# Time-translational symmetry in statistical dynamics dictates Einstein relation, Green-Kubo formula, and their generalizations

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A stochastic dynamics has a natural decomposition into a drift capturing mean rate of change and a martingale increment capturing randomness. They are two statistically uncorrelated, but not necessarily independent, components contributing to the overall fluctuations of the dynamics, representing the uncertainties in the past and in the future. We show that fluctuation-dissipation relations of the two aforementioned components, such as the Einstein relation and the Green-Kubo formula, can be formulated for any stochastic process with a steady state, without additional supposition of the process being Markovian, reversible, or linear. Further, by considering the adjoint process defined by the time reversal at the steady state, we show that reversibility in equilibrium leads to an additional symmetry in the covariance between system's state and drift. Potential directions of further generalizing our results to processes without steady states is briefly discussed.

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## I. INTRODUCTION

Each step, small or large, of a complex motion can be represented by a "stochastic noise part" (noise) and a "deterministic average rate part" (drift) whose interplay gives rise to the fluctuation-dissipation relation (FDR), a central result in statistical physics. From a dynamical systems point of view, the stochasticity of time evolution implies divergent potential moves from a state in the state space (1-to-many with probabilities) while a dissipative drift represents a contracting vector field of average motions from various initial states (many-to-1 mapping in discrete state space). When these two "opposing" tendencies strike a balance and yield a stationary process, the FDR appears.

There are at least two quantitative manifestations of the above physical picture: On the one hand, the classic FDR in linear response theory, following Onsager's regression hypothesis [1], is a set of relations between a system's relaxation-after-perturbation near an equilibrium and autocorrelation of spontaneous equilibrium fluctuations [2–5]. Extensions of this result to nonequilibrium systems are discussed in recent works [6–8]. On the other hand, the Einstein relation and the Green-Kubo formula (GKF) are between components with different statistical characteristics, dissipative drift vs fluctuating noise, within a stationary process without a perturbation [9,10]. To illustrate, using Langevin's equation for the velocity of a Brownian particle that follows

$$m\frac{\mathrm{d}V}{\mathrm{d}t} = \underbrace{-\eta V}_{\text{drift}} + \underbrace{\sqrt{2k_BT\eta}\,\xi(t)}_{\text{noise}}, \tag{1}$$

$\xi(t)$ being a standard white noise, one gets stationary

$$\mathbb{E}[\Delta V(t)\Delta V(t+\tau)] = (k_BT/m)e^{-\eta\tau/m}, \tag{2}$$

where $\mathbb{E}[\cdot]$ denotes expectation and $\Delta V(t) := V(t) - \mathbb{E}[V(t)]$. Then,

$$\underbrace{D = \frac{k_BT}{\eta}}_{\text{Einstein relation}} \underbrace{= \int_0^\infty \mathbb{E}[\Delta V(t)\Delta V(t+\tau)]\mathrm{d}\tau}_{\text{Green-Kubo formula}}, \tag{3}$$

in which $V(t)$ is a stationary process, and $D$ is the long-time limit of the mean square displacement of $X(t)$, the integration of $V(t)$: $\mathbb{E}[(X(t)-X(0))^2] \sim 2Dt$.

In this paper, we shall refer relations directly between the diffusive noise and the dissipative drift as generalized Einstein relation (GER) and relations involving time correlation function as the GKF. Extensions of these to the nonequilibrium realm have also been explored: for an $n$-dimensional linear irreversible Ornstein-Uhlenbeck process, GER takes the form of the Lyapunov matrix equation, connecting to the theory of linear stability and control [11,12],

$$2\mathbf{D} = \boldsymbol{\Xi}\mathbf{B}^{\mathsf{T}} + \mathbf{B}\boldsymbol{\Xi}, \tag{4}$$

where $\boldsymbol{\Xi}$, $\mathbf{B}$, and $\mathbf{D}$ are matrices of the stationary covariance between states, the linear relaxation, and the diffusion. A nonlinear GKF for nonequilibrium steady states in continuous time Markov processes was also established in Ref. [13,14]:

$$\mathbb{E}\big[D(X_t)\big] = \int_0^\infty \mathbb{E}\big[b(X_t)b(X_{t+\tau})\big]\mathrm{d}\tau, \tag{5}$$

where the stationary $X_t$ follows a nonlinear stochastic differential equation with drift $b(X_t)$ and diffusion $D(X_t)$.

In this paper, we show that "the fluctuating noise" and "the dissipative drift", where the latter being a conditional

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expectation, can be used as defining properties for a decomposition of general stationary processes, without additional supposition of the system being Markovian, reversible, linear, etc. In terms of this decomposition, a GER can be formulated. The formalism clearly illustrates, actually it defines, the GER as the consequence of stationarity of a process in which the stochasticity is balanced by dissipation. In the past, the stationary Fokker-Planck equation for a Markov process poses a mathematical relation among three: (i) the stationary distribution, (ii) the dissipative drift, and (iii) the stochastic noise strength [15]. For most of the applications, one solves (i) based on (ii) and (iii) [14,16]. Alternatively, given (i) and (iii), (ii) admits a general decomposition in terms of the other two [17–19]. All these previous results are now encompassed in the GER [Eq. (15) below] and the GKF in Eq. (20), broadly generalizing Eq. (4) and Eq. (5), respectively.

A key mathematical insight contributing to our result is a general decomposition of stochastic processes discovered by Doob [15,20]: a stochastic step in the time evolution of a process, infinitesimal or large, can always be written as the sum of a "drift part" that captures the average increment and a "noise part" that captures the stochasticity [21]. The latter parts from all steps constitute a martingale [15], which is a process that has no (conditional) gain or loss on average: a fair game. In stochastic thermodynamics, the theory of martingale has played an important role in studying stopping time statistics [22–24]. Here, we discover that the martingale increment is uncorrelated to the past, which leads to a clear cut of two uncorrelated contributions to the fluctuations of the overall stochastic dynamics, as shown in Eq. (13).

For Markov processes with detailed balance, our GER leads to another characterization of equilibrium steady state: by considering a process and its adjoint process, we show that the covariance matrix between the state and its drift is symmetric if the process is reversible. Various forms of the GKF, as corollaries, can be derived for the adjoint drift. The 1-to-many and many-to-1 features in the dynamics can also be identified, representing uncertainties in the future and in the past respectively, with the fluctuations of drift and adjoint drift under Doob decompositions of a process and its adjoint.

All results point to the time stationarity being central to FDR. The search for a similar relationship, between noise and drift, in sweeping dynamics that does not reach stationarity [12] naturally arises. We briefly discuss one class of sweeping processes whose exponentiation becomes a martingale in the Discussion.

## II. DOOB DECOMPOSITION

We consider a general discrete time $n$-dimensional ($n$-D) stochastic process, not necessarily Markovian, $\mathbf{X}_t \in \mathbb{R}^n$, $t \in \mathbb{N}$. Continuous time processes can be discussed by considering the infinitesimal d$t$ and taking the continuous time limit. We use $\mathbf{X}_{0:t}$ to denote the entire stochastic trajectory from time 0 to time $t$. The change of the value of the state of the system from time $t$ to $t+1$ has a natural decomposition by the conditional expectation:

$$\delta\mathbf{X}_t := \mathbf{X}_{t+1} - \mathbf{X}_t = \delta\mathbf{A}_t(\mathbf{X}_{0:t}) + \delta\mathbf{M}_t(\mathbf{X}_{0:t+1}), \tag{6}$$

where

$$\delta\mathbf{A}_t := \mathbb{E}[\mathbf{X}_{t+1}|\mathbf{X}_{0:t}] - \mathbf{X}_t \tag{7}$$

and

$$\delta\mathbf{M}_t := \mathbf{X}_{t+1} - \mathbb{E}[\mathbf{X}_{t+1}|\mathbf{X}_{0:t}]. \tag{8}$$

The first term $\delta\mathbf{A}_t$ in the decomposition is the conditional average change of $\mathbf{X}_t$, a function of entire, non-Markovian $\mathbf{X}_{0:t}$, that captures the average dynamics of $\mathbf{X}_t$, $\mathbb{E}[\delta\mathbf{X}_t|\mathbf{X}_{0:t}] = \delta\mathbf{A}_t$. Hence, the increment $\delta\mathbf{A}_t$ is referred as the *drift* of $\mathbf{X}_t$. The second term $\delta\mathbf{M}_t$ captures the 1-to-many randomness in the change of $\mathbf{X}_t$ conditioned on one past trajectory $\mathbf{X}_{0:t}$, there are many possible next states $\mathbf{X}_{t+1}$ diverging from the average.

The noise term $\delta\mathbf{M}_t$ has a zero (conditional) mean:

$$\mathbb{E}[\delta\mathbf{M}_t|\mathbf{X}_{0:t}] = 0 \text{ and } \mathbb{E}[\delta\mathbf{M}_t] = 0. \tag{9}$$

In this paper, expectation without conditioning represent averaging over all random variables involved, e.g., over the whole path $\mathbf{X}_{0:t+1}$ for $\mathbb{E}[\delta\mathbf{M}_t]$. The existence of this decomposition of a general process in Eq. (6) into the sum of two processes is known as the *Doob decomposition theorem* [15,20].

The decomposed process $\mathbf{M}_t = \sum_{k=0}^{t-1}\delta\mathbf{M}_k$ satisfies

$$\mathbb{E}[\mathbf{M}_t|\mathbf{X}_{0:s}] = \mathbf{M}_s, \text{ for all } 0 \leqslant s \leqslant t, \tag{10}$$

due to the zero conditional gain in every increment. In the theory of probability, such a process is called a *martingale* [15,25]. Typical examples of martingales are an unbiased random walk in discrete time and a Brownian motion in the continuous time.

The zero (conditional) mean properties of the martingale increment in Eq. (9) implies that $\delta\mathbf{M}_t$ is an increment uncorrelated to the past (but not necessarily independent): for an arbitrary path scalar variable of $\mathbf{X}_{0:t}$, $f(\mathbf{X}_{0:t}, t)$, the covariance between $f$ and any component of $\delta\mathbf{M}_t$, say the $i$th one denoted as $\delta M_t^{(i)}$, is zero:

$$\mathrm{Co}\mathbb{V}\big[f(\mathbf{X}_{0:t}, t), \delta M_t^{(i)}\big] = 0. \tag{11}$$

This leads to the following two important results. To present them in a more concise way, we will use $[\![\mathbf{u}, \mathbf{w}]\!]$ to denote the covariance matrix between two vector random variables $\mathbf{u}$ and $\mathbf{w}$ in this paper. Specifically, the $i, j$ component of $[\![\mathbf{u}, \mathbf{w}]\!]$ is $\mathrm{Co}\mathbb{V}[u_i, w_j]$. Here and below, covariance is averaging over the whole trajectory $\mathbf{X}_{0:t+1}$, a notation consistent with the expectation (without conditioning) $\mathbb{E}[\cdot]$ used throughout the paper.

First, the martingale increments at different times are uncorrelated $[\![\delta\mathbf{M}_t, \delta\mathbf{M}_s]\!] = \mathbf{0}$. This shows that a martingale has an ever-increasing, additive fluctuation,

$$[\![\mathbf{M}_t, \mathbf{M}_t]\!] = \sum_{k=0}^{t-1}[\![\delta\mathbf{M}_k, \delta\mathbf{M}_k]\!]. \tag{12}$$

The scalar version of this, the variance of $M_t$ satisfying $\mathbb{V}[M_t] = \sum_{k=0}^{t-1}\mathbb{V}[\delta M_k]$, is a discrete-time analog of Itô isometry [25] and is, in a sense, more general than Itô isometry: the martingale in Itô isometry is the Brownian motion which has independent increments whereas Eq. (12) doesn't require independency in the increments.

Second, the uncertainty of increment $\delta\mathbf{X}_t$ actually has two uncorrelated sources identified by the Doob decomposition in

Eq. (6),

$$[\![\delta\mathbf{X}_t, \delta\mathbf{X}_t]\!] = [\![\delta\mathbf{A}_t, \delta\mathbf{A}_t]\!] + [\![\delta\mathbf{M}_t, \delta\mathbf{M}_t]\!]. \quad (13)$$

The two sources of the uncertainty in $\delta\mathbf{X}_t$ are rather disjoint conceptually. Since $\delta\mathbf{A}_t$ is a function of the past path $\mathbf{X}_{0:t}$, the fluctuation of $\delta\mathbf{A}_t$ is really about the uncertainty of the past. On the other hand, the uncertainty of $\delta\mathbf{M}_t$ is about the fluctuation in the conditional mapping from $\mathbf{X}_t$ to $\mathbf{X}_{t+1}$. If the conditional mapping is deterministic, then $\delta\mathbf{M}_t = 0$ but $[\![\delta\mathbf{A}_t, \delta\mathbf{A}_t]\!]$ could still be nonzero if there is uncertainty in the initial condition and/or the past state.

These two results shown above are valid for general processes. Assumptions such as Markovian, stationarity, or detailed balance are not needed. In fact, the Doob decomposition can also be applied to an arbitrary path variable $\mathcal{U}_t(\mathbf{X}_{0:t})$. The decomposition then becomes $\delta\mathcal{U}_t = \delta A_{\mathcal{U}_t} + \delta M_{\mathcal{U}_t}$ where $\delta A_{\mathcal{U}_t} := \mathbb{E}[\mathcal{U}_{t+1}|\mathbf{X}_{0:t}] - \mathcal{U}_t$ and $\delta M_{\mathcal{U}_t} := \mathcal{U}_{t+1} - \mathbb{E}[\mathcal{U}_{t+1}|\mathbf{X}_{0:t}]$. The results presented above still hold.

We note here that two special classes of processes can be identified with the Doob decomposition and are the natural extension of a martingale. If the drift of a scalar process is always non-negative, then the process is called a *submartingale.* If the drift of a scalar process is always nonpositive, then the process is called a *supermartingale.* An important example of *submartingale* in stochastic thermodynamics is the housekeeping heat $\mathcal{Q}_{\text{hk}}$. In fact, the housekeeping heat $\mathcal{Q}_{\text{hk}}$ belongs to a special class of submartingale where $\exp(-\mathcal{Q}_{\text{hk}})$ becomes a martingale [26–28]. Other types of entropy production in stochastic thermodynamics has a non-negative average drift but their drifts are not guaranteed to be non-negative before expectation, and are in general not submartingale [28].

## III. RESULTS

### A. Generalized Einstein relation

If the process $\mathbf{X}_t$ reaches a steady state, the probability distribution of state no longer changes in time. For those stationary $\mathbf{X}_t$, all its cumulants will be fixed in time. The average state of $\mathbf{X}_t$ would be constant in time, meaning that the average drift of the observable would be zero at the steady state $\mathbb{E}_*[\delta\mathbf{A}_t] = 0$ where $\mathbb{E}_*[\cdot]$ means expectation for the stationary process. For the evolution of the covariance matrix, we have

$$\delta[\![\mathbf{X}_t, \mathbf{X}_t]\!] := [\![\mathbf{X}_{t+1}, \mathbf{X}_{t+1}]\!] - [\![\mathbf{X}_t, \mathbf{X}_t]\!] \quad (14a)$$

$$= [\![\delta\mathbf{A}_t, \mathbf{X}_t]\!] + [\![\delta\mathbf{A}_t, \mathbf{X}_t]\!]^{\mathsf{T}} + [\![\delta\mathbf{X}_t, \delta\mathbf{X}_t]\!] \quad (14b)$$

where $\mathsf{T}$ denotes the transpose of a matrix. This shows that the covariance of states always have a source $[\![\delta\mathbf{X}_t, \delta\mathbf{X}_t]\!]$ given by the fluctuation of transitions. Stationarity of $\mathbf{X}_t$ is achieved by the balance between the drift and the fluctuation such that $\delta[\![\mathbf{X}_t, \mathbf{X}_t]\!] = \mathbf{0}$,

$$[\![\delta\mathbf{A}_t, \mathbf{X}_t]\!]_* + [\![\delta\mathbf{A}_t, \mathbf{X}_t]\!]_*^{\mathsf{T}} = -[\![\delta\mathbf{X}_t, \delta\mathbf{X}_t]\!]_*, \quad (15)$$

where $[\![\mathbf{u}, \mathbf{w}]\!]_*$ denotes covariance matrix of $\mathbf{u}$ and $\mathbf{w}$ when the process is stationary. This shows that the symmetric part of $[\![\delta\mathbf{A}_t, \mathbf{X}_t]\!]_*$ is negative definite. In physics, the drift $\delta\mathbf{A}_t$ in a stable process is directly related to the dissipation of the dynamics. Equation (15) is thus a generally valid *Einstein relation* (GER) implied by stationarity. In a scalar process,

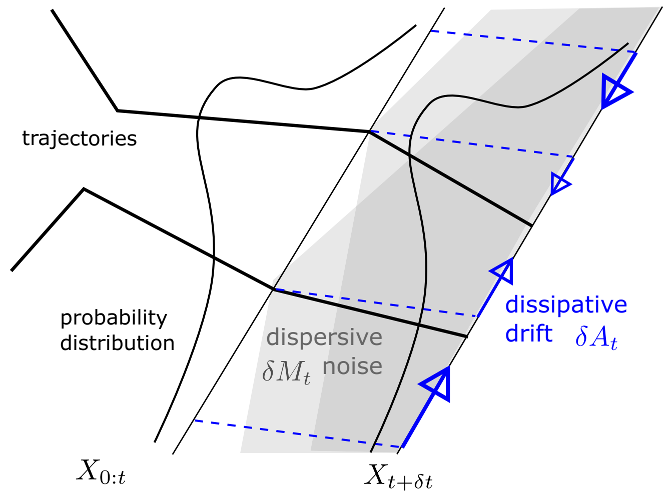


FIG. 1. Two trajectory realizations of the stochastic process are depicted in black solid lines. The noise is dispersive in each step, drawn as shaded area to represented all possibilities. The drift is drawn as blue arrows, "dissipative" in the sense that it is on average pointing inward: it dissipates the level of $X_t$. Fluctuation-dissipation relations emerge as the balance between the dissipative drift and the dispersive noise necessary for a time-translational symmetry in the probability distribution of state to form in stationary processes.

Eq. (15) reduces to $2\text{Co}\mathbb{V}_*(\delta A_t, X_t) = -\mathbb{V}_*[\delta X_t]$ which shows that the drift $\delta A_t$, on average, has an opposite sign of the value of $X_t$ as a "dissipation" to $X_t$. This negative covariance implies that the dissipative drifts $\delta A_t$ at different states are on average pointing inward, as a contracting vector field in continuous state space and many-to-1 mapping in discrete state space. A demonstration of the concept discussed above is shown in Fig. 1. In fact, the above result can be extended to arbitrary observable of the process, $U_t(\mathbf{X}_t)$, e.g., the energy of the system. The Doob decomposition of its dynamics becomes $\delta U_t = \delta A_{U_t} + \delta M_{U_t}$, where $\delta A_{U_t} := \mathbb{E}[U_{t+1}|\mathbf{X}_{0:t}] - U_t$ and $\delta M_{U_t} := U_{t+1} - \mathbb{E}[U_{t+1}|\mathbf{X}_{0:t}]$. The GER then becomes

$$2\text{Co}\mathbb{V}_*(\delta A_{U_t}, U_t) = -\mathbb{V}_*[\delta U_t], \quad (16)$$

which clearly portraits a relation between fluctuation $\mathbb{V}_*[\delta U_t]$ and the energy dissipation $\delta A_{U_t}$.

In Ornstein-Uhlenbeck (OU) processes described by the stochastic differential equation $\text{d}\mathbf{X}_t = -\mathbf{B}\mathbf{X}_t\text{d}t + \mathbf{\Gamma}\text{d}\mathbf{W}_t$ where $\mathbf{W}_t$ is the $n$-D Brownian motion, we have $\delta\mathbf{A}_t = -\mathbf{B}\mathbf{X}_t\text{d}t$ and $[\![\text{d}\mathbf{X}_t, \text{d}\mathbf{X}_t]\!]_* = 2\mathbf{D}\text{d}t$, where $\mathbf{D} = \mathbf{\Gamma}\mathbf{\Gamma}^{\mathsf{T}}/2$ is the diffusion matrix. Equation (15) then reduces to the Einstein relation for linear systems given by the Lyapunov matrix equation in Eq. (4) [12].

The GER in Eq. (15) is valid for any stationary processes. Conditions such as Markovian or detailed balance are not needed. It is a necessary condition for the stationarity of fluctuation and covariance. We note that the stationarity of $\mathbf{X}_t$ actually requires all of its cumulants to be fixed in time. Thus, any martingale, supermartingale, or submartingale will not satisfy the GER since a martingale has an ever-increasing variance and both supermartingale and submartingale have a monotonic drift.

### B. Green-Kubo formula

Equations (14b) and (15) further allow us to derive a general Green-Kubo formula (GKF) for a stationary processes [4,13,14]. We note that for $t \geqslant 0$, we have

$$[\![\delta\mathbf{A}_t, \delta\mathbf{A}_0]\!] = [\![\mathbf{X}_{t+1}, \delta\mathbf{A}_0]\!] - [\![\mathbf{X}_t, \delta\mathbf{A}_0]\!]. \quad (17)$$

Therefore,

$$\sum_{k=0}^{\infty}[\![\delta\mathbf{A}_k, \delta\mathbf{A}_0]\!] = [\![\mathbf{X}_\infty, \delta\mathbf{A}_0]\!] - [\![\mathbf{X}_0, \delta\mathbf{A}_0]\!]. \quad (18)$$

Assuming that $\mathbf{X}_t$ has a finite correlation time, the first term on the right-hand side is zero. Then, by applying Eq. (15) to the above equation, we get a general GKF that relates autocorrelation of the dissipative drift $\delta\mathbf{A}_t$ to the fluctuation of $\delta\mathbf{M}_t$ at steady state,

$$[\![\delta\mathbf{X}_t, \delta\mathbf{X}_t]\!]_* = \sum_{k=0}^{\infty}\left\{[\![\delta\mathbf{A}_k, \delta\mathbf{A}_0]\!]_* + [\![\delta\mathbf{A}_k, \delta\mathbf{A}_0]\!]_*^{\mathsf{T}}\right\}, \quad (19)$$

which becomes

$$[\![\delta\mathbf{M}_t, \delta\mathbf{M}_t]\!]_* = \sum_{k=-\infty}^{\infty}[\![\delta\mathbf{A}_k, \delta\mathbf{A}_0]\!]_* \quad (20)$$

by using Eq. (13) and stationarity. Equation (20) shows that the GKF is really a relation between the drift $\delta\mathbf{A}_t$ and the martingale increment $\delta\mathbf{M}_t$. The results for continuous time processes derived in the past [13,14] lost this important insight since the continuous time processes considered have $\delta\mathbf{A}_t = O(\mathrm{d}t)$ and $\delta\mathbf{M}_t = O(\sqrt{\mathrm{d}t})$, which makes the covariance of the drift higher order.

### C. Adjoint processes and adjoint drift

The Doob decomposition shown in Eq. (6) is with respect to the forward probability measure $\mathbb{P}$. In Markov processes with steady states, we can consider the Doob decomposition given by the adjoint probability measure $\mathbb{P}^\dagger$ (i.e., the decomposition in the adjoint process) where the transition probability is given by

$$\mathbb{P}^\dagger\{\mathbf{X}_{t+1} = \mathbf{y}|\mathbf{X}_t = \mathbf{x}\} = \frac{\pi(\mathbf{y})}{\pi(\mathbf{x})}\mathbb{P}\{\mathbf{X}_{t+1} = \mathbf{x}|\mathbf{X}_t = \mathbf{y}\}, \quad (21)$$

where $\pi$ is the invariant distribution. The adjont Doob decomposition is then

$$\delta\mathbf{X}_t = \delta\mathbf{A}_t^\dagger + \delta\mathbf{M}_t^\dagger, \quad (22)$$

with $\delta\mathbf{A}_t^\dagger := \mathbb{E}^\dagger[\mathbf{X}_{t+1}|\mathbf{X}_t] - \mathbf{X}_t$ and $\delta\mathbf{M}_t^\dagger := \mathbf{X}_{t+1} - \mathbb{E}^\dagger[\mathbf{X}_{t+1}|\mathbf{X}_t]$. Here, the conditional expectation in the adjoint process is done with the transition probability in Eq. (21):

$$\mathbb{E}^\dagger[\mathbf{X}_{t+1}|\mathbf{X}_t] = \sum_{\mathbf{y}}\mathbf{y}\mathbb{P}^\dagger\{\mathbf{X}_{t+1} = \mathbf{y}|\mathbf{X}_t\}. \quad (23)$$

The covariance between $\mathbf{X}_t$ and $\delta\mathbf{A}_t$ and the covariance between $\mathbf{X}_t$ and $\delta\mathbf{A}_t^\dagger$ are only subject to a transpose at steady state,

$$[\![\mathbf{X}_t, \delta\mathbf{A}_t]\!]_* = [\![\mathbf{X}_t, \delta\mathbf{A}_t^\dagger]\!]_*^{\mathsf{T}}. \quad (24)$$

This gives us a neater expression of the GER in Eq. (15),

$$[\![\mathbf{X}_t, \delta\mathbf{A}_t + \delta\mathbf{A}_t^\dagger]\!]_* = -[\![\delta\mathbf{X}_t, \delta\mathbf{X}_t]\!]_*. \quad (25)$$

This allows one to show that for reversible (detailed balanced) systems where the forward and the adjoint processes are the same, we have $\delta\mathbf{A}_t = \delta\mathbf{A}_t^\dagger$ and thus

$$[\![\mathbf{X}_t, \delta\mathbf{A}_t]\!]_* = -\tfrac{1}{2}[\![\delta\mathbf{X}_t, \delta\mathbf{X}_t]\!]_*, \quad (26)$$

telling us that the covariance matrix $[\![\mathbf{X}_t, \delta\mathbf{A}_t]\!]_*$ is symmetric and negative-definite. This gives yet another characterization of detailed balance and is the generalization of $\mathbf{B\Xi}$ being symmetric for reversible OU processes [12].

We note here that the GKF also have two sibling expressions in terms of the adjoint drift for continuous time Markov chain [13]:

$$[\![\delta\mathbf{X}_t, \delta\mathbf{X}_t]\!]_* = \sum_{k=0}^{\infty}[\![\delta\mathbf{A}_k, \delta\mathbf{A}_0^\dagger]\!]_* + [\![\delta\mathbf{A}_k, \delta\mathbf{A}_0^\dagger]\!]_*^{\mathsf{T}} \quad (27)$$

and

$$[\![\delta\mathbf{X}_t, \delta\mathbf{X}_t]\!]_* = \sum_{k=0}^{\infty}[\![\delta\mathbf{A}_k^\dagger, \delta\mathbf{A}_0^\dagger]\!]_* + [\![\delta\mathbf{A}_k^\dagger, \delta\mathbf{A}_0^\dagger]\!]_*^{\mathsf{T}}. \quad (28)$$

They can be derived from a similar approach.

### D. Continuous Markov processes

Here we consider a continuous Markov process (diffusion process) as another example. This gives the generalization to the results in OU processes [11,12] and establishes an interesting connection to the landscape cycle potentials theory in stochastic thermodynamics [19].

Before delving into continuous Markov processes, we first note that the covariance matrix between the system's state and its drift $[\![\mathbf{X}_t, \delta\mathbf{A}_t]\!]_*$, as an matrix, can always be decomposed to a symmetric part and an antisymmetric part:

$$[\![\mathbf{X}_t, \delta\mathbf{A}_t]\!]_* = [\text{symmetric}] + [\text{anti-symmetric}]. \quad (29)$$

Our discussion above tells us two things: (1) the symmetric part is related to the fluctuation of the process as shown by our GER in Eq. (15); (2) the antisymmetric part only exists in nonequilibrium systems, i.e., it characterizes the nonequilibrium driving force. We show here that this antisymmetric part as nonequilibrium driving force actually have been identified in diffusion [19].

A continuous process can be described either by stochastic differential equations,

$$\mathrm{d}\mathbf{X}_t = [\mathbf{b}(\mathbf{X}_t) + \nabla\cdot\mathbf{D}(\mathbf{X}_t)]\mathrm{d}t + \boldsymbol{\Gamma}(\mathbf{X}_t)\mathrm{d}\mathbf{W}_t, \quad (30)$$

where $\mathbf{D} = \boldsymbol{\Gamma}\boldsymbol{\Gamma}^{\mathsf{T}}/2$ is the diffusion matrix and $\mathbf{W}_t$ is the Brownian motion, or by the Fokker-Planck equation

$$\partial_t p(\mathbf{x}, t) = -\nabla\cdot[\mathbf{b}(\mathbf{x})p(\mathbf{x}, t) - \mathbf{D}(\mathbf{x})\nabla p(\mathbf{x}, t)]. \quad (31)$$

In an infinitesimal time step, the drift and noise are then $\delta\mathbf{A}_t = (\mathbf{b} + \nabla\cdot\mathbf{D})\mathrm{d}t$ and $\delta\mathbf{M}_t = \boldsymbol{\Gamma}\mathrm{d}\mathbf{W}_t$. Treating the Fokker-Planck equation as an equation for continuity equation for probability, the term $\mathbf{J}(\mathbf{x}, t) := \mathbf{b}p(\mathbf{x}, t) - \mathbf{D}\nabla p(\mathbf{x}, t)$ can be identified as the probability flux of the system. At the steady state, the system is described by the stationary probability density $\pi(\mathbf{x})$ and the probability flux $\mathbf{J}^*(\mathbf{x}) = \mathbf{b}(\mathbf{x})\pi(\mathbf{x}) - \mathbf{D}(\mathbf{x})\nabla\pi(\mathbf{x})$, which is divergence-free.

Using the divergence-free property, the bivector potential $\mathbf{A}(\mathbf{x})$ of the stationary probability flux can be identified by $\mathbf{J}^* = \nabla\times\mathbf{A}$ and can be understood as a cyclic probability flux [29]. Further, by defining the cyclic probability velocity $\mathbf{Q} :=$

$\mathbf{A}/\pi$ and the scalar potential landscape $\Phi(\mathbf{x}) := -\ln \pi(\mathbf{x})$, a general vector field decomposition

$$\mathbf{b} = -\mathbf{D}\nabla\Phi - \mathbf{Q}\nabla\Phi + \nabla \times \mathbf{Q} \tag{32}$$

can be derived [19]. Now, quantities defined on the bivectorial cycles in diffusion, e.g., $\mathbf{A}$ and $\mathbf{Q}$, are represented by antisymmetric matrices [29]. By using integration by part, $\mathbf{Q} = -\mathbf{Q}^\mathsf{T}$ and $\mathbf{D} = \mathbf{D}^\mathsf{T}$, the covariance $[\![\mathbf{X}_t, \delta\mathbf{A}_t]\!]_* = [\![\mathbf{X}_t, \mathbf{b} + \nabla\cdot\mathbf{D}]\!]_* \mathrm{d}t$ can be further rewritten as

$$[\![\mathbf{X}_t, \delta\mathbf{A}_t]\!]_* = \mathbb{E}_*[\mathbf{Q} - \mathbf{D}]\mathrm{d}t. \tag{33}$$

This shows that

$$[\![\mathbf{X}_t, \delta\mathbf{A}_t]\!]_* + [\![\mathbf{X}_t, \delta\mathbf{A}_t]\!]_*^\mathsf{T} = -2\mathbb{E}_*[\mathbf{D}]\mathrm{d}t, \tag{34}$$

which is exactly the continuous-time version of Eq. (19).

Note that Eq. (33) is exactly the diffusion version of the symmetric-antisymmetric decomposition of the covarariance matrix discussed above at Eq. (29). With $\mathbf{Q}$ understood as the cycle velocity in continuous processes [19,29], $\mathbb{E}_*[\mathbf{Q}]$ in fact characterizes the nonequilibrium driving force in the system. $\mathbf{Q} = \mathbf{0}$ corresponds to detailed balanced systems, implying that the covariance $[\![\mathbf{X}_t, \delta\mathbf{A}_t]\!]_*$ is a symmetric and negative-definite matrix in detailed balanced systems. This echoes the central result in stochastic thermodynamics: a dynamic object, such as the covariance between the system's state and its drift shown here, can be decomposed into its underlying equilibrium part and a nonequilibrium cyclic driving force part. Such decomposition fundamentally originates from the irreversibility decomposition of stochastic dynamics in stochastic thermodynamics, as summarized in Ref. [19].

Let us now remark on some practical values of the FDR we derived at Eq. (33). The vector field decomposition in Eq. (32) has shown us that a diffusion process has an equilibrium component $-\mathbf{D}\nabla\Phi$ and a cyclic component $-\mathbf{Q}\nabla\Phi + \nabla\times\mathbf{Q}$, with a scalar potential $\Phi$, a symmetric matrix potential $\mathbf{D}$, and an antisymmetric bivector potential $\mathbf{Q}$ [19]. However, it is challenging to get the functional form of $\mathbf{Q}$ analytically: one needs to solve $\mathbf{A}$ from $\mathbf{J}^* = \nabla\times\mathbf{A}$ and the invariant probability density $\pi$. The FDR of diffusion processes we derived here thus have at least two practical values. On the one hand, the covariance matrix $[\![\mathbf{X}_t, \delta\mathbf{A}_t]\!]_* = [\![\mathbf{X}_t, \mathbf{X}_{t+\mathrm{d}t} - \mathbf{X}_t]\!]_* \mathrm{d}t$ can be rather easily computed from trajectory data from experiments. The FDR shown in Eq. (33) thus gives us a practical way to compute the average $\mathbf{D}$ and average $\mathbf{Q}$ at the steady state from trajectory data. On the other hand, we know from our FDR that the process is nondetailed balanced if the $[\![\mathbf{X}_t, \delta\mathbf{A}_t]\!]_*$ is not symmetric. Compared to the standard probability flux calculation, this is a much simpler way to determine whether a process $\mathbf{X}_t$ is reversible or not. The level of the antisymmetric part $\mathbb{E}_*[\mathbf{Q}]$ further indicates how nonequilibrium the process is.

## IV. DISCUSSIONS

### A. Reversed decomposition

The Doob decomposition decomposes the dynamics $\delta\mathbf{X}_t$ into a drift part $\delta\mathbf{A}_t$ and a martingale part $\delta\mathbf{M}_t$. One of our key results is that the uncertainty of the dynamics has a resulting uncorrelated decomposition into the fluctuation of the past and the fluctuation of the 1-to-many mapping marching toward the future as shown in Eq. (13). Here, we show another decomposition that relates explicitly the fluctuation of the dynamics to the many-to-1 uncertainty in the dynamics.

We can decompose $\delta\mathbf{X}_t$ by conditioning on the state one step in the future,

$$\delta\mathbf{X}_t = \delta\mathbf{R}_t + \delta\mathbf{N}_t, \tag{35}$$

where

$$\delta\mathbf{R}_t = \mathbf{X}_{t+1} - \mathbb{E}[\mathbf{X}_t|\mathbf{X}_{t+1}] \tag{36a}$$

$$\delta\mathbf{N}_t = \mathbb{E}[\mathbf{X}_t|\mathbf{X}_{t+1}] - \mathbf{X}_t. \tag{36b}$$

This is also an uncorrelated decomposition, $[\![\delta\mathbf{R}_t, \delta\mathbf{N}_t]\!] = \mathbf{0}$, which leads us to another fluctuation decomposition,

$$[\![\delta\mathbf{X}_t, \delta\mathbf{X}_t]\!] = [\![\delta\mathbf{R}_t, \delta\mathbf{R}_t]\!] + [\![\delta\mathbf{N}_t, \delta\mathbf{N}_t]\!]. \tag{37}$$

$\delta\mathbf{R}_t$ can be thought of as the backward drift and $\delta\mathbf{N}_t$ is a quantification of the many-to-1 uncertainty in the dynamics. Therefore, Eq. (37) and Eq. (13) together link the many-to-1 uncertainty and 1-to-many uncertainty with forward and backward drift,

$$[\![\delta\mathbf{X}_t, \delta\mathbf{X}_t]\!] = [\![\delta\mathbf{A}_t, \delta\mathbf{A}_t]\!] + [\![\delta\mathbf{M}_t, \delta\mathbf{M}_t]\!] \tag{38a}$$

$$= [\![\delta\mathbf{R}_t, \delta\mathbf{R}_t]\!] + [\![\delta\mathbf{N}_t, \delta\mathbf{N}_t]\!]. \tag{38b}$$

For Markov processes, the backward drift becomes the adjoint drift at steady state $\delta\mathbf{R}_t = -\delta\mathbf{A}_t^\dagger$. In fact, the decomposition in Eq. (35) is actually from the Doob decomposition of the reversed process $\mathbf{Z}_t = \mathbf{X}_{-t}$. The past and the future is conditionally independent if conditioned on the present in Markov processes:

$$P_{\mathbf{X}_{0:t}|\mathbf{X}_{t+1:\infty}}(\mathbf{x}_{0:t}|\mathbf{x}_{t+1:\infty}) = P_{\mathbf{X}_{0:t}|\mathbf{X}_{t+1}}(\mathbf{x}_{0:t}|\mathbf{x}_{t+1}). \tag{39}$$

This means that the conditional expectation $\mathbb{E}[\mathbf{X}_t|\mathbf{X}_{t+1}]$ in Eq. (35) is the same as conditioning the whole future $\mathbb{E}[\mathbf{X}_t|\mathbf{X}_{t+1:\infty}]$. The decomposed process is thus

$$\mathbf{N}_t = \sum_{k=0}^{t-1} \delta\mathbf{N}_k = \sum_{k=0}^{t-1} (\mathbb{E}[\mathbf{X}_t|\mathbf{X}_{t+1:\infty}] - \mathbf{X}_t), \tag{40}$$

a *reversed martingale*, or called *backward martingale* in mathematics [15], for Markov processes.

### B. Exponential martingale and worklike observable

The GER discussed above is for general stationary processes. It, however, excludes any sweeping dynamics such as martingale, submartingale, and supermartingale. Here, we present that a specific type of submartingale in continuous processes actually have a fluctuation-drift relation. We consider a process $\mathcal{E}_t$ whose exponentiation $e^{-\mathcal{E}_t}$ becomes a martingale. Stochastic calculus tells us that the drift $\mu_t$ and the fluctuation level $\sigma_t$ in the stochastic differential equation of $\mathcal{E}_t$, $\mathrm{d}\mathcal{E}_t = \mu_t \mathrm{d}t + \sigma_t \mathrm{d}W_t$ is related by

$$2\mu_t = \sigma_t^2. \tag{41}$$

This shows that the process $\mathcal{E}_t$ is a submartingale and has a fluctuation-drift relation induced by the requirement of being a martingale after exponentiation. A famous example for $\mathcal{E}_t$ in stochastic thermodynamics is the housekeeping heat $\mathcal{Q}_{\mathrm{hk}}$ [26,27].

Here, we consider the process $\mathcal{E}_t$ is worklike if its infinitesimal difference $\mathrm{d}\mathcal{E}_t$ can be expressed as

$$\boldsymbol{f}(\mathbf{X}_t) \circ \mathrm{d}\mathbf{X}_t := \boldsymbol{f}\left(\mathbf{X}_t + \tfrac{1}{2}\mathrm{d}\mathbf{X}_t\right) \cdot \mathrm{d}\mathbf{X}_t \quad (42a)$$

$$= \boldsymbol{f}(\mathbf{X}_t) \cdot \mathrm{d}\mathbf{X}_t + \mathbf{D} \cdot (\nabla \boldsymbol{f})\mathrm{d}t, \quad (42b)$$

where the empty circle $\circ$ denotes Stratonovich midpoint integration (with an inner product involved) and the solid dot $\cdot$ denotes the standard inner product. The process $\mathcal{E}_t$ then satisfies a Cauchy-Schwarz inequality given the inner product $\langle \mathbf{u}, \mathbf{w} \rangle := \mathbb{E}[\mathbf{u} \cdot \mathbf{D}^{-1}\mathbf{w}]$,

$$\left(\mathbb{E}\left[\frac{\mathrm{d}\mathcal{E}_t}{\mathrm{d}t}\right]\right)^2 \leqslant \mathbb{E}\left[\frac{\mathrm{d}\mathcal{S}_{\mathrm{tot}}}{\mathrm{d}t}\right] \frac{\mathbb{V}[\mathrm{d}\mathcal{E}_t]}{2\mathrm{d}t}, \quad (43)$$

which is an instantaneous version of the recently-celebrated thermodynamic uncertainty relation [30,31]. The proof of this follows quite directly from Refs. [32,33]. A key step is to recognize that $\mathbb{V}[\mathrm{d}\mathcal{E}_t] = 2\mathbb{E}[\boldsymbol{f} \cdot \mathbf{D}\boldsymbol{f}]\mathrm{d}t$. Further, by Eq. (41) and time integration, one gets

$$\mathbb{E}[\mathcal{E}_t] \leqslant \mathbb{E}[\mathcal{S}_{\mathrm{tot}}]. \quad (44)$$

The total entropy production is the upper bound of any worklike $\mathcal{E}_t$ process. The force $\boldsymbol{f}$ should satisfy $\boldsymbol{f} \cdot \mathbf{D}\boldsymbol{f} = \mathbf{b} \cdot \boldsymbol{f} + \nabla \cdot (\mathbf{D}\boldsymbol{f})$ for a worklike process to be a martingale after exponentiation. Examples for such a process $\mathcal{E}_t$ include the housekeeping heat $\mathcal{Q}_{\mathrm{hk}}$ [26,27] and the heat dissipation $\mathcal{Q} := \mathbf{D}^{-1}\mathbf{b} \circ \mathrm{d}\mathbf{X}_t$ in diffusion processes if the vector field $\mathbf{b}$ is divergence-free.

### C. Summary

In this paper, we summarize and extend the Einstein relation and the Green-Kubo formula to nonequilibrium, nonlinear and non-Markovian systems in a covariance formalism. Two underlying components contributing to a stochastic change of a system's state were identified: a "deterministic" drift summarizing the past and a noise representing the stochasticity of one step toward the future. Stationarity of the process requires a dissipative drift to balance out the fluctuation generated by noise, which is the origin of our general fluctuation-dissipation relations. Reversibility and Markovian property are not needed but can impose a further symmetry in the covariance between the state and the drift. General relations between the fluctuation and the drift of sweeping dynamics remains to be investigated. Generally speaking, a symmetry is needed to dictate a fluctuation-drift relation.

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approach would need to consider the Doob-Meyer decomposition theorem for continuous time processes [34,35].

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