1; \forall i\). \(\hat{A}_k\) is the rate matrix for the dual process, defined from the fourth line in terms of dual rate constants \(\hat{k}_{ij}\).

The change coming from the kinetic term when the action (26) is written in dual variables is
\[
- (d\tau \phi^p) \phi_p = - (d\tau \varphi^p) \varphi_p + d\tau \log n_p \varphi^p \varphi_p,
\] (99)

and the term involving \(d\tau \log n_p\) is the one that must be subtracted by a path-weighting function to cause the observable and response fields to exchange roles. Note that this term — the path-integral version of the time derivative of the log-density function of Hatano and Sasa — is defined entirely from the overlap \(\langle \phi_\tau | \phi_\tau \rangle\) of the coherent states between insertions of the Peliti representation of unity at adjacent times. In the case of detailed balance as with the 2-state example, it becomes the excess work of Crooks.

The action for the dual generating functional,
\[
S_{\text{Crooks}} = \int d\tau \left\{ - (d\tau \phi^i) \phi + \psi^T_i(\phi^i) \hat{A}_k \psi_Y(\phi) - \phi^i \left[ \text{diag} (d\tau \log n) \right] \phi \right\}
= \int d\tau \left\{ - (d\tau \varphi^i) \varphi + \psi^T_i(\varphi^i) \hat{A}_k \psi_Y(\varphi) \right\},
\] (100)

is the general memory-erasing form for stochastic CRNs. For the two-state model, it recovers the forms (52, 53).

### B. Similarity transforms on the complex network and on the state space

Fig. 4 summarizes the parallel action of the adjoint dualization transform on the adjacency matrix \(A_k\) and the transition rate matrix \(T\). The fixed set of reactions among complexes generate the full matrix of transition rates among states. As we note in (53, 54), the step of interposing complexes between chemical species and reaction events, thus placing stoichiometric constraints between species and complexes, rather than between species and reactions directly, allows the complex matrix to behave as an ordinary directed network for a random walk. Therefore the vector of 1s on complexes \(i\) annihilates \(\hat{A}_k\) on the left, as the vector of 1s on states \(n\) annihilates \(T\) on the left in Eq. (12).

Under adjoint dualization, both matrices are similarity transformed by rescaling, \(\hat{A}_k\) with a vector of complex activities \(\psi_Y(n)\), \(T\) with the vector of probabilities \(\rho\) in which those activities would be observed. The adjoint adjacency matrix \(\hat{A}_k\) generates the adjoint transition rates among states. In systems with detailed balance, \(\hat{A}_k = \hat{A}_k^T\), and thus both \(\hat{A}_k\) and \(T\) are self-adjoint. Details are provided in App. E. Self-duality of the Liouville operator for networks with detailed-balance equilibrium is similar to Hermiticity of the Hamiltonian for systems with microscopic reversibility.

We see both why nonlinear CRNs can transform as simply as linear processes under dualization, and also that the adjoint construction from Eq. (97) is much simpler than would be expected from the general transformation (49). The former is true because the adjacency
Complexes \( \mathbb{A}_{kji} \) \( \rightarrow \) States \( T_{n'n} \)

\[ \dot{\mathbb{A}}_{kji} = \frac{1}{\psi Y_j(n)} \mathbb{A}_{kji} \psi Y_j(n) \rightarrow (\bar{T})_{n'n} = \frac{1}{2n} T_{n'n} \mathbb{A}_{n} \]

FIG. 1: The adjacency matrix \( \mathbb{A}_k \) and the one-step transition matrix \( T \) under dualization. The fixed matrix \( \mathbb{A}_k \) generates a transition matrix \( T \) of rank equal to that of the state space. Dualization to form the adjoint generating functional acts on both matrices by a rescaling similarity transform. For the adjacency matrix, the scale factor is a function of average numbers, and for the transition matrix it is the vector of state probabilities.

matrix transforms as an ordinary graph Laplacian for linear or non-linear processes; all complexity is cordoned off in the estimates of \( \bar{n} \). Note, however, that whereas the transition matrix is transformed by all components of \( \rho \), Eq. (47) is defined from simple products of the \( P \) components of the mean number vector \( \bar{n} \). Exact calculation of \( \bar{n} \) formally depends on calculation of \( \rho \), because in general moment hierarchies do not truncate [55, 56]. However, approximate or parametric inversions based on mean values are simpler and more robust than those that require explicit estimation of all moments.

The condition that assures many of the stronger simplifications among fluctuation theorems – principle among them the equivalence of the backward and the adjoint versions of duality – is detailed balance. The simplification associated with the similarity transforms we have just exhibited for CRNs – that the low-dimensional information in the scale factors \( \psi_Y(n) \) contain all the information in the densities \( \rho \) – is the weaker condition of complex balance. For complex-balanced steady states, the distributions are products of Poisson distributions on individual \( n_k \), or sections through such products, and \( \psi_Y(n) = (\Psi_Y(n))_j \), a result known as the Anderson-Cracium-Kurtz theorem [57].

C. Worked examples

We close with a pair of worked examples to show how dual graphical models characterizing the propagation of information in the response fields are derived from the graphical models of the underlying stochastic process.

1. A simple cycle with no dynamical reversibility

The first example is a 3-cycle of purely irreversible events, with two of the complexes involving pairs of particles. The reaction schema (with generally time-dependent rate constants) is

\[
\begin{align*}
A & \xrightarrow{k_1} 2B \\
2B & \xrightarrow{k_2} 2C \\
2C & \xrightarrow{k_3} A.
\end{align*}
\]

The rate matrix written explicitly is

\[ \mathbb{A}_k = \begin{bmatrix} -k_1 & 0 & k_3 \\ k_1 & -k_2 & 0 \\ 0 & k_2 & -k_3 \end{bmatrix}, \]

and the stoichiometric matrix is

\[ Y = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 2 \end{bmatrix}, \]

in terms of which the stationary-path equation of motion for the field \( \phi \) becomes

\[
0 \rightarrow d_\tau \phi + Y \mathbb{A}_k \psi_Y(\phi)
\]

\[ = d_\tau \phi + Y \begin{bmatrix} -k_1 & 0 & k_3 \\ k_1 & -k_2 & 0 \\ 0 & k_2 & -k_3 \end{bmatrix} \begin{bmatrix} \psi_A(\phi) \\ \psi_B(\phi) \\ \psi_C(\phi) \end{bmatrix}. \]

The vector of complex activities on the non-equilibrium steady-state solution is given by

\[ \begin{bmatrix} \psi_A(\bar{n}) \\ \psi_B(\bar{n}) \\ \psi_C(\bar{n}) \end{bmatrix} = \begin{bmatrix} n_A \\ n_B \\ n_C \end{bmatrix} \propto \begin{bmatrix} 1/k_1 \\ 1/k_2 \\ 1/k_3 \end{bmatrix}. \]

From this, the steady-state concentrations can be computed, and the duality transform [56] becomes

\[ \phi_A = \frac{\varphi_A}{k_1}, \quad \phi_B = \frac{\varphi_B}{\sqrt{k_2}} \quad \phi_C = \frac{\varphi_C}{\sqrt{k_3}} \]

\[ \phi_A^\dagger = k_1 \varphi_A^\dagger, \quad \phi_B^\dagger = \sqrt{k_2} \varphi_B^\dagger \quad \phi_C^\dagger = \sqrt{k_3} \varphi_C^\dagger. \]

The adjacency matrix in the dual generating functional, from Eq. (47), is then

\[ \dot{\mathbb{A}}_k = \begin{bmatrix} -k_1 & 0 & k_3 \\ k_2 & -k_2 & 0 \\ 0 & k_3 & -k_3 \end{bmatrix}. \]

In the dual theory, the stationary-path background for the observable field \( \varphi \) is given by \( \bar{\varphi} \equiv 1 \). We write the stationary-path equation of motion for the response field in its transpose form, for the sake of comparison to the un-weighted equation of motion [104], as

\[
0 = -d_\tau \varphi^\dagger T + \frac{\partial \psi_T^\dagger(\varphi)}{\partial \varphi^\dagger} \mathbb{A}_k \psi_Y(\varphi^\dagger)
\]

\[ \rightarrow -d_\tau \varphi^\dagger T + Y \begin{bmatrix} -k_1 & k_2 & 0 \\ 0 & -k_2 & k_3 \\ k_1 & 0 & -k_3 \end{bmatrix} \begin{bmatrix} \psi_A(\varphi^\dagger) \\ \psi_B(\varphi^\dagger) \\ \psi_C(\varphi^\dagger) \end{bmatrix}. \]
If the adjacency matrix had admitted a detailed-balance solution, then by Eq. (98), Eq. (108) would simply have described the process of Eq. (108) with a mirror-image trajectory for the rate constants. In this fully-irreversible model, the graphs for the original process, and for the dual process, shown in Fig. 2 exhibit two further features. In the dual process, the only elementary moves are the opposites of those in the underlying process. The positions of the rate constants are also moved to different links in the graph, as well as their time-courses’ becoming mirror images.

FIG. 2: Left graphic: original CRN with simple cycle. Right graphic: dual CRN that propagates the inference field.

2. An example in which a cycle co-occurs with symmetric bi-directional links

The second example combines the irreversible cycle of the previous example with a conventional microscopically-reversible sub-network, to show that duality is not always as simple as shuffling rate constants on an existing complex network.

The reaction schema is

\[
\begin{align*}
A & \xrightarrow{k_1} 2B \\
2B & \xrightarrow{k_2} 2C \\
2C & \xrightarrow{k_3} A \\
2B & \xrightarrow{k_4} D \\
2C & \xrightarrow{k_4} D,
\end{align*}
\]

and the rate matrix written explicitly is

\[
A_k = \begin{bmatrix}
-k_1 & 0 & k_3 & 0 \\
-k_2 & (k_2 + k_3) & 0 & k_4 \\
0 & k_2 & (k_3 + k_4) & k_4 \\
0 & k_4 & k_4 & -2k_4
\end{bmatrix}.
\]

The powers of species activities appearing in the complex-activity vector \(\psi(\mathbf{u})\) on the non-equilibrium steady state may be solved as

\[
\begin{bmatrix}
\mathbf{u}_A \\
\mathbf{u}_B \\
\mathbf{u}_C \\
\mathbf{u}_D
\end{bmatrix}
\propto
\begin{bmatrix}
(2k_2 + k_4)/2k_1k_2 \\
(2k_3 + k_4)/2k_2k_3 \\
(2k_2 + k_3 + k_4)/2k_2k_3 \\
(k_2 + k_3 + k_4)/2k_2k_3
\end{bmatrix}.
\]

The rate constants in the dual matrix \(\tilde{A}_k\) now have a more complex form, shown on the complex-network graphs for the original and dual processes in Fig. 3. The graphs refer to writing the equation of motion for the response field transposed, as in the previous example. All but one of the dual reaction rates are non-trivial functions of the equilibrium across the network.

FIG. 3: Top graphic: original CRN with both a totally asymmetric loop and a totally-symmetric conversion. Bottom graphic: dual CRN with respect to the canonical CRN on the same topology (see development in the text). The dual graph now has structural asymmetry in the two-directional rates connected to complex \(D\), emphasized by distinguishing their arcs.

VI. CONCLUDING REMARKS

The substitution of measures on trajectories to produce an expression of the form \(E_P (P^*/P) \equiv 1\) is a tautology; particular classes of such transformations rise to significance when they are identified by an interpretation linking a class of measurements. The use of the underlying measure on reversed trajectories was the first such group to be extensively developed in fluctuation theorems \(2, 3, 9, 10\); its interpretation was time reversal and it linked work along paths with total entropy production. The entropy produced in the bath is the equilibrium entropy by the local-equilibrium assumption. The entropy in the explicitly resolved stochastic process is still the usual Shannon form. It would become an equilibrium entropy if the system were held in a fixed state by an external boundary condition, as it is momentarily held in that state by the waiting time for transitions in the stochastic process.

Hatano and Sasa \(15\) showed that the underlying measure is not the only one with a fluctuation-theorem in-
terpretation, and even if it exists, it may not be a useful measure for questions involving nonequilibrium systems. However, they provided an alternative in the adjoint measure. Its interpretation is the reversal of probability currents in the instantaneous steady-state distribution, and it links the quantity identified by Oono and Paniconi [18] as housekeeping heat, with the change in Shannon entropy of these steady states. Housekeeping heat is still defined in terms of a near-equilibrium approximation for the bath, making this interpretation of the adjoint fluctuation theorem somewhat contingent on the system [20].

We have therefore developed the adjoint fluctuation theorems in terms that are independent of any external thermodynamic interpretations of the rate constants, emphasizing instead generating functionals, memory erasure, and inference, and we have developed some of the consequences for correlation functions at the level of generality of stochastic CRNs.

We would like to regard the two measures studied so far as two early cases within a more general duality concept captured by fluctuation theorems. One can imagine designing adjoint transformations to yield measures of other aspects of non-equilibrium structure, as the Hatano-Sasa construction measures changes in system Shannon entropy under a Langevin equation, using excess heat. We hope that a generating-functional framing is helpful in developing that generalization systematically.

Acknowledgments

DES thanks the Physics Department at Stockholm University for support during visits in 2014, 2016, 2017 and 2018 when the bulk of this work was carried out. The authors are grateful to Massimiliano Esposito, David Lacoste, Sreekanth Manikandan, Luca Peliti and Gatien Verley for very helpful discussions and references.

Appendix A: Definitions, notation, and standard constructions for the Doi-Peliti generating functional

Here we briefly review the operator-algebra construction of Doi [12, 43] for moment-generating functions, and the Peliti coherent-state expansion [44, 45] that creates a functional-integral representation of extended-time generating functions and functionals. More didactic reviews may be found in [51, 63, 64].

1. The Doi operator algebra construction

Following the notations [12] to represent complex arguments and their partial derivatives as raising and lowering operators, with the operator commutator [19], the Doi algebra [42, 43] defines a Hilbert space of generating functions and an inner product that corresponds to projection. These are written as right and left “ground states”, with the correspondences

\[ 1 \rightarrow |0\rangle \quad \int d^p z \delta^p(z) \rightarrow (0| . \quad (A1) \]

A moment-generating function is a polynomial in the components of z multiplying the number 1, which in the Doi algebra is the action of a polynomial of the raising operators acting on the left ground state. Each monomial is a basis vector for this space,

\[ \prod_{p=1}^{P} z_p^n \times 1 \rightarrow \prod_{p=1}^{P} a_p \dagger \rho_p |0\rangle \equiv |n\rangle ; \quad (A2) \]

the basis vectors are termed number states.

Under the mapping (A2) the analytic function \( \Phi(z) \) becomes a state vector \( |\Phi\rangle \), given by

\[ \Phi(z) = \sum_n \rho_n \prod_{p=1}^{P} z_p^n \times 1 \rightarrow \sum_n \rho_n |n\rangle \equiv |\Phi\rangle . \quad (A3) \]

All number states have unit normalization in an inner product known as the Glauber norm, given by

\[ (0|e^{\sum_p a_p} |n) = 1, \quad \forall n. \quad (A4) \]

As a consequence, the Glauber norm of each generating function is simply the trace of the underlying probability density:

\[ (0| e^{\sum_p a_p} |\Phi\rangle = \sum_n \rho_n = 1. \quad (A5) \]

The Doi algebra may be seen simply as a way to use integration and \( \delta \)-functions to change the variable argument of a generating function from a complex argument \( z \) to a formal argument \( a \dagger \). The compact notation it provides for an inner product becomes very convenient when an evolving generating function must be projected onto a basis at each of a large sequence of time intervals, as is done to integrate the equations of motion. The inverse transform, from variables \( a \dagger \) back to analytic argument \( z \), is given by the inner product Eq. (21) in the text, of which the Glauber norm (A5) is a special case.

2. The Peliti coherent-state expansion and path integral

In the Doi Hilbert-space representation, time evolution [20] is formally reduced to quadrature by exponentiation in the Liouville operator:

\[ |\Phi_T\rangle = T e^{-\int_0^T d\tau L_\tau} |\Phi_0\rangle . \quad (A6) \]

Here the subscript \( L_\tau \) indicates that the parameters in \( L \) may be explicit functions of time, and \( T \) stands for
time-ordering of the exponential, written as a product of terms over successive small time slices.

The 2FFI representation introduced by Peliti \cite{44, 45} provides a way to evaluate the quadrature \((A6)\) by expanding the arbitrary evolving generating function in a basis of coherent states, which were introduced in Eq. \((22)\). Coherent states are eigenstates of all coefficients in the lowering operator:

$$a_p |\phi\rangle = \phi_p |\phi\rangle. \quad (A7)$$

A sequence of insertions of the representation of unity \((24)\), formed from the outer product of left and right coherent states (projection operators and their conjugate generating functions), defines a skeletonized functional integral, in which the values of \(\phi\) and \(\phi^\dagger\) at each time become field-variables of integration. In the continuum limit defined by letting the spacing between insertions \(\delta \tau \to 0\), the functional measure of integration is denoted and defined as

$$\int_0^T D\phi^\dagger D\phi = \lim_{\delta \tau \to 0} \prod_{k=0}^{T/\delta \tau} \int D\phi^\dagger_{k\delta \tau} D\phi_{k\delta \tau} \pi^p. \quad (A8)$$

From the quadrature \((A6)\), the insertion of this skeletonized measure, with Eq. \((21)\) used to change variable back from \(a^\dagger\) to a complex surface argument \(z\), produces the functional integral representation \((29)\) for the generating function of the time-dependent density \(\rho\) evolved from time \(\tau = 0\) to time \(\tau = T\).

**Appendix B: The Feinberg decomposition for stochastic CRNs**

The main feature in our use of Doi-Peliti representations for stochastic Chemical Reaction Networks is a decomposition due to Feinberg \cite{39, 62}, which recognizes complexes as formal objects distinct from species, and factors the representation of reactions into independent events that occur on the complex network, and stoichiometric relations that connect removal or addition of a complex to removal or addition of a set of species. The complex network can be represented by an ordinary directed graph, and the stochastic process on this network is equivalent to a simple random walk on this graph. The stoichiometric relations are represented by links of a distinct type, giving a way to represent the multi-hypergraph of the CRN with a bipartite ordinary graph, with two kinds of nodes (species and complexes) and two kinds of links (reactions and stoichiometric connections).

The work of Feinberg typically represents only the complex network explicitly, and we follow this convention in Sec. \(\ref{sec:feinberg}\). Elsewhere \cite{55, 57, 68} we have used the bipartite graph representation to more fully represent the multi-hypergraph.

To obtain a representation for the transition matrix of a stochastic CRN, we begin with a matrix representation for the adjacency/rate structure on the complex network:

$$k_{ik} \equiv \sum_{(i,j)} (w_j - w_i) k_{ji} w^T_i. \quad (B1)$$

Here \(i\) and \(j\) index complexes, and the ordered pair \((i, j)\) indexes a reaction from complex \(i\) to complex \(j\). We will later assign a probability of formation to each complex in state \(n\), and imagine these probabilities written as a column vector indexed by \(i\). \(w_i\) is then a vector which is an indicator function with value 1 at index \(i\), and \(w^T_i\) is a transpose which selects the formation probability at complex \(i\). The parameter \(k_{ji}\) is the rate constant for complex \(i\), if formed, to be converted to complex \(j\).

An important theorem for CRNs \cite{33, 32} is that the existence and uniqueness of steady states of the time evolution \((1)\) is for some cases determined by the topology of the adjacency matrix, independent of its rate structure as long as the rates are nonzero. We will represent the topology by referring to an adjacency matrix with all rates set (arbitrarily) to unity, denoted by

$$A_{lop} \equiv \sum_{(i,j)} (w_j - w_i) w^T_i. \quad (B2)$$

For the simple case where complexes are formed from species by sampling without replacement in a well-mixed reactor (the only case we will develop here; some more general cases are considered in \cite{67}), the probability to form complex \(i\) is given by a truncated factorial of the species numbers \(\{n_p\}\), which we denote by the function

$$\Psi_{Y_i}(n) = \prod_p \frac{n_p!}{(n_p - y^i_p)!}. \quad (B3)$$

Here the \(y^i_p\) are non-negative integer-valued stoichiometric coefficients, giving the number of members from species \(p\) that form complex \(i\).

In the Doi algebra, the operator that will produce the combinatorial factor \((B3)\) for complex \(i\) when acting on a number state \(|n\rangle\), and the conjugate operator that will create the particles in complex \(i\), are both given by the same function taking respectively \(a\) and \(a^\dagger\) as arguments. We denote these by

$$\psi_{Y_i}(a) \equiv \prod_p a^y^i_p, \quad \psi_{Y_i}(a^\dagger) \equiv \prod_p a^\dagger y^i_p. \quad (B4)$$

In the transition matrix, when complex \(i\) is consumed and complex \(j\) is produced, the generator \(T\) adds probability to the state \(|n\rangle\) from the state \(|n + y^j - y^i\rangle\), for which each \(n_p\) is offset to \(n_p + y^j_p - y^i_p\). The shift operator that produces the index offset \(n_p \to n_p + y^i\) is also given by

$$\psi_{Y_i}(e^{\partial / \partial n}) \equiv \prod_p e^{y^j_p \partial / \partial n_p} = e^{y^j T \partial / \partial n}. \quad (B5)$$

Here \(y^j\) is a column vector with components \(y^j_p\), and \(y^j T\) is its transpose, forming an inner product with
the vector $\partial/\partial n \equiv [\partial/\partial n_p]$. The complementary shift
operator for $n_p \rightarrow n_p - y^j$ is $\psi_{y^j}(e^{-\partial/\partial n})$, and the two
operators commute.

From these definitions, the expression \[27\] for the transition matrix and \[28\] for the Liouville operator follow.

Appendix C: Importance Sampling and relations to saddle-point methods

Here we review basic concepts and terms associated with Importance Sampling, which are helpful in interpreting the roles and meanings of the observable and response fields in DP functional integrals. Although there is no process identical to sample estimation in the 2FFI
representation, many of the same criteria and interpretations apply to stationary-point expansions, which are a type of saddle-point approximation. In the interest of brevity, we simplify from the general notation of the text for binomial distributions, and assign reduced names for distribution parameters.

1. Altering the performance of sample estimators by Importance Sampling

Consider the problem of estimation by sampling a variable $n \in 0,\ldots,N$ from a binomial distribution with parameter $p$:

$$
\rho_n = p^n (1-p)^{N-n} \binom{N}{n}.
$$

(C1)

Expectations in $\rho$ are defined as in Eq. \[14\].

Sample estimation may perform poorly if the support of the observable $\mathcal{O}$ falls outside the range where $\rho$ produces many samples; or if the mean depends on an interaction between the shape of $\mathcal{O}$ and the shape of $\rho$, as is often the case if $\rho$ must be sampled in a “tail”.

It may be possible to mitigate both problems by drawing samples, not from the original distribution $\rho$, but rather from a tilted distribution $\tilde{\rho}$. In order to obtain an unbiased estimator for the mean, the observable $\mathcal{O}$ must be multiplied by a weight function that compensates for the tilt of the sample distribution. The key observation behind the protocol known as Importance Sampling (IS) \[54\] is that the tilt may be chosen so that sample values of the weighted observable cluster closer to their mean than did those of the unweighted observable. If the binomial parameter $p$ is tilted to a new parameter $q$, the expectation \[14\] becomes

$$
\langle \mathcal{O} \rangle = \sum_{n=0}^{N} \binom{N}{n} p^n (1-p)^{N-n} \mathcal{O}_n q^n (1-q)^{N-n} \binom{N}{n} \mathcal{O}_n, \quad n \geq 0.
$$

(C2)

The tilted density $\tilde{\rho}$ is termed the importance distribution, and the residual correction factor that converts $\mathcal{O}$ into $\tilde{\mathcal{O}}$ is termed the likelihood ratio. The original density $\rho$ is termed the nominal distribution. The likelihood ratio under an exponential tilting is also known as the Radon-Nikodym derivative of the map from the nominal probability measure $\rho$ to the importance measure $\tilde{\rho}$.

Suppose, for instance, that $\mathcal{O}_n = \varphi^n$ for some constant $\varphi$. Then if we choose

$$
q = \frac{\varphi p}{1-p + \varphi p},
$$

the likelihood-weighted observable

$$
\tilde{\mathcal{O}}_n = \left( \frac{1-p}{1-q} \right)^N \left( \frac{p (1-q) \varphi}{q (1-p)} \right)^n = \left( \frac{1-p}{1-q} \right)^N \times 1^n,
$$

(C4)

at all $n$. Whereas the values of the original observable $\mathcal{O}_n$ are dispersed in $n$, and the shape of $\rho_n$ is needed to compute the mean from them, the values of $\tilde{\mathcal{O}}_n$ are tightly compressed around the mean (here, they are perfectly collapsed onto it), and the shape of $\tilde{\rho}_n$ does not matter.

2. Use of tilting in saddle-point methods

The criterion of minimizing variance in sample-estimation is related to approximation procedures such as saddle-point expansions, for which exponential tilting also is commonly employed \[53\]. For the same distribution $\rho$ and exponential observable $\mathcal{O}_n = \varphi^n$, the leading exponential dependence in the sum \[14\] defining $\langle \mathcal{O} \rangle$ is given by

$$
\frac{1}{N} \log (\mathcal{O}_n \rho_n) \sim \frac{n}{N} \log \left( \frac{n}{N p \varphi} \right) + \frac{N-n}{N} \log \left( \frac{N-n}{N (1-p)} \right),
$$

(C5)

(where $\sim$ indicates the omission of higher-order corrections in the Stirling formula for factorials).

The saddle point of the argument in Eq. \[14\] is the value $\tilde{n}$ where $d \log (\mathcal{O}_n \rho_n) / dn = 0$, given by

$$
\frac{\tilde{n}}{N - \tilde{n}} = \frac{p \varphi}{1-p}.
$$

(C6)

Thus $\tilde{n}/N = q$ from Eq. \[53\], the same saddle-point value that would be obtained by approximating the tilted
distribution $\tilde{\rho}$ alone. In the saddle-point approximation $\sum_n O_n \rho_n$ is replaced by the leading-exponential term

$$\sum_n O_n \rho_n \sim O_n \rho_n \approx e^{-N \log \left( \frac{\sum_n O_n \rho_n}{N^N} \right)} = \left( \frac{1 - \bar{n}/N}{1 - p} \right)^N = (O). \quad (C7)$$

For this case, the optimal IS-tilt is the one that, in stationary-point approximation, maximally insulates the resulting observable $\tilde{O}$ from sample fluctuations, and in complementary fashion brings the identification of the observable.

The duality transformation (44), which can be used to absorb path weighting terms in the class of the NEWRs, has exactly the effect of exchanging a Radon-Nikodym derivative between an observable field that behaves as the mean of an importance distribution, and a response field that carries a complementary likelihood ratio. When the path weighting is done in such a way that the stationary points of either the observable or the response field become fixed points of the forward or backward equations (respectively, in the dual or the original variables), it has the effect of maximally separating the values of one field from the distribution dynamics of the other, as seen in the above example.

Appendix D: Supporting algebra for elementary stationary-path solutions

This appendix provides supporting algebra for the stationary-point evaluations of the four free field theories introduced in Sec. III. We keep surface arguments $z_{aT}$ and $z_{bT}$, and their variations explicit whether they are $O(\delta \tau^0)$ or $1 + O(\delta \tau)$. The four cases are contrasted according to whether the absence or presence of dynamics (respectively) preserves or dissipates the terminal values of stationary paths, and according to whether (by duality transformation) the response fields or observable fields are fixed points of the respective backward and forward equations.

1. Identity path-integral at a single time, followed by discrete tilting

The first variational derivatives in the action (40) lead to stationary-path conditions for $\phi^\dagger$ of

$$d_\tau \phi^\dagger_a = 0, \quad d_\tau \phi^\dagger_b = 0. \quad (D1)$$

The surface terms at $\tau = T$ from variation of $\phi$ set the boundary values of $\phi^\dagger$ equal to the arguments

$$\phi^\dagger_a)_{T} = z_a, \quad \phi^\dagger_b)_{T} = z_b. \quad (D2)$$

The stationary-path conditions for $\phi$ are likewise

$$d_\tau \phi_a = 0, \quad d_\tau \phi_b = 0. \quad (D3)$$

Their boundary values are set by the variations of $\phi^\dagger$ at $\tau = 0$, to give

$$\phi^\dagger_a)_{0} = \frac{\partial \log \psi_0}{\partial (\phi^\dagger_a)_{0}} = \frac{N}{1 - \bar{x}_a}, \quad \phi^\dagger_b)_{0} = \frac{\partial \log \psi_0}{\partial (\phi^\dagger_b)_{0}} = \frac{N}{1 - \bar{x}_b}. \quad (D4)$$

Because we have chosen to vary $z_a, z_b$ within the contour $\tilde{O}$, the denominators in Eq. (D4) equal 2 at all values of $z_b - z_a$. The solutions $\phi, \phi^\dagger$, and $\bar{n}$ are then constant at the values in Eq. (44).

2. Continuous tilting at a single time using a 2-field functional integral

Because the duality transform (44) converts the action (42) into the stationary form (44), the variations are the same as in the previous case except for their boundary values. First variational derivatives give

$$d_\tau \phi^\dagger_a = 0, \quad d_\tau \phi^\dagger_b = 0; \quad (D5)$$

$$d_\tau \phi_a = 0, \quad d_\tau \phi_b = 0. \quad (D6)$$

The surface terms at $\tau = T$ from variation of the $\phi$ fields set the response fields equal to the arguments

$$\phi^\dagger a)_{T} = z_a T (1 - x_{T - \delta \tau}) \quad \phi^\dagger b)_{T} = z_b T (1 + x_{T - \delta \tau}) = (1 + x_{T}), \quad (D7)$$

The $0$ boundary values for $\phi$ take a simple form due to the duality transform because we have chosen $z_\phi = \bar{x}_\phi$:

$$\phi^\dagger a)_{0} = \frac{\partial \log \psi_0}{\partial (\phi^\dagger a)_{0}} = \frac{N}{(\bar{\phi}^\dagger a)_{0} + (\phi^\dagger b)_{0}}, \quad (\phi^\dagger b)_{0} = \frac{\partial \log \psi_0}{\partial (\phi^\dagger b)_{0}} = \frac{N}{(\phi^\dagger a)_{0} + (\phi^\dagger b)_{0}}. \quad (D8)$$

Thus both $\phi$ and $\phi^\dagger$ are constant at their boundary values. In particular, $\bar{n}$, which is an invariant under the duality transform, is given by

$$\bar{n}_a = \phi^\dagger_a \phi_a = \phi^\dagger a \phi_a = \frac{N}{2} (1 - x_{\tau}), \quad \bar{n}_b = \phi^\dagger_b \phi_b = \phi^\dagger b \phi_b = \frac{N}{2} (1 + x_{\tau}). \quad (D9)$$

Inverting the duality transform gives the $\tau$-dependent values for $\phi$ and $\phi^\dagger$ of Eq. (45).

Note in particular, with reference to Eq. (36), that the stationary values for the response fields correspond to

$$\phi^\dagger a)_{\tau} = \frac{1 - x_{\tau}}{1 + x_{\tau}} = \prod_{\tau = \tau' + d\tau}^T \left( \frac{\psi_{a \tau'}}{\psi_{a \tau' - d\tau}} \right), \quad (D10)$$

$$\phi^\dagger b)_{\tau} = \frac{1 + x_{\tau}}{1 - x_{\tau}} = \prod_{\tau = \tau' + d\tau}^T \left( \frac{\psi_{b \tau'}}{\psi_{b \tau' - d\tau}} \right). \quad (D10)$$
the values of the likelihood ratio from the IS decomposition of the tilted generating function.

3. Retarded time evolution under the un-tilted stochastic process

The introduction of dynamics along the contour $\tau$ changes the character of stationary paths by dissipating the boundary data at $\tau = T$ (the weight variables $z_a$, $z_b$) and $\tau = 0$ (the distribution parameter $\bar{x}_0$), and gradually substituting the influence of the rate parameter $\tilde{z}$ in the transition matrix \[.\] The observable fields are evolved with retarded dynamics, and the response fields with advanced dynamics. Unlike either of the single-time weighting protocols, the nominal distribution -- the distribution reported by $\bar{n}$ -- becomes a dynamical function of $\tau$, sensitive to both initial and final data as well as the history of rates $\tilde{z}$.

Variation of the observable fields $\phi$ in the action $S_{\text{dyn}}$ from Eq. \[\text{[17]}\] gives advanced equations of motion for the response fields with source $\tilde{z}$.

$$(-d_{\tau} + 1) \left( \phi_b^{\dagger} - \phi_a^{\dagger} \right)_\tau = 0,$$
$$-d_{\tau} \left( \phi_b^{\dagger} + \phi_a^{\dagger} \right) = \tilde{z} \left( \phi_b^{\dagger} - \phi_a^{\dagger} \right). \tag{D11}$$

The surface variation at $\tau = T$ again produces the assignments \[\text{[12]}\]. The solutions for these in terms of the arguments $z_a$, $z_b$ of the generating function at time $T$ are

$$\left( \phi_b^{\dagger} - \phi_a^{\dagger} \right)_\tau = (z_b - z_a) e^{-(T-\tau)},$$
$$\left( \phi_b^{\dagger} + \phi_a^{\dagger} \right)_\tau = (z_b + z_a) + (z_b - z_a) \int_\tau^T d\tau' e^{-(T-\tau')} \tilde{z} \tau'. \tag{D12}$$

At $z_a = z_b = 1$ we have the usual \[\text{[33, 64]}\] fixed-point solutions $\phi_b^{\dagger} = \phi_a^{\dagger} \equiv 1$.

Variation of the response fields $\phi^\dagger$ fields gives the retarded equations of motion for the observable fields

$$d_{\tau} \left( \phi_b + \phi_a \right) = 0,$$
$$(d_{\tau} + 1) \left( \phi_b - \phi_a \right) = \tilde{z} \left( \phi_b + \phi_a \right), \tag{D13}$$
and the variation at $\tau = 0$ again gives the surface conditions \[\text{[D3]}\].

\[
\left( \phi_b^{\dagger} - \phi_a^{\dagger} \right)_\tau = \left( \phi_b^{\dagger} - \phi_a^{\dagger} \right)_T = \left( \phi_b^{\dagger} + \phi_a^{\dagger} \right) \int_\tau^T d\tau' e^{-(T-\tau')} \tilde{z} \tau',
\]

\[
= (z_bT - z_aT) (1 - \tilde{z} \tau^2) e^{-(T-\tau)} + (\phi_b^{\dagger} + \phi_a^{\dagger}) \left[ \tilde{z} \tau + \int_\tau^T d\tau' e^{-(T-\tau')} \partial_{\tilde{z}} \tilde{z} \tau' \right]. \tag{D17}
\]

When $z_{bT} = z_{aT}$, the first term in the second line of Eq. \[\text{[D17]}\] vanishes, $\left( \phi_b^{\dagger} + \phi_a^{\dagger} \right) = z_{bT} + z_{aT}$, and
\((\tilde{\varphi}_b^i - \tilde{\varphi}_a^i)\) evolves under an advanced response to \(x\), dual in both time and field conjugation to the retarded response that \(\varphi_b - \varphi_a\) shows in Eq. \((D13)\).

The variation of response fields \(\varphi^i\) gives the equations of motion for the observable fields \(\varphi\)

\[
(d_\tau + 1) (\tilde{\varphi}_b - \tilde{\varphi}_a) = 0,
\]

\[
d_\tau (\tilde{\varphi}_b + \tilde{\varphi}_a) = \mathcal{L} (\tilde{\varphi}_b - \tilde{\varphi}_a), \tag{D18}
\]

and again recovers the surface conditions \((D8)\). Thus \(\tilde{\varphi}_b = \tilde{\varphi}_a = N/2\), independent of the trajectory \(x\). The observable field in the dual variables has become a fixed point of its forward equation – the role played by the response function (with respect to the backward equation) in an unweighted time evolution of a plain distribution as noted following Eq. \((D12)\).

The components of the number field again satisfy \(\tilde{n}_b + \tilde{n}_a = N\) at all times, but the difference value \((\tilde{n}_a - \tilde{n}_b)\) satisfies Eq. \((E3)\), with \(\bar{x}\) obeying the advanced equation of motion \((E13)\) and \(\bar{x}_T = \bar{x}_T\).

To compare the field interpretations to the non-dynamical case with cumulative tilting, we convert back using the duality transform \((E13)\), to obtain

\[
\frac{1}{2} (\tilde{\varphi}_b^i + \tilde{\varphi}_a^i) = 1 - \frac{x_{\tau}}{1 - x_{\tau}} \int_\tau^T d\tau' e^{-\tau' - \tau} \partial_{\tau'} x_{\tau'},
\]

\[
\frac{1}{2} (\tilde{\varphi}_b^i - \tilde{\varphi}_a^i) = \frac{1}{1 - x_{\tau}^2} \int_\tau^T d\tau' e^{-\tau' - \tau} \partial_{\tau'} x_{\tau'},
\]

\[
(\tilde{\varphi}_b + \tilde{\varphi}_a) = N,
\]

\[
(\tilde{\varphi}_b - \tilde{\varphi}_a) = N\bar{x}_T. \tag{D19}
\]

By construction the observable fields are the same. For the response fields, the quantity \(x_{\tau} - \bar{x}\) in Eq. \((D10)\) is replaced with the integral \(\int_\tau^T d\tau' e^{-\tau' - \tau} \partial_{\tau'} x_{\tau'}\) in Eq. \((D19)\).

**Appendix E: Supporting algebra for Green’s function computation in action-angle variables**

The retarded and advanced Green’s functions for number fields are solutions to the inhomogeneous differential equations involving \(n\) in the second and fourth lines of Eq. \((E7)\), corresponding to Eq. \((D3)\) in coherent-state fields.

However, whereas the diffusion kernel \(D_\tau\) in Eq. \((E7)\) leads to the characteristic decay rate 1 (the lower-right entry in Eq. \((D7)\)), the two decay rates appearing in the second and fourth lines of Eq. \((E7)\) are non-obvious functions of \(x\) and \(\eta\) or \(\bar{\eta}\), which evaluate respectively to

\[
\text{ch} \: \bar{\eta} + \text{zh} \: \bar{\eta} = 1,
\]

\[
\text{ch} \: \bar{\eta} - \text{zh} \: \bar{\eta} = \left(1 + \bar{x}^2\right) - 2 \bar{x} \bar{x}\left(1 - \bar{x}^2\right) = 1 - d_\tau \log (1 - \bar{x}^2). \tag{E1}
\]

The argument of the decaying exponential, which is \(\tau - \tau'\) in Eq. \((E8)\) for coherent-state fields, remains \(\tau - \tau'\) for number fields in the un-tilted stochastic process, but is replaced with the integral

\[
\bar{Y}_\tau^{\tau'} = \int_{\tau}^{\tau'} d\tau'' \left(\text{ch} \: \bar{\eta} - \text{zh} \: \bar{\eta}\right) = (\tau - \tau') + \log \left(1 - \bar{x}^2\right)
\]

\[
(1 - \bar{x}^2) \tag{E2}
\]

in the tilted generating functional.

Using these in the equations \((E8)\) for the Keldysh kernel, one can check that both are solved by the functions

\[
M = \frac{N}{4} (1 - \bar{x}^2), \quad \bar{M} = \frac{N}{4} (1 - \bar{x}^2), \tag{E3}
\]

with the appropriate retarded solution \((E8)\) for \(x_T\) in the case of \(M\) and the advanced solution \((E4)\) for \(x_T\) in the case of \(\bar{M}\). The quadrature form of Eq. \((E8)\) for the kernel \(M\) is

\[
\bar{M}_T = e^{-2Y_\tau^{\tau'}} \bar{M}_T + \int_{\tau}^{\tau'} d\tau'' e^{-2Y_\tau^{\tau''}} \frac{N}{2} (1 - \bar{x}_T^{\tau''}). \tag{E4}
\]

Collecting these evaluations together gives the expression \((E9)\) for the Green’s functions in the text.

**Appendix F: Rate matrix and duality for microscopically reversible systems**

Microscopic reversibility requires that the rate matrix have a form

\[
\bar{k}_k \equiv \sum_{(i,j)} (w_j - w_i) \left(k_{ji} u_i^T - k_{ij} u_j^T\right), \tag{F1}
\]

in which the rate constants can be expressed in terms of single-complex and transition-state chemical potentials, as

\[
k_{ji} = e^{-\beta [\mu_{(i)} - \mu_{(j)}]} = e^{-\beta (\mu_{(i)} - (\mu_{(i)} + \mu_{(j)})/2)} e^{\beta (\mu_{(i)} - \mu_{(j)})/2},
\]

\[
k_{ij} = e^{-\beta [\mu_{(j)} - \mu_{(i)}]} = e^{-\beta (\mu_{(j)} - (\mu_{(i)} + \mu_{(j)})/2)} e^{\beta (\mu_{(j)} - \mu_{(i)})/2}. \tag{F2}
\]

Here the single-complex chemical potentials \(\mu_{(i)}\) are expressed in terms of the one-particle potentials \(\mu_{(i)}\) for each species, and the stoichiometric coefficients, as

\[
\mu_{(i)} = \sum_{p} p_{ij} \mu_{(i)}. \tag{F3}
\]

\(\langle ij \rangle\) denotes the un-ordered pair of \(i\) and \(j\), and \(\mu_{(ij)}\) denotes the single-complex transition-state free energy (equal to a chemical potential in energy units) for the reactions \((ij)\) and \((ji)\), the same in both directions under the assumption that these are elementary reactions. Eq. \((F1)\) then becomes
\[ \hat{A}_k \equiv \sum_{(i,j)} (w_j - w_i) e^{-\beta \left[ \mu_{(i)} - \frac{1}{2} \left( \mu_i + \mu_j \right) \right]} \left( e^{\beta \frac{2}{3} (\mu_i - \mu_j)^2 w_i^T} - e^{\beta \frac{2}{3} (\mu_i - \mu_j)^2 w_j^T} \right). \]  

(F4)

The detailed-balance equilibrium satisfies
\[ \mu_i \propto e^{-\beta \mu_i}, \]  
from which (choosing the normalization for convenience), the dual variables become
\[ \phi_p \equiv e^{-\beta \mu_p} \varphi_p, \]
\[ \phi_p^\dagger \equiv e^{\beta \mu_p} \varphi_p^\dagger. \]  

(F5)

The complex activities in Eq. (7) then transform as
\[ \psi_i(\phi) = e^{-\beta \mu_i} \psi_i(\varphi), \]
\[ \psi_i(\phi^\dagger) = e^{\beta \mu_i} \psi_i^\dagger(\varphi^\dagger). \]  

(F7)

For the form (F1) of \( \hat{A}_k \), the rate matrix for the dual complex network becomes
\[ \tilde{\hat{A}}_k = \hat{A}_k^T. \]  

(F8)

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[75] Note that the term “backward process”, which we adopt from [11], is not a reference to the Kolmogorov-backward equation, which also figures in our development.

[76] For stationary Markov chains, this is the actual steady-state solution, and may be used directly as such.

[77] This result is implicit in that the representation we have used elsewhere [52] for stochastic population processes is the same one produced by CRNs [53, 54], which we will use below.

[78] An example is the standard formulation of the Transient Fluctuation Theorems in terms of a generating functional for the path work; see [11].

[79] In this respect the Peliti functional integral may be understood as an extension of the Poisson representation of Gardiner and Chaturvedi [69, 70]. For an application of their method to Large Deviations and fluctuation theorems, see [71].

[80] The relation between the forward and backward equations was developed by Kolmogorov for stochastic differential equations, where the forward equation is also known as the *Fokker-Planck* equation. [11].

[81] The properties of analytic functions can lead in some cases to powerful and elegant methods to derive the asymptotic behavior of coefficients in the series of generating functions [72]. Many results do not require the full machinery of analyticity, however, and employ only the formal power series [72]. We introduce the analytic representation here because it clarifies some interpretations that are often implicit in the abstract linear-algebra formalism, in which the operator $a$ (introduced below) is treated as a “continuous-valued” argument, an interpretation that is manifest for its antecedent $z$ and otherwise obscure.

[82] An unfortunate collision of terms causes the adjective *com’plex* of complex variables and the noun *com,plex* for CRN reactants or products to take the same English orthography. We will attempt to use language that avoids ambiguity.

[83] See [27] for an application of this freedom to replace pathological cases of Hatano-Sasa duality, where for instance the steady-state distribution may be everywhere non-smooth, with reference distributions that have the same support in the state space as the dynamical distribution.

[84] This means that the naïve measure in the new variables produces the correct fluctuation statistics, and is free of anomalies. The representation of unity in these fields is derived directly in Li et al. [74].

[85] Note that this means the Hamiltonian-conjugate fields with respect to the conserved volume element of the DP construction correspond to the Legendre dual fields with respect to the equilibrium entropy.

[86] This choice is WLOG if the null complex never appears in the CRN as a source or sink; it is forced if the null complex does appear, because for that complex $\psi_{\text{null}} \equiv 1$. 