

Properties of the dissipation functions for passive and active systemsHarsh Soni *School of Physical Sciences, IIT Mandi, Kamand, Mandi, HP 175005, India*

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The dissipation function for a system is defined as the natural logarithm of the ratio between probabilities of a trajectory and its time-reversed trajectory, and its probability distribution follows a well-known relation called the fluctuation theorem. Using the generic Langevin equations, we derive the expressions of the dissipation function for passive and active systems. For passive systems, the dissipation function depends only on the initial and the final values of the dynamical variables of the system, not on the trajectory of the system. Furthermore, it does not depend explicitly on the reactive or dissipative coupling coefficients of the generic Langevin equations. In addition, we study a one-dimensional case numerically to verify the fluctuation theorem with the form of the dissipation function we obtained. For active systems, we define the work done by active forces along a trajectory. If the probability distribution of the dynamical variables is symmetric under time reversal, in both cases, the average rate of change of the dissipation function with trajectory duration is nothing but the average entropy production rate of the system and reservoir.

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Irreversibility of a system can be quantified by using the dissipation function which is defined as the natural logarithm of the ratio of the probability density of a trajectory to that of its time-reversed trajectory. The probability distribution function of the dissipation function exhibits an interesting symmetry relation known as the fluctuation theorem [1–3]. The fluctuation theorem has been substantially explored using theory [4–12] and experiment [13–19]. For stochastic processes, it has been investigated mainly for the single-particle or single-variable case [5,6,20]. Moreover, little attention has been paid to the systems described by the Langevin equations with multiplicative noise, except for a few studies [12,20].

This paper discusses the fluctuation relations for a wide class of systems described by the generic Langevin equations [21,22]. Assuming that the slow variables of a system vary much slower than its microscopic degrees of freedom, one can consider that the system is always in local thermodynamic equilibrium at temperature T . The dynamics of such systems is well-explained by the generic Langevin equations. We consider the active as well as passive systems. We use the path integral approach to calculate the probability density of a trajectory of the system with α -discretization [20,23,24].

Our main results are as follows. We first show that the generic Langevin equations describe a passive system, irrespective of the value of α . We then derive the expression of the dissipation function for passive systems relaxing toward thermodynamic equilibrium. Interestingly, the dissipation function is independent of the trajectory followed by the system; it only depends on the initial and the final values of the dynamical variables of the system. Moreover, it is not an explicit function of the coefficients appearing in the generic

Langevin equation. Using Brownian dynamics simulation, we also verify the fluctuation theorem for a one-dimensional (1D) single-particle problem with state-dependent diffusion. Finally, we construct an expression of the dissipation function for the active systems, and we define the work done by the active forces. For both active and passive systems, the average rate of change of the dissipation function with the time duration is the same as the rate of change of the entropy of the system and reservoir, assuming that the probability distribution of the dynamical variables is invariant under time reversal.

In Sec. II, we will discuss passive systems, and in Sec. III, we will explore active systems.

II. PASSIVE SYSTEMS

This section is arranged as follows. In the next Sec. II A, we summarize the generic Langevin equations. We then calculate the ratio of the probabilities of a trajectory and its time-reversed trajectory (see Sec. II B). In Sec. II C, fluctuation relations and the dissipation function for the passive systems are presented. In Sec. II D, we talk about the quenched systems, along with an example of a system of a single colloidal particle.

A. Generic Langevin equations

Here we consider a passive system relaxing toward equilibrium. Its macroscopic dynamics is described by a set of n number of slow variables $\mathbf{A} \equiv \{A_1, A_2, \dots, A_n\}$. Let $A_i \rightarrow s_i A_i$ under time reversal, where $s_i = 1$ and $s_i = -1$ if A_i is even and odd under time reversal, respectively; e.g., $s_i = 1$ for position and $s_i = -1$ for momentum. The generic Langevin equations for the system at temperature T can be written in

the following form [21,22]:

$$\frac{dA_i}{dt} = -\Gamma_{ij} \frac{\partial \mathcal{H}}{\partial A_j} + k_B T \frac{\partial \Gamma_{ij}}{\partial A_j} + \eta_i(t), \quad (1)$$

where \mathcal{H} is the coarse-grained or effective Hamiltonian of the system and the coefficients Γ_{ij} satisfy the following property:

$$\Gamma_{ij} = s_i s_j \Gamma_{ji}. \quad (2)$$

In Eq. (1), the terms with $s_i s_j = -1$ are the Poisson bracket or reactive terms, whereas the terms with $s_i s_j = 1$ are the dissipative terms [25]. The last term $\eta_i(t)$ represents the rapid fluctuations due to the dynamics of the microscopic degrees of freedom of the system. We assume that $\eta_i(t)$ is white Gaussian noise, and its autocorrelation function is given by

$$\langle \eta_i(t) \eta_j(t') \rangle = 2k_B T \Gamma_{ij}^s \delta(t - t'), \quad (3)$$

where $\Gamma_{ij}^s \equiv (\Gamma_{ij} + \Gamma_{ji})/2$ is the symmetric part of Γ_{ij} . From Eq. (2), Γ_{ij}^s shows the following symmetry property:

$$\Gamma_{ij}^s = s_i s_j \Gamma_{ij}^s. \quad (4)$$

Further, it is assumed to be invertible. Here in Eq. (1), we use Einstein notation, which will be carried through the rest of the paper, unless otherwise stated. Writing $\eta_i(t)$ as the linear combination of time series of the white Gaussian noise $\xi_j(t)$ having no correlation with each other, i.e., $\langle \xi_i(t) \xi_j(t') \rangle = \delta_{ij} \delta(t - t')$:

$$\eta_i(t) = N_{ij} \xi_j(t), \quad (5)$$

where, from Eq. (3), N_{ij} is given by the solution of the equations:

$$N_{ik} N_{jk} = 2k_B T \Gamma_{ij}^s. \quad (6)$$

Since N_{ik} must be real, Γ_{ij}^s must have positive eigenvalues [26]. As Γ_{ij}^s is considered to be invertible, N_{ik} is invertible as well. It should be noted that N_{jk} is not uniquely defined by the above equation. However, N_{jk} is just a dummy matrix which does not appear anywhere in the final results. Substituting (5) into Eq. (1):

$$\frac{dA_i}{dt} = -\Gamma_{ij} \frac{\partial \mathcal{H}}{\partial A_j} + k_B T \frac{\partial \Gamma_{ij}}{\partial A_j} + N_{ij} \xi_j(t). \quad (7)$$

The above stochastic equations have no ambiguity when N_{ij} does not depend explicitly on \mathbf{A} . However, N_{ij} is the function of \mathbf{A} for many systems; in such cases, the above equations are not well-defined unless their discrete scheme is specified. We here use α -discretization method to discretize the above equations [20,23,24], which leads to a drift of $\alpha N_{ij} \partial N_{ij} / \partial A_l$ to the value of A_i due to the noise term [24,27]. On the contrary, the noise terms in the generic Langevin equations represent the thermal fluctuations and do not contribute to the average dynamics of the slow variables. One can eliminate the noise-induced drift by adding a correction term $-\alpha N_{ij} \partial N_{ij} / \partial A_l$ to Eq. (7). Therefore, the generic Langevin equations can be completely described as follows:

$$\frac{dA_i}{dt} = -\Gamma_{ij} \frac{\partial \mathcal{H}}{\partial A_j} + k_B T \frac{\partial \Gamma_{ij}}{\partial A_j} - \alpha N_{ij} \frac{\partial N_{ij}}{\partial A_l} + N_{ij} \xi_j \quad (8)$$

$$\equiv \mathcal{F}_i + N_{ij} \xi_j, \quad (9)$$

with their discrete form

$$dA_i(l) = \epsilon \mathcal{F}_i(\bar{\mathbf{A}}_l^f) + \sqrt{\epsilon} N_{ij}(\bar{\mathbf{A}}_l^f) \xi_j^l, \quad (10)$$

where ϵ is the time step, $dA_i(l) \equiv A_i(\epsilon l) - A_i[\epsilon(l-1)]$, $\bar{\mathbf{A}}_l^f \equiv \alpha \mathbf{A}(\epsilon l) + (1-\alpha) \mathbf{A}[\epsilon(l-1)]$,

$$\mathcal{F}_i \equiv -\Gamma_{ij} \frac{\partial \mathcal{H}}{\partial A_j} + k_B T \frac{\partial \Gamma_{ij}}{\partial A_j} - \alpha N_{ij} \frac{\partial N_{ij}}{\partial A_l}, \quad (11)$$

and

$$\xi_j^l \equiv \frac{1}{\sqrt{\epsilon}} \int_{(l-1)\epsilon}^{l\epsilon} \xi_j(t) dt, \quad (12)$$

are the series of random numbers having normal distribution with standard deviation 1 and mean 0. The parameter α can take any ‘‘absolute constant’’ between 0 and 1; $\alpha = 0$ and $\alpha = 1/2$ cases are referred to as Itô and Stratonovich methods, respectively. As we have another parameter α in the problem now, one of the questions we ask here is, do different values of α correspond to different systems? If yes, do all the values of α belong to passive systems?

Based on the behavior under time reversal, dividing \mathcal{F}_i into the following three parts \mathcal{F}_i^s , \mathcal{F}_i^a , and \mathcal{F}_i^N :

$$\mathcal{F}_i^s(\mathbf{A}) = -\Gamma_{ij}^s \frac{\partial \mathcal{H}}{\partial A_j} + k_B T \frac{\partial \Gamma_{ij}^s}{\partial A_j}, \quad (13)$$

$$\mathcal{F}_i^a(\mathbf{A}) = -\Gamma_{ij}^a \frac{\partial \mathcal{H}}{\partial A_j} + k_B T \frac{\partial \Gamma_{ij}^a}{\partial A_j}, \quad (14)$$

$$\mathcal{F}_i^N = -\alpha N_{kj} \frac{\partial N_{ij}}{\partial A_k}, \quad (15)$$

where $\Gamma_{ij}^a \equiv (\Gamma_{ij} - \Gamma_{ji})/2$ is the antisymmetric part of Γ_{ij} . From Eq. (2), Γ_{ij}^a exhibits the following symmetry property (not in Einstein notation):

$$\Gamma_{ij}^a = -s_i s_j \Gamma_{ij}^a. \quad (16)$$

Since $\mathcal{H}(s \circ \mathbf{A}) = \mathcal{H}(\mathbf{A})$ and $\Gamma_{ij}^s(s \circ \mathbf{A}) = \Gamma_{ij}^s(\mathbf{A})$ [21], from Eqs. (4) and (16), under time reversal,

$$\mathcal{F}^s(\mathbf{A}) \rightarrow \mathcal{F}^s(s \circ \mathbf{A}) = s \circ \mathcal{F}^s(\mathbf{A}), \quad (17)$$

$$\mathcal{F}^a(\mathbf{A}) \rightarrow \mathcal{F}^a(s \circ \mathbf{A}) = -s \circ \mathcal{F}^a(\mathbf{A}), \quad (18)$$

where \circ stands for Hadamard product, i.e., $s \circ \mathbf{A} \equiv \{s_1 A_1, s_2 A_2, \dots, s_n A_n\}$. For given Γ_{ij}^s , $\mathcal{F}_i^s(\mathbf{A})$ and $\mathcal{F}_i^a(\mathbf{A})$ do not depend on N_{ij} . In general, \mathcal{F}_i^N does not follow any of the above time reversal symmetries.

B. The ratio between the probability densities of a trajectory and its time-reversed trajectory

Let $p_0(\mathbf{A})$ be the probability distribution function of \mathbf{A} at $t = 0$. In $\epsilon \rightarrow 0$ limit, the probability density of a trajectory of the system $(\mathbf{A}_0, \mathbf{A}_1, \mathbf{A}_2, \dots, \mathbf{A}_N)$ [here $\mathbf{A}_l \equiv \mathbf{A}(l\epsilon)$] between

$t = 0$ and $t = \tau \equiv N\epsilon$ is given by [12] (see Appendix A)

$$\begin{aligned}
 P \simeq & p_0(\mathbf{A}_0) \prod_{l=1}^N \left(\frac{(2k_B T)^{-1/2}}{(2\pi\epsilon)^{n/2}} \exp \left\{ -\frac{1}{4\epsilon k_B T} [dA_i(l) - \epsilon \mathcal{F}_i^s(\bar{\mathbf{A}}_l^f) - \epsilon \mathcal{F}_i^a(\bar{\mathbf{A}}_l^f)] (\Gamma^{s-1})_{ij}(\bar{\mathbf{A}}_l^f) [dA_j(l) - \epsilon \mathcal{F}_j^s(\bar{\mathbf{A}}_l^f) - \epsilon \mathcal{F}_j^a(\bar{\mathbf{A}}_l^f)] \right. \right. \\
 & \left. \left. - \alpha \left[(dA_i(l) - \epsilon \mathcal{F}_i^s(\bar{\mathbf{A}}_l^f) - \epsilon \mathcal{F}_i^a(\bar{\mathbf{A}}_l^f)) \left[(\Gamma^{s-1})_{ij} \frac{\partial \Gamma_{jk}^s}{\partial A_k} \right]_{\bar{\mathbf{A}}_l^f} + \epsilon \left[\frac{\partial \mathcal{F}_i^s}{\partial A_i} + \frac{\partial \mathcal{F}_i^a}{\partial A_i} \right]_{\bar{\mathbf{A}}_l^f} \right] \right\} \det(\Gamma^s(\bar{\mathbf{A}}_l^f))^{-1/2} \right. \\
 & \left. \times \exp \left\{ \alpha^2 \epsilon k_B T \left[\frac{\partial^2 \Gamma_{ij}^s}{\partial A_i \partial A_j} - \frac{\partial \Gamma_{ik}^s}{\partial A_k} (\Gamma^{s-1})_{ij} \frac{\partial \Gamma_{jp}^s}{\partial A_p} \right]_{\bar{\mathbf{A}}_l^f} \right\} \right). \quad (19)
 \end{aligned}$$

The $\epsilon^{3/2}$ - and higher-order terms have been neglected here. It is apparent from the above expression that, for given Γ_{ij}^s , P is independent of N_{ij} . So no statistical property of the system has a dependence upon the choice of N_{ik} . Therefore, as mentioned earlier, N_{ik} is merely a dummy matrix. The probability density P depends on α ; thus, the different values

of α correspond to different systems. Later in this subsection, we will see that Eq. (8) provides the dynamics of a passive system for any α . The time-reversed trajectory of the trajectory $(\mathbf{A}_0, \mathbf{A}_1, \mathbf{A}_2, \dots, \mathbf{A}_N)$ would be $(s \circ \mathbf{A}_N, s \circ \mathbf{A}_{N-1}, \dots, s \circ \mathbf{A}_1)$, so its probability density can be calculated by replacing A_i by $s \circ A_{N-i}$ in the above equation; that is, (see Appendix B)

$$\begin{aligned}
 P_r \simeq & \prod_{l=1}^N \left(\frac{(2k_B T)^{-1/2}}{(2\pi\epsilon)^{n/2}} \exp \left\{ -\frac{1}{4\epsilon k_B T} [-dA_i(l) - \epsilon \mathcal{F}_i^s(\bar{\mathbf{A}}_l^r) + \epsilon \mathcal{F}_i^a(\bar{\mathbf{A}}_l^r)] (\Gamma^{s-1})_{ij}(\bar{\mathbf{A}}_l^r) [-dA_j(l) - \epsilon \mathcal{F}_j^s(\bar{\mathbf{A}}_l^r) + \epsilon \mathcal{F}_j^a(\bar{\mathbf{A}}_l^r)] \right. \right. \\
 & \left. \left. - \alpha \left[(-dA_i(l) - \epsilon \mathcal{F}_i^s(\bar{\mathbf{A}}_l^r) + \epsilon \mathcal{F}_i^a(\bar{\mathbf{A}}_l^r)) \left[(\Gamma^{s-1})_{ij} \frac{\partial \Gamma_{jk}^s}{\partial A_k} \right]_{\bar{\mathbf{A}}_l^r} + \epsilon \left[\frac{\partial \mathcal{F}_i^s}{\partial A_i} - \frac{\partial \mathcal{F}_i^a}{\partial A_i} \right]_{\bar{\mathbf{A}}_l^r} \right] \right\} \det(\Gamma^s(\bar{\mathbf{A}}_l^r))^{-1/2} \right. \\
 & \left. \times \exp \left\{ \alpha^2 \epsilon k_B T \left[\frac{\partial^2 \Gamma_{ij}^s}{\partial A_i \partial A_j} - \frac{\partial \Gamma_{ik}^s}{\partial A_k} (\Gamma^{s-1})_{ij} \frac{\partial \Gamma_{jp}^s}{\partial A_p} \right]_{\bar{\mathbf{A}}_l^r} \right\} \right) p_0(s \circ \mathbf{A}_N). \quad (20)
 \end{aligned}$$

In $\epsilon \rightarrow 0$ limit, the ratio P/P_r takes the following form (see Appendix C4):

$$\frac{P}{P_r} = \frac{p_0(\mathbf{A}(0))}{p_0(s \circ \mathbf{A}(\tau))} \exp \left[-\frac{1}{k_B T} (\mathcal{H}(\mathbf{A}(\tau)) - \mathcal{H}(\mathbf{A}(0))) \right]. \quad (21)$$

In the stationary state, $p_0(\mathbf{A}) = \exp(-\mathcal{H}(\mathbf{A})/k_B T)/\mathcal{Z}$ (see Appendix H), the above equation then yields

$$P = P_r. \quad (22)$$

It implies that any system whose dynamics is given by Eq. (8) has the time reversal symmetry in its stationary state, regardless of the value of α . Hence, Eq. (8) describes a passive system for any value of α between 0 and 1.

C. Fluctuation relations and the dissipation function for the passive systems

One can readily show that [12] the dissipation function \mathcal{R}_τ for the trajectory $(\mathbf{A}_0, \mathbf{A}_1, \mathbf{A}_2, \dots, \mathbf{A}_N)$ defined as

$$\mathcal{R}_\tau = \ln \left(\frac{P}{P_r} \right) \quad (23)$$

satisfies the relation

$$\frac{\mathcal{P}(\mathcal{R}_\tau = X)}{\mathcal{P}(\mathcal{R}_\tau = -X)} = \exp(X), \quad (24)$$

where \mathcal{P} is the probability distribution of \mathcal{R}_τ . The above relation is known as the fluctuation theorem [2,5]. From

Eq. (21),

$$\mathcal{R}_\tau = \ln \frac{p_0(\mathbf{A}(0))}{p_0(s \circ \mathbf{A}(\tau))} - \frac{1}{k_B T} [\mathcal{H}(\mathbf{A}(\tau)) - \mathcal{H}(\mathbf{A}(0))]. \quad (25)$$

Intriguingly, \mathcal{R}_τ does not depend explicitly on Γ_{ij} . Moreover, it depends only the initial and final values of \mathbf{A} , not on the trajectory followed by \mathbf{A} . Note that the ratio P/P_r in Eq. (21) also has the same functional properties.

One can also define the dissipation function for the system as follows [1]:

$$\mathcal{R}'_\tau = \ln \frac{p(\mathbf{A}(0), \mathbf{A}(\tau); \tau)}{p(s \circ \mathbf{A}(\tau), s \circ \mathbf{A}(0); \tau)}, \quad (26)$$

where $p(\mathbf{A}(0), \mathbf{A}(\tau); \tau)$ is the net probability that the system goes from $\mathbf{A}(0)$ to $\mathbf{A}(\tau)$ in time τ :

$$p(\mathbf{A}(0), \mathbf{A}(\tau); \tau) = \sum P, \quad (27)$$

where the summation is performed over all the trajectories between $\mathbf{A}(0)$ and $\mathbf{A}(\tau)$. Since the ratio P/P_r is independent of the trajectory between $\mathbf{A}(0)$ and $\mathbf{A}(\tau)$, $\mathcal{R}'_\tau = \mathcal{R}_\tau$.

The integrated form of the relation (24) is

$$\langle \exp(-\mathcal{R}_\tau) \rangle = 1, \quad (28)$$

where angular bracket stands for the ensemble average. Using this relation, one can show that [5,28]

$$\langle \mathcal{R}_\tau \rangle \geq 0. \quad (29)$$

In equilibrium, $P = P_r$, thus $\langle \mathcal{R}_\tau \rangle = \mathcal{R}_\tau = 0$. So $\langle \mathcal{R}_\tau \rangle$ behaves like the change in the entropy of system and it can be used to evaluate that how far the system is from equilibrium. Since the solution of the Fokker-Planck equation corresponding to Eq. (8) does not depend on α , $\langle \mathcal{R}_\tau \rangle$ is constant in α (see Appendix I).

Generalizing the expression of the dissipation function given in Eq. (25) for the trajectories starting at arbitrary time t :

$$\mathcal{R}_\tau(t) = \ln \frac{p_t(\mathbf{A}(t))}{p_t(\mathbf{s} \circ \mathbf{A}(t + \tau))} - \frac{1}{k_B T} [\mathcal{H}(\mathbf{A}(t + \tau)) - \mathcal{H}(\mathbf{A}(t))]. \quad (30)$$

The instantaneous irreversibility can be evaluated by calculating $\mathcal{R}_\tau(t)$ in $\tau \rightarrow 0$ limit, that is,

$$\mathcal{R}_\tau(t) \simeq \dot{s}(t)\tau + \ln \frac{p_t(\mathbf{A}(t + \tau))}{p_t(\mathbf{s} \circ \mathbf{A}(t + \tau))}, \quad (31)$$

where

$$\dot{s}(t) = - \left. \frac{d}{dt'} \left(\ln p_t(\mathbf{A}(t')) + \frac{1}{k_B T} \mathcal{H}(\mathbf{A}(t')) \right) \right|_{t'=t}. \quad (32)$$

As discussed in Appendix E, $k_B \dot{s}(t)$ is nothing but the rate of change of total entropy of the system and the reservoir [see Eq. (E6)]. According to Eq. (31), the irreversible behavior of the system results from entropy production and from the asymmetric behavior of $p_t(\mathbf{A})$ under time reversal. If $p_t(\mathbf{s} \circ \mathbf{A}) \neq p_t(\mathbf{A})$, the system is instantaneously irreversible since

$$\mathcal{R}_0(t) = \ln \frac{p_t(\mathbf{A}(t))}{p_t(\mathbf{s} \circ \mathbf{A}(t))} \neq 0. \quad (33)$$

Since $\mathcal{H}(\mathbf{s} \circ \mathbf{A}) = \mathcal{H}(\mathbf{A})$, the equilibrium probability distribution $p_{\text{eq}}(\mathbf{A}) \equiv \exp(-\mathcal{H}(\mathbf{A})/k_B T)/\mathcal{Z}$ always follows the symmetry property $p_{\text{eq}}(\mathbf{s} \circ \mathbf{A}) = p_{\text{eq}}(\mathbf{A})$; it is a fundamental property of $p_{\text{eq}}(\mathbf{A})$. The nonzero value of $\langle \mathcal{R}_0(t) \rangle$ for an out-of-equilibrium system signifies that the system violates this symmetry. Note that $\langle \mathcal{R}_0(t) \rangle \geq 0$. An example of such systems is as follows: consider a colloidal particle moving with a nonzero average velocity \mathbf{v}_0 and having the probability distribution $p_0(\mathbf{v}) = C \exp(-(\mathbf{v} - \mathbf{v}_0)^2/2)$, at $t = 0$. Under time reversal $\mathbf{v} \rightarrow -\mathbf{v}$, so $\mathbf{s} = \{-1, -1, -1\}$. Hence, $p_0(\mathbf{s} \circ \mathbf{v}) \neq p_0(\mathbf{v})$.

For the $p_t(\mathbf{s} \circ \mathbf{A}) = p_t(\mathbf{A})$ case, $\mathcal{R}_0(t) = 0$, so from Eq. (31),

$$\dot{s}(t) = \lim_{\tau \rightarrow 0} \frac{\mathcal{R}_\tau(t)}{\tau}. \quad (34)$$

Thus, the average rate of change of $\mathcal{R}_\tau(t)$ with τ is the same as the rate of the total entropy production of the system and the reservoir; from Eq. (29), the second law of thermodynamics is evident, $\dot{s}(t) > 0$. In the next subsection, we discuss a broad class of passive systems with $p_t(\mathbf{s} \circ \mathbf{A}) = p_t(\mathbf{A})$.

The form of the dissipation function used by Seifert *et al.* [5] is briefly discussed in Appendix F.

D. The dissipation function for quenched systems

Here we consider that the system is initially in a thermodynamic equilibrium state and the state variables of the

system $\boldsymbol{\beta} \equiv \{\beta_1, \beta_2, \dots, \beta_n\}$ are abruptly changed at $t = 0$. Then the system will start evolving toward the equilibrium state corresponding to the modified values of $\boldsymbol{\beta}$. Writing the coarse-grained Hamiltonian of the system as the function of $\boldsymbol{\beta}$: $\mathcal{H} \equiv \mathcal{H}(\mathbf{A}; \boldsymbol{\beta})$. Let $\boldsymbol{\beta} = \boldsymbol{\beta}_I$ at $t = 0$ then

$$p_0(\mathbf{A}) = \frac{1}{\mathcal{Z}(\boldsymbol{\beta}_I)} \exp \left[-\frac{\mathcal{H}(\mathbf{A}; \boldsymbol{\beta}_I)}{k_B T} \right]. \quad (35)$$

From Eq. (25), for a quench from $\boldsymbol{\beta} = \boldsymbol{\beta}_I$ to $\boldsymbol{\beta} = \boldsymbol{\beta}_F$ at $t = 0$, the dissipation function for the system takes the following form:

$$\mathcal{R}_\tau = \frac{1}{k_B T} [\mathcal{H}(\mathbf{A}(0); \boldsymbol{\beta}_F) - \mathcal{H}(\mathbf{A}(0); \boldsymbol{\beta}_I) - (\mathcal{H}(\mathbf{A}(\tau); \boldsymbol{\beta}_F) - \mathcal{H}(\mathbf{A}(\tau); \boldsymbol{\beta}_I))]. \quad (36)$$

We will now discuss an example of quenched systems.

1. Colloidal particle in a harmonic potential well

Consider a colloidal particle trapped in a harmonic potential $U = k\mathbf{r}^2/2$, where k is the stiffness of the potential. Imagine that initially the particle is in thermodynamic equilibrium with $k = k_0$ and the value of k is instantaneously changed from k_0 to k_1 at $t = 0$ [15]. Ignoring the kinetic energy, the coarse-grained Hamiltonian for this system would be simply $\mathcal{H} = U$. Then, from Eq. (36), the dissipation function for a trajectory between $\mathbf{r} = \mathbf{r}_0$ and $\mathbf{r} = \mathbf{r}_\tau$ in time τ is given by

$$R_\tau = \frac{1}{2}(k_0 - k_1)(\mathbf{r}_\tau^2 - \mathbf{r}_0^2). \quad (37)$$

The above expression was derived by Carberry *et al.* [15,29] for spatially uniform diffusion constant. As we have considered the dependence of Γ_{ij} on \mathbf{A} in the derivation of \mathcal{R}_τ , the above expression of the dissipation function is more general; it is valid for the systems having state dependent diffusion as well. To verify our prediction, we numerically solve the Langevin equation for a colloidal particle with the diffusion coefficient varying with position. For simplicity, we consider the 1D case. From Eq. (8), the overdamped Langevin equation for the colloidal particle reads

$$\frac{dx}{dt} = -\frac{1}{k_B T} D(x) kx + (1 - \alpha) \frac{dD(x)}{dx} + \sqrt{2D(x)} \eta(t), \quad (38)$$

with its discrete form [see Eq. (10)]

$$x(t + dt) = x(t) - \frac{1}{k_B T} D(\bar{x}^f) k \bar{x}^f + (1 - \alpha) \left[\frac{dD(x)}{dx} \right]_{\bar{x}^f} + \sqrt{2D(\bar{x}^f) dt} \eta_t, \quad (39)$$

where $\bar{x}^f = \alpha x(t + dt) + (1 - \alpha)x(t)$ and $D(x)$ is the state-dependent diffusion. The above equation is a self-consistent equation of $x(t + dt)$ for given $x(t)$. There are many examples of the systems having state-dependent diffusion; e.g., a colloidal particle near a wall [23]. We here consider a hypothetical system having Gaussian profile of the diffusion coefficient:

$$D(x) = D_0 \exp \left(-\frac{x^2}{L^2} \right). \quad (40)$$

To obtain the trajectory of the particle, at each time step, we solve the Eq. (39) for $x(t + dt)$ with fixed point

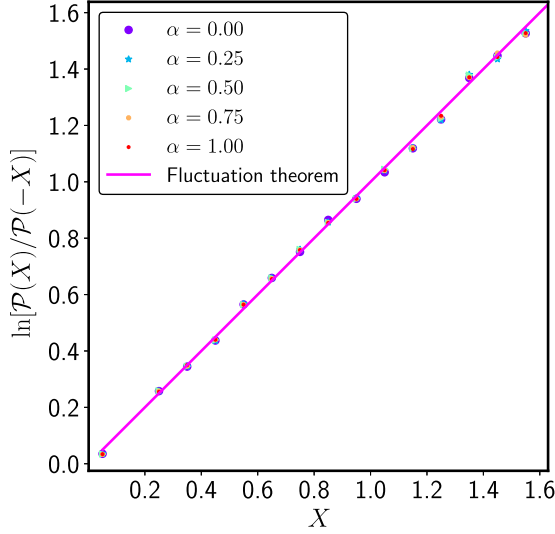


FIG. 1. $\ln[\mathcal{P}(X)/\mathcal{P}(-X)]$ vs X for a 1D colloidal particle in a potential well $U = kx^2/2$ with the diffusion coefficient $D(x) = D_0 \exp(-x^2/L^2)$, where \mathcal{P} is the probability distribution function for the dissipation function given by Eq. (37). The value of k is suddenly changed from $k = k_0$ to $k = k_1$ at $t = 0$. Here $L/\sqrt{k_1/k_B T} = 1$, $k_1/k_0 = 4$, the time duration of the trajectory $\tau = 3k_B T/D_0 k_1$, and 800 000 trajectories are used for the statistics.

iteration method with the accuracy of 10^{-4} . In Fig. 1, we show $\ln[\mathcal{P}(X)/\mathcal{P}(-X)]$ vs X : clearly, the dissipation function given by Eq. (37) obeys the fluctuation relation, for all the values of α .

III. THE DISSIPATION FUNCTION FOR ACTIVE SYSTEMS

In this section, we consider the active systems [30] whose dynamics is governed by the equations of motion having the following form:

$$\frac{dA_i}{dt} = \mathcal{F}_i + \mathcal{X}_i + N_{ij}\xi_j(t), \quad (41)$$

where the addition term \mathcal{X}_i represents the active driving forces. Due to the presence of the active forces, the active systems are always away from equilibrium. However, they can achieve a nonequilibrium steady state. Writing \mathcal{X}_i as the sum of two terms \mathcal{X}_i^s and \mathcal{X}_i^a such that $\mathcal{X}^s(s \circ \mathbf{A}) = s \circ \mathcal{X}^s(\mathbf{A})$ and $\mathcal{X}^a(s \circ \mathbf{A}) = -s \circ \mathcal{X}^a(\mathbf{A})$ [see Eqs. (G3) and (G4) in Appendix G]. It should be noted that N_{ij} serves as a dummy matrix here as well because the form of P will be the same as that in Eq. (19), except that \mathcal{F}_i^s and \mathcal{F}_i^a will have additional active components \mathcal{X}_i^s and \mathcal{X}_i^a , respectively. Following the approach used in Sec. II B, we obtain the following expression of the dissipation function:

$$\begin{aligned} \mathcal{R}_\tau(t) = \ln \frac{p_t(\mathbf{A}(t))}{p_t(s \circ \mathbf{A}(t + \tau))} - \frac{1}{k_B T} [\mathcal{H}(\mathbf{A}(t + \tau)) \\ - \mathcal{H}(\mathbf{A}(t))] + \frac{1}{k_B T} \int_t^{t+\tau} w(t') dt', \end{aligned} \quad (42)$$

where

$$\begin{aligned} w(t) = \frac{\partial \mathcal{H}(\mathbf{A}(t))}{\partial A_i} \mathcal{X}_i^a(\mathbf{A}(t)) - k_B T \frac{\partial \mathcal{X}_i^a(\mathbf{A}(t))}{\partial A_i} \\ + (\Gamma^{s-1})_{ij}(\mathbf{A}(t)) \mathcal{X}_j^s(\mathbf{A}(t)) \left[\frac{dA_i}{dt} - \mathcal{Y}_i^a(\mathbf{A}(t)) \right] \end{aligned} \quad (43)$$

and

$$\mathcal{Y}_i^a = \mathcal{X}_i^a + \frac{\partial \mathcal{H}}{\partial A_k} \Gamma_{ki}^a - k_B T \frac{\partial \Gamma_{ki}^a}{\partial A_k}. \quad (44)$$

The integration in Eq. (43) is performed using midpoint rule. In contrast to passive systems, $\mathcal{R}_\tau(t)$ here depends on Γ_{ij} , though not on α . Moreover, $\mathcal{R}_\tau(t)$ is trajectory-dependent, so $\langle \mathcal{R}_\tau(t) \rangle$ is a function of α because the probability density P of a trajectory depends on α [as in passive systems, see Eq. (19)]. The ensemble average of $w(t)$ is given by (with an assumption, see Appendix G)

$$\begin{aligned} \langle w(t) \rangle = \left\langle \left(\frac{dA_i}{dt} - \frac{\partial \mathcal{H}}{\partial A_k} \Gamma_{ki}^a + k_B T \frac{\partial \Gamma_{ki}^a}{\partial A_k} \right) (\Gamma^{s-1})_{ij} \mathcal{X}_j^s \right\rangle \\ - \left\langle \left(\frac{dA_i}{dt} - \mathcal{Y}_i^a \right) (\Gamma^{s-1})_{ij} \mathcal{X}_j^a \right\rangle, \end{aligned} \quad (45)$$

where the first term is the average rate of work done by active force $(\Gamma^{s-1})_{ij} \mathcal{X}_j^s$ and the second term is by the active force $(\Gamma^{s-1})_{ij} \mathcal{X}_j^a$. So $w(t)$ can be interpreted as the rate of work done by active forces along the trajectory at time t . For $p_t(s \circ \mathbf{A}) = p_t(\mathbf{A})$, the rate of change of dissipation function with τ [see Eqs. (34) and (42)] is given by

$$\dot{s}(t) = \frac{1}{k_B T} w(t) - \frac{d}{dt'} \left(\ln p_t(\mathbf{A}(t')) + \frac{1}{k_B T} \mathcal{H}(\mathbf{A}(t')) \right) \Big|_{t'=t}, \quad (46)$$

and its average reads (see Appendix G)

$$\begin{aligned} \langle \dot{s}(t) \rangle = \frac{1}{k_B T} \left\langle \left(\frac{J_i(\mathbf{A}, t)}{p_t(\mathbf{A})} - \mathcal{Y}_i^a(\mathbf{A}) \right) (\Gamma^{s-1})_{ij}(\mathbf{A}) \right. \\ \left. \times \left(\frac{J_j(\mathbf{A}, t)}{p_t(\mathbf{A})} - \mathcal{Y}_j^a(\mathbf{A}) \right) \right\rangle, \end{aligned} \quad (47)$$

where $J_i(\mathbf{A}, t)$ is the probability current for \mathbf{A} [23]:

$$\begin{aligned} J_i(\mathbf{A}, t) = \left(-\Gamma_{ij}^s(\mathbf{A}) \frac{\partial \mathcal{H}(\mathbf{A})}{\partial A_j} + \mathcal{Y}_i^a(\mathbf{A}) + \mathcal{X}_i^s(\mathbf{A}) \right) p_t(\mathbf{A}) \\ - k_B T \Gamma_{ij}^s(\mathbf{A}) \frac{\partial p_t(\mathbf{A})}{\partial A_j}. \end{aligned} \quad (48)$$

Using Eq. (6), it is easy to show that $\langle \dot{s}(t) \rangle > 0$, as expected from the integrated fluctuation theorem (28). Again, $k_B \langle \dot{s}(t) \rangle$ is nothing but the rate of the total entropy production of the system and the reservoir (see Appendix E).

As discussed for the passive systems in Sec. II C, for $p_t(s \circ \mathbf{A}) \neq p_t(\mathbf{A})$ case, time reversal asymmetry in $p_t(\mathbf{A})$ also contributes to irreversibility. This contribution can also be observed in the stationary states of many active systems. Active systems with polar alignment [31–34] are examples of this type of system; as the velocities of the particles are globally aligned, the velocity distribution is not an even function for these systems. The passive systems, being in equilibrium in their stationary states, cannot demonstrate this irreversibility.

A few special cases for the active systems are as follows: (a) If initially the system is in equilibrium (that is, $\mathcal{X}_i = 0$) and the active term \mathcal{X}_i is switched on at $t = 0$, then $p_0(\mathbf{A}) = \exp(-\mathcal{H}(\mathbf{A})/k_B T)/\mathcal{Z}$. In this case, \mathcal{R}_τ is just the net work

done by the active forces during the trajectory [see Eq. (42)]:

$$\mathcal{R}_\tau = \frac{1}{k_B T} \int_0^\tau w(t') dt'. \quad (49)$$

(b) In the stationary state (i.e., in $t \rightarrow \infty$ limit), the time averaged work done by the active forces,

$$w_{\text{av}} = \lim_{\tau \rightarrow \infty} \frac{1}{\tau} \int_t^{t+\tau} dt' w(t'), \quad (50)$$

is independent of t . So, in $\tau \rightarrow \infty$ limit, in Eq. (42), the last term is proportional to τ and we can ignore the first two terms. Then,

$$\mathcal{R}_\tau \simeq \frac{1}{k_B T} \int_t^{t+\tau} w(t') dt' \quad (51)$$

$$\simeq \frac{1}{k_B T} w_{\text{av}} \tau. \quad (52)$$

From Eq. (24), the probability distribution $\mathcal{P}_w(w_{\text{av}})$ of w_{av} satisfies the relation

$$X = \lim_{\tau \rightarrow \infty} k_B T \frac{1}{\tau} \ln \frac{\mathcal{P}_w(w_{\text{av}} = X)}{\mathcal{P}_w(w_{\text{av}} = -X)}. \quad (53)$$

This is called the steady-state fluctuation theorem [28].

IV. CONCLUSION

Starting with the generic Langevin equations, using path integral approach, we first calculated the ratio of the probability densities of a trajectory and its time-reversed trajectory for passive systems using α -discretization: it is independent of the value of α . Irrespective of the value of α , the stationary solutions of generic Langevin equations have time reversal symmetry, so the generic Langevin equations with any value of α describes a passive system. Next we calculated the dissipation function for the passive systems which is found to be independent of the trajectory of the system, it depends only on the initial and the final values of the dynamical variables of the system. Furthermore, it is not an explicit function of coefficients of the generic Langevin equations. We also verify the fluctuation theorem for a 1D particle trapped in a potential well whose stiffness is suddenly changed, with the state-dependent diffusion. Finally, we obtained the expression of the dissipation function for active systems and defined the work done by the active forces. For both passive and active systems, the average of the rate of change of dissipation function with the duration of the trajectory is just the entropy production rate of the system and the reservoir.

APPENDIX A: THE PROBABILITY DENSITY OF A TRAJECTORY FOR PASSIVE SYSTEMS

The generic Langevin equations for passive systems in discrete form [see Eq. (10)]:

$$dA_i(l) = \epsilon \mathcal{F}_i(\bar{\mathbf{A}}_l^f) + \sqrt{\epsilon} N_{ij}(\bar{\mathbf{A}}_l^f) \xi_j^l, \quad (A1)$$

where $dA_i(l) \equiv A_i(\epsilon l) - A_i(\epsilon(l-1))$, $\bar{\mathbf{A}}_l^f \equiv \alpha \mathbf{A}(\epsilon l) + (1-\alpha) \mathbf{A}(\epsilon(l-1))$, and

$$\mathcal{F}_i \equiv -\Gamma_{ij} \frac{\partial \mathcal{H}}{\partial A_j} + k_B T \frac{\partial \Gamma_{ij}}{\partial A_j} - \alpha N_{ij} \frac{\partial N_{ij}}{\partial A_i}. \quad (A2)$$

Solving the above equations for ξ_i^l , we obtain

$$\xi_i^l = \frac{1}{\sqrt{\epsilon}} (N^{-1})_{ij}(\bar{\mathbf{A}}_l^f) (dA_j(l) - \epsilon \mathcal{F}_j(\bar{\mathbf{A}}_l^f)). \quad (A3)$$

Since ξ_i^l are the uncorrelated series of random numbers having normal distribution with zero mean and variance one, the probability density function of a trajectory of the system ($\mathbf{A}_0, \mathbf{A}_1, \mathbf{A}_2, \dots, \mathbf{A}_N$) [here $\mathbf{A}_l \equiv \mathbf{A}(l\epsilon)$] between $t = 0$ and $t = \tau \equiv N\epsilon$ is given by [12]

$$P = p_0(\mathbf{A}_0) |\mathcal{J}| \prod_{l=1}^N \frac{1}{(2\pi)^{n/2}} \exp \left[-\frac{1}{2\epsilon} [dA_i(l) - \epsilon \mathcal{F}_i(\bar{\mathbf{A}}_l^f)] (N^{-1})_{ki}(\bar{\mathbf{A}}_l^f) (N^{-1})_{kj}(\bar{\mathbf{A}}_l^f) [dA_j(l) - \epsilon \mathcal{F}_j(\bar{\mathbf{A}}_l^f)] \right], \quad (A4)$$

where $p_0(\mathbf{A})$ is the probability distribution of \mathbf{A} at $t = 0$ and \mathcal{J} is the Jacobean determinant for the transformation of the variables of the probability density function from the ξ_i^l to $A_j(\epsilon m)$. From Eq. (A3), the $Nn \times Nn$ Jacobean matrix for the variable transformation is given by

$$\begin{aligned} \mathcal{J}_{jm}^{il} &= \frac{\partial \xi_i^l}{\partial A_j(\epsilon m)} \\ &= \frac{1}{\epsilon^{1/2}} \left[\left[\frac{\partial (N^{-1})_{ik}}{\partial A_j} \right]_{\bar{\mathbf{A}}_l^f} dA_k(l) - \epsilon \left[\frac{\partial (N^{-1})_{ik}}{\partial A_j} \mathcal{F}_k + \frac{\partial \mathcal{F}_k}{\partial A_j} (N^{-1})_{ik} \right]_{\bar{\mathbf{A}}_l^f} \right] (\alpha \delta_{lm} + (1-\alpha) \delta_{(l-1)m}) + (N^{-1})_{ij}(\bar{\mathbf{A}}_l^f) (\delta_{lm} - \delta_{(l-1)m}) \\ &= \frac{1}{\epsilon^{1/2}} \left[\left[\frac{\partial (N^{-1})_{ik}}{\partial A_j} \right]_{\bar{\mathbf{A}}_l^f} (dA_k(l) - \epsilon \mathcal{F}_k(\bar{\mathbf{A}}_l^f)) - \epsilon \left[\frac{\partial \mathcal{F}_k}{\partial A_j} (N^{-1})_{ik} \right]_{\bar{\mathbf{A}}_l^f} \right] (\alpha \delta_{lm} + (1-\alpha) \delta_{(l-1)m}) + (N^{-1})_{ij}(\bar{\mathbf{A}}_l^f) (\delta_{lm} - \delta_{(l-1)m}). \end{aligned} \quad (A5)$$

The above matrix is a block triangular matrix of $n \times n$ submatrices with fixed (l, m) , so its determinant will be the multiplication of all the diagonal submatrices (i.e., with $l = m$):

$$\mathcal{J} = \prod_{l=1}^N \frac{1}{\epsilon^{n/2}} \det(\mathbf{M}(l)), \quad (\text{A6})$$

where

$$\begin{aligned} M_{ij}(l) &= (N^{-1})_{ij}(\bar{\mathbf{A}}_l^f) + \alpha \left[\frac{\partial(N^{-1})_{ik}}{\partial A_j} \right]_{\bar{\mathbf{A}}_l^f} (dA_k(l) - \epsilon \mathcal{F}_k(\bar{\mathbf{A}}_l^f)) - \epsilon \alpha \left[\frac{\partial \mathcal{F}_k}{\partial A_j} (N^{-1})_{ik} \right]_{\bar{\mathbf{A}}_l^f} \\ &= (N^{-1})_{ip}(\bar{\mathbf{A}}_l^f) \left[\delta_{pj} + \alpha \left[N_{pq} \frac{\partial(N^{-1})_{qk}}{\partial A_j} \right]_{\bar{\mathbf{A}}_l^f} (dA_k(l) - \epsilon \mathcal{F}_k(\bar{\mathbf{A}}_l^f)) - \alpha \epsilon \left[\frac{\partial \mathcal{F}_p}{\partial A_j} \right]_{\bar{\mathbf{A}}_l^f} \right]. \end{aligned} \quad (\text{A7})$$

Using the power series expression of $\ln(\det(\mathbf{I} + \delta \mathbf{B}))$ for any matrix \mathbf{B} in $\delta \rightarrow 0$ limit (such that $\|\delta \mathbf{B}\| < 1$), that is,

$$\ln(\det(\mathbf{I} + \delta \mathbf{B})) = [\text{Tr}[\mathbf{B}]\delta - \frac{1}{2}\text{Tr}[\mathbf{B} \cdot \mathbf{B}]\delta^2 + \mathcal{O}(\delta^3)], \quad (\text{A8})$$

the determinant of $\mathbf{M}(l)$ can be written as

$$\begin{aligned} \det(\mathbf{M}(l)) &= \det(N^{-1}(\bar{\mathbf{A}}_l^f)) \exp \left[\alpha \left[\left[N_{jq} \frac{\partial(N^{-1})_{qk}}{\partial A_j} \right]_{\bar{\mathbf{A}}_l^f} (dA_k(l) - \epsilon \mathcal{F}_k(\bar{\mathbf{A}}_l^f)) - \epsilon \left[\frac{\partial \mathcal{F}_j}{\partial A_j} \right]_{\bar{\mathbf{A}}_l^f} \right] \right. \\ &\quad \left. - \frac{1}{2} \alpha^2 \left[N_{pq} \frac{\partial(N^{-1})_{qk}}{\partial A_j} N_{jr} \frac{\partial(N^{-1})_{ri}}{\partial A_p} \right]_{\bar{\mathbf{A}}_l^f} dA_k(l) dA_i(l) + \mathcal{O}(\epsilon^{3/2}) \right], \\ &= \det(N^{-1}(\bar{\mathbf{A}}_l^f)) \exp \left[-\alpha \left[\left[(N^{-1})_{qk} \frac{\partial N_{jq}}{\partial A_j} \right]_{\bar{\mathbf{A}}_l^f} (dA_k(l) - \epsilon \mathcal{F}_k(\bar{\mathbf{A}}_l^f)) + \epsilon \left[\frac{\partial \mathcal{F}_j}{\partial A_j} \right]_{\bar{\mathbf{A}}_l^f} \right] - \frac{1}{2} \alpha^2 \epsilon \left[\frac{\partial N_{pm}}{\partial A_j} \frac{\partial N_{jm}}{\partial A_p} \right]_{\bar{\mathbf{A}}_l^f} + \mathcal{O}(\epsilon^{3/2}) \right]. \end{aligned} \quad (\text{A9})$$

Note that $dA_k(l)$ has a $\epsilon^{1/2}$ -term, so $dA_i(l)dA_k(l)$ is of the order of ϵ . Relations (D1) and (D6) (see Appendix D) have been used to get the last term of the above equation. Equation (A7) then reads

$$\begin{aligned} \mathcal{J} &= \prod_{l=1}^N \frac{1}{\epsilon^{n/2}} \det(N^{-1}(\bar{\mathbf{A}}_l^f)) \exp \left[-\alpha \left[\left[(N^{-1})_{qk} \frac{\partial N_{jq}}{\partial A_j} \right]_{\bar{\mathbf{A}}_l^f} (dA_k(l) - \epsilon \mathcal{F}_k(\bar{\mathbf{A}}_l^f)) + \epsilon \left[\frac{\partial \mathcal{F}_j}{\partial A_j} \right]_{\bar{\mathbf{A}}_l^f} \right] \right. \\ &\quad \left. - \frac{1}{2} \alpha^2 \epsilon \left[\frac{\partial N_{pm}}{\partial A_j} \frac{\partial N_{jm}}{\partial A_p} \right]_{\bar{\mathbf{A}}_l^f} + \mathcal{O}(\epsilon^{3/2}) \right]. \end{aligned} \quad (\text{A10})$$

Substituting the above expression of \mathcal{J} into Eq.(A4):

$$\begin{aligned} P &= p_0(\mathbf{A}_0) \prod_{l=1}^N \left\{ \frac{1}{(2\pi\epsilon)^{n/2}} |\det(N^{-1}(\bar{\mathbf{A}}_l^f))| \exp \left[-\frac{1}{2\epsilon} [dA_i(l) - \epsilon \mathcal{F}_i(\bar{\mathbf{A}}_l^f)] (N^{-1})_{ki}(\bar{\mathbf{A}}_l^f) (N^{-1})_{kj}(\bar{\mathbf{A}}_l^f) [dA_j(l) - \epsilon \mathcal{F}_j(\bar{\mathbf{A}}_l^f)] \right] \right. \\ &\quad \left. \times \exp \left[-\alpha \left[(dA_i(l) - \epsilon \mathcal{F}_i(\bar{\mathbf{A}}_l^f)) \left[(N^{-1})_{ji} \frac{\partial N_{kj}}{\partial A_k} \right]_{\bar{\mathbf{A}}_l^f} + \epsilon \left[\frac{\partial \mathcal{F}_i}{\partial A_i} \right]_{\bar{\mathbf{A}}_l^f} \right] - \frac{1}{2} \alpha^2 \epsilon \left[\frac{\partial N_{pm}}{\partial A_j} \frac{\partial N_{jm}}{\partial A_p} \right]_{\bar{\mathbf{A}}_l^f} + \mathcal{O}(\epsilon^{3/2}) \right] \right\}. \end{aligned} \quad (\text{A11})$$

From Eq. (2), $(N^{-1})_{ki}(N^{-1})_{kj} = (\Gamma^{s-1})_{ij}/2k_B T$, so

$$\begin{aligned} P &= p_0(\mathbf{A}_0) \prod_{l=1}^N \left\{ \frac{(2k_B T)^{-1/2}}{(2\pi\epsilon)^{n/2}} \det(\Gamma^s(\bar{\mathbf{A}}_l^f))^{-1/2} \exp \left[-\frac{1}{4\epsilon k_B T} [dA_i(l) - \epsilon \mathcal{F}_i(\bar{\mathbf{A}}_l^f)] (\Gamma^{s-1})_{ij}(\bar{\mathbf{A}}_l^f) [dA_j(l) - \epsilon \mathcal{F}_j(\bar{\mathbf{A}}_l^f)] \right] \right. \\ &\quad \left. \times \exp \left[-\alpha \left[(dA_i(l) - \epsilon \mathcal{F}_i(\bar{\mathbf{A}}_l^f)) \left[(N^{-1})_{ji} \frac{\partial N_{kj}}{\partial A_k} \right]_{\bar{\mathbf{A}}_l^f} + \epsilon \left[\frac{\partial \mathcal{F}_i}{\partial A_i} \right]_{\bar{\mathbf{A}}_l^f} \right] - \frac{1}{2} \alpha^2 \epsilon \left[\frac{\partial N_{pm}}{\partial A_j} \frac{\partial N_{jm}}{\partial A_p} \right]_{\bar{\mathbf{A}}_l^f} + \mathcal{O}(\epsilon^{3/2}) \right] \right\}. \end{aligned} \quad (\text{A12})$$

Now let us break \mathcal{F}_i into two terms,

$$\mathcal{F}_i^0 = -\Gamma_{ij} \frac{\partial \mathcal{H}}{\partial A_j} + k_B T \frac{\partial \Gamma_{ij}}{\partial A_j} \quad (\text{A13})$$

and

$$\mathcal{F}_i^N = -\alpha N_{ij} \frac{\partial N_{ij}}{\partial A_i}. \quad (\text{A14})$$

Replacing \mathcal{F}_i by $\mathcal{F}_i^0 + \mathcal{F}_i^N$ in Eq. (A12):

$$\begin{aligned}
P = p_0(\mathbf{A}_0) \prod_{l=1}^N & \left\{ \frac{(2k_B T)^{-1/2}}{(2\pi\epsilon)^{n/2}} \det(\mathbf{\Gamma}^s(\bar{\mathbf{A}}_l^f))^{-1/2} \exp \left[-\frac{1}{4\epsilon k_B T} [dA_i(l) - \epsilon \mathcal{F}_i^0(\bar{\mathbf{A}}_l^f)] (\mathbf{\Gamma}^{s-1})_{ij}(\bar{\mathbf{A}}_l^f) [dA_j(l) - \epsilon \mathcal{F}_j^0(\bar{\mathbf{A}}_l^f)] \right] \right. \\
& \times \exp \left[-\alpha \left[(dA_i(l) - \epsilon \mathcal{F}_i^0(\bar{\mathbf{A}}_l^f)) \left[(N^{-1})_{ji} \frac{\partial N_{kj}}{\partial A_k} \right]_{\bar{\mathbf{A}}_l^f} + \epsilon \left[\frac{\partial \mathcal{F}_i^0}{\partial A_i} \right]_{\bar{\mathbf{A}}_l^f} \right] \right] \\
& \times \exp \left[\frac{1}{2k_B T} \mathcal{F}_i^N(\bar{\mathbf{A}}_l^f) (\mathbf{\Gamma}^{s-1})_{ij}(\bar{\mathbf{A}}_l^f) [dA_j(l) - \epsilon \mathcal{F}_j^0(\bar{\mathbf{A}}_l^f)] - \frac{\epsilon}{4k_B T} [\mathcal{F}_i^N (\mathbf{\Gamma}^{s-1})_{ij} \mathcal{F}_j^N]_{\bar{\mathbf{A}}_l^f} \right] \\
& \left. \times \exp \left[\alpha \epsilon \left[\mathcal{F}_i^N (N^{-1})_{ji} \frac{\partial N_{kj}}{\partial A_k} - \frac{\partial \mathcal{F}_i^N}{\partial A_i} \right]_{\bar{\mathbf{A}}_l^f} - \frac{1}{2} \alpha^2 \epsilon \left[\frac{\partial N_{pm}}{\partial A_j} \frac{\partial N_{jm}}{\partial A_p} \right]_{\bar{\mathbf{A}}_l^f} + \mathcal{O}(\epsilon^{3/2}) \right] \right\}. \quad (\text{A15})
\end{aligned}$$

Using Eq. (6) (that is, $N_{ik}N_{jk} = 2k_B T \Gamma_{ij}^s$), one can write

$$\begin{aligned}
(N^{-1})_{ji} \frac{\partial N_{kj}}{\partial A_k} &= \delta_{im} (N^{-1})_{jm} \frac{\partial N_{kj}}{\partial A_k} \\
&= (\mathbf{\Gamma}^{s-1})_{ip} \mathbf{\Gamma}_{pm}^s (N^{-1})_{jm} \frac{\partial N_{kj}}{\partial A_k} \\
&= \frac{1}{2k_B T} (\mathbf{\Gamma}^{s-1})_{ip} N_{pj} \frac{\partial N_{kj}}{\partial A_k} \\
&= \frac{1}{2k_B T} (\mathbf{\Gamma}^{s-1})_{ip} \left(\frac{\partial (N_{kj} N_{pj})}{\partial A_k} - N_{kj} \frac{\partial N_{pj}}{\partial A_k} \right) \\
&= (\mathbf{\Gamma}^{s-1})_{ip} \frac{\partial \mathbf{\Gamma}_{pk}^s}{\partial A_k} + \frac{1}{2k_B T \alpha} (\mathbf{\Gamma}^{s-1})_{ip} \mathcal{F}_p^N. \quad (\text{A16})
\end{aligned}$$

With the above expression, Eq. (A15) reduces to

$$\begin{aligned}
P = p_0(\mathbf{A}_0) \prod_{l=1}^N & \left\{ \frac{(2k_B T)^{-1/2}}{(2\pi\epsilon)^{n/2}} \det(\mathbf{\Gamma}^s(\bar{\mathbf{A}}_l^f))^{-1/2} \exp \left[-\frac{1}{4\epsilon k_B T} [dA_i(l) - \epsilon \mathcal{F}_i^0(\bar{\mathbf{A}}_l^f)] (\mathbf{\Gamma}^{s-1})_{ij}(\bar{\mathbf{A}}_l^f) [dA_j(l) - \epsilon \mathcal{F}_j^0(\bar{\mathbf{A}}_l^f)] \right] \right. \\
& - \alpha \left[(dA_i(l) - \epsilon \mathcal{F}_i^0(\bar{\mathbf{A}}_l^f)) \left[(\mathbf{\Gamma}^{s-1})_{ij} \frac{\partial \mathbf{\Gamma}_{jk}^s}{\partial A_k} \right]_{\bar{\mathbf{A}}_l^f} + \epsilon \left[\frac{\partial \mathcal{F}_i^0}{\partial A_i} \right]_{\bar{\mathbf{A}}_l^f} \right] \\
& \left. \times \exp \left[\frac{\epsilon}{4k_B T} \left[\mathcal{F}_i^N (\mathbf{\Gamma}^{s-1})_{ij} \left(\mathcal{F}_j^N + 4\alpha k_B T \frac{\partial \mathbf{\Gamma}_{jk}^s}{\partial A_k} \right) - 4\alpha k_B T \frac{\partial \mathcal{F}_i^N}{\partial A_i} - 2k_B T \alpha^2 \frac{\partial N_{pm}}{\partial A_j} \frac{\partial N_{jm}}{\partial A_p} \right]_{\bar{\mathbf{A}}_l^f} + \mathcal{O}(\epsilon^{3/2}) \right] \right\}. \quad (\text{A17})
\end{aligned}$$

Using the relation $N_{ik}N_{jk} = 2k_B T \Gamma_{ij}^s$, further simplifying the last term of the above equation yields

$$\begin{aligned}
P = p_0(\mathbf{A}_0) \prod_{l=1}^N & \left\{ \frac{(2k_B T)^{-1/2}}{(2\pi\epsilon)^{n/2}} \det(\mathbf{\Gamma}^s(\bar{\mathbf{A}}_l^f))^{-1/2} \exp \left[-\frac{1}{4\epsilon k_B T} [dA_i(l) - \epsilon \mathcal{F}_i^0(\bar{\mathbf{A}}_l^f)] (\mathbf{\Gamma}^{s-1})_{ij}(\bar{\mathbf{A}}_l^f) [dA_j(l) - \epsilon \mathcal{F}_j^0(\bar{\mathbf{A}}_l^f)] \right] \right. \\
& - \alpha \left[(dA_i(l) - \epsilon \mathcal{F}_i^0(\bar{\mathbf{A}}_l^f)) \left[(\mathbf{\Gamma}^{s-1})_{ij} \frac{\partial \mathbf{\Gamma}_{jk}^s}{\partial A_k} \right]_{\bar{\mathbf{A}}_l^f} + \epsilon \left[\frac{\partial \mathcal{F}_i^0}{\partial A_i} \right]_{\bar{\mathbf{A}}_l^f} \right] \\
& \left. \times \exp \left[\alpha^2 \epsilon k_B T \left[\frac{\partial^2 \mathbf{\Gamma}_{ij}^s}{\partial A_i \partial A_j} - \frac{\partial \mathbf{\Gamma}_{ik}^s}{\partial A_k} (\mathbf{\Gamma}^{s-1})_{ij} \frac{\partial \mathbf{\Gamma}_{jp}^s}{\partial A_p} \right]_{\bar{\mathbf{A}}_l^f} + \mathcal{O}(\epsilon^{3/2}) \right] \right\}. \quad (\text{A18})
\end{aligned}$$

We further split \mathcal{F}_i^0 into the two terms,

$$\mathcal{F}_i^s(\mathbf{A}) = -\mathbf{\Gamma}_{ij}^s \frac{\partial \mathcal{H}}{\partial A_j} + k_B T \frac{\partial \mathbf{\Gamma}_{ij}^s}{\partial A_j} \quad (\text{A19})$$

and

$$\mathcal{F}_i^a(\mathbf{A}) = -\mathbf{\Gamma}_{ij}^a \frac{\partial \mathcal{H}}{\partial A_j} + k_B T \frac{\partial \mathbf{\Gamma}_{ij}^a}{\partial A_j}, \quad (\text{A20})$$

such that, under time reversal [see Eqs. (17) and (18)],

$$\mathcal{F}^s(\mathbf{A}) \rightarrow \mathcal{F}^s(\mathbf{s} \circ \mathbf{A}) = \mathbf{s} \circ \mathcal{F}^s(\mathbf{A}), \quad (\text{A21})$$

$$\mathcal{F}^a(\mathbf{A}) \rightarrow \mathcal{F}^a(\mathbf{s} \circ \mathbf{A}) = -\mathbf{s} \circ \mathcal{F}^a(\mathbf{A}). \quad (\text{A22})$$

Equation (A17) then becomes

$$\begin{aligned} P = p_0(\mathbf{A}_0) \prod_{l=1}^N & \left\{ \frac{(2k_B T)^{-1/2}}{(2\pi\epsilon)^{n/2}} \exp \left[-\frac{1}{4\epsilon k_B T} [dA_i(l) - \epsilon \mathcal{F}_i^s(\bar{\mathbf{A}}_l^f) - \epsilon \mathcal{F}_i^a(\bar{\mathbf{A}}_l^f)] (\Gamma^{s-1})_{ij}(\bar{\mathbf{A}}_l^f) [dA_j(l) - \epsilon \mathcal{F}_j^s(\bar{\mathbf{A}}_l^f) - \epsilon \mathcal{F}_j^a(\bar{\mathbf{A}}_l^f)] \right. \right. \\ & - \alpha \left[(dA_i(l) - \epsilon \mathcal{F}_i^s(\bar{\mathbf{A}}_l^f) - \epsilon \mathcal{F}_i^a(\bar{\mathbf{A}}_l^f)) \left[(\Gamma^{s-1})_{ij} \frac{\partial \Gamma_{jk}^s}{\partial A_k} \right]_{\bar{\mathbf{A}}_l^f} + \epsilon \left[\frac{\partial \mathcal{F}_i^s}{\partial A_i} + \frac{\partial \mathcal{F}_i^a}{\partial A_i} \right]_{\bar{\mathbf{A}}_l^f} \right] \left. \right] \det(\Gamma^s(\bar{\mathbf{A}}_l^f))^{-1/2} \\ & \times \exp \left[\alpha^2 \epsilon k_B T \left[\frac{\partial^2 \Gamma_{ij}^s}{\partial A_i \partial A_j} - \frac{\partial \Gamma_{ik}^s}{\partial A_k} (\Gamma^{s-1})_{ij} \frac{\partial \Gamma_{jp}^s}{\partial A_p} \right]_{\bar{\mathbf{A}}_l^f} + \mathcal{O}(\epsilon^{3/2}) \right] \left. \right\}. \quad (\text{A23}) \end{aligned}$$

Clearly, for given Γ_{ij}^s , P is independent of the choice of N_{ij} .

APPENDIX B: THE PROBABILITY DENSITY FOR THE TIME-REVERSED TRAJECTORY

As the time-reversed trajectory of the trajectory $(\mathbf{A}_0, \mathbf{A}_1, \mathbf{A}_2, \dots, \mathbf{A}_N)$ is $(\mathbf{s} \circ \mathbf{A}_N, \mathbf{s} \circ \mathbf{A}_{N-1}, \dots, \mathbf{s} \circ \mathbf{A}_1)$, under time reversal, $\mathbf{A}_l \rightarrow \mathbf{s} \circ \mathbf{A}_{N-l}$ and therefore,

$$\begin{aligned} dA_i(l) &= A_i(\epsilon l) - A_i(\epsilon(l-1)) \\ &\rightarrow s_i(A_i(\epsilon(N-l)) - A_i(\epsilon(N-l+1))) \\ &\rightarrow -s_i dA_i(N-l+1), \end{aligned} \quad (\text{B1})$$

(Einstein's convention is not used here) and

$$\begin{aligned} \bar{\mathbf{A}}_l^f &= \alpha \mathbf{A}_l + (1-\alpha) \mathbf{A}_{l-1} \\ &\rightarrow (\alpha \mathbf{s} \circ \mathbf{A}_{N-l} + (1-\alpha) \mathbf{s} \circ \mathbf{A}_{N-l+1}) \rightarrow \mathbf{s} \circ \bar{\mathbf{A}}_{N-l+1}^r, \end{aligned} \quad (\text{B2})$$

where $\bar{\mathbf{A}}_l^r \equiv (1-\alpha) \mathbf{A}(l) + \alpha \mathbf{A}(l-1)$. With the above transformations, using the relation $\Gamma_{ij}^s = s_i s_j \Gamma_{ij}^s$ and Eqs. (A21), (A22), and (A23), we obtain the following expression of the probability density of the time-reversed trajectory:

$$\begin{aligned} P_r = \prod_{l=1}^N & \left\{ \frac{(2k_B T)^{-1/2}}{(2\pi\epsilon)^{n/2}} \exp \left[-\frac{1}{4\epsilon k_B T} [-dA_i(l') - \epsilon \mathcal{F}_i^s(\bar{\mathbf{A}}_{l'}^r) + \epsilon \mathcal{F}_i^a(\bar{\mathbf{A}}_{l'}^r)] (\Gamma^{s-1})_{ij}(\bar{\mathbf{A}}_{l'}^r) [-dA_j(l') - \epsilon \mathcal{F}_j^s(\bar{\mathbf{A}}_{l'}^r) + \epsilon \mathcal{F}_j^a(\bar{\mathbf{A}}_{l'}^r)] \right. \right. \\ & - \alpha \left[(-dA_i(l') - \epsilon \mathcal{F}_i^s(\bar{\mathbf{A}}_{l'}^r) + \epsilon \mathcal{F}_i^a(\bar{\mathbf{A}}_{l'}^r)) \left[(\Gamma^{s-1})_{ij} \frac{\partial \Gamma_{jk}^s}{\partial A_k} \right]_{\bar{\mathbf{A}}_{l'}^r} + \epsilon \left[\frac{\partial \mathcal{F}_i^s}{\partial A_i} - \frac{\partial \mathcal{F}_i^a}{\partial A_i} \right]_{\bar{\mathbf{A}}_{l'}^r} \right] \left. \right] \det(\Gamma^s(\bar{\mathbf{A}}_{l'}^r))^{-1/2} \\ & \times \exp \left[\alpha^2 \epsilon k_B T \left[\frac{\partial^2 \Gamma_{ij}^s}{\partial A_i \partial A_j} - \frac{\partial \Gamma_{ik}^s}{\partial A_k} (\Gamma^{s-1})_{ij} \frac{\partial \Gamma_{jp}^s}{\partial A_p} \right]_{\bar{\mathbf{A}}_{l'}^r} + \mathcal{O}(\epsilon^{3/2}) \right] \left. \right\} p_0(\mathbf{s} \circ \mathbf{A}_N), \quad (\text{B3}) \end{aligned}$$

where $l' = N-l+1$. In the above equation, the index l' runs from N to 1 so we can replace $\prod_{l=1}^N$ by $\prod_{l'=N}^1 \equiv \prod_{l'=1}^N$. Hence,

$$\begin{aligned} P_r = \prod_{l=1}^N & \left\{ \frac{(2k_B T)^{-1/2}}{(2\pi\epsilon)^{n/2}} \exp \left[-\frac{1}{4\epsilon k_B T} [-dA_i(l) - \epsilon \mathcal{F}_i^s(\bar{\mathbf{A}}_l^r) + \epsilon \mathcal{F}_i^a(\bar{\mathbf{A}}_l^r)] (\Gamma^{s-1})_{ij}(\bar{\mathbf{A}}_l^r) [-dA_j(l) - \epsilon \mathcal{F}_j^s(\bar{\mathbf{A}}_l^r) + \epsilon \mathcal{F}_j^a(\bar{\mathbf{A}}_l^r)] \right. \right. \\ & - \alpha \left[(-dA_i(l) - \epsilon \mathcal{F}_i^s(\bar{\mathbf{A}}_l^r) + \epsilon \mathcal{F}_i^a(\bar{\mathbf{A}}_l^r)) \left[(\Gamma^{s-1})_{ij} \frac{\partial \Gamma_{jk}^s}{\partial A_k} \right]_{\bar{\mathbf{A}}_l^r} + \epsilon \left[\frac{\partial \mathcal{F}_i^s}{\partial A_i} - \frac{\partial \mathcal{F}_i^a}{\partial A_i} \right]_{\bar{\mathbf{A}}_l^r} \right] \left. \right] \det(\Gamma^s(\bar{\mathbf{A}}_l^r))^{-1/2} \\ & \times \exp \left[\alpha^2 \epsilon k_B T \left[\frac{\partial^2 \Gamma_{ij}^s}{\partial A_i \partial A_j} - \frac{\partial \Gamma_{ik}^s}{\partial A_k} (\Gamma^{s-1})_{ij} \frac{\partial \Gamma_{jp}^s}{\partial A_p} \right]_{\bar{\mathbf{A}}_l^r} + \mathcal{O}(\epsilon^{3/2}) \right] \left. \right\} p_0(\mathbf{s} \circ \mathbf{A}_N). \quad (\text{B4}) \end{aligned}$$

APPENDIX C: CALCULATION OF THE RATIO BETWEEN THE PROBABILITY DENSITIES OF A TRAJECTORY AND ITS TIME-REVERSED TRAJECTORY

Using relations (D2) and (D3), expanding $N_{ij}(\bar{A}_l^f)$ and $N_{ij}(\bar{A}_l^r)$ around $\mathbf{A} = \bar{\mathbf{A}}_l \equiv (\mathbf{A}_l + \mathbf{A}_{l-1})/2$:

$$N_{ij}(\bar{A}_l^f) = N_{ij}(\bar{\mathbf{A}}_l) + \frac{2\alpha - 1}{2} \left[\frac{\partial N_{ij}}{\partial A_k} \right]_{\bar{\mathbf{A}}_l} dA_k(l) + \frac{1}{2} \left(\frac{2\alpha - 1}{2} \right)^2 \left[\frac{\partial^2 N_{ij}}{\partial A_k \partial A_m} \right]_{\bar{\mathbf{A}}_l} dA_k(l) dA_m(l) + \mathcal{O}(\epsilon^{3/2}), \quad (\text{C1})$$

$$N_{ij}(\bar{A}_l^r) = N_{ij}(\bar{\mathbf{A}}_l) - \frac{2\alpha - 1}{2} \left[\frac{\partial N_{ij}}{\partial A_k} \right]_{\bar{\mathbf{A}}_l} dA_k(l) + \frac{1}{2} \left(\frac{2\alpha - 1}{2} \right)^2 \left[\frac{\partial^2 N_{ij}}{\partial A_k \partial A_m} \right]_{\bar{\mathbf{A}}_l} dA_k(l) dA_m(l) + \mathcal{O}(\epsilon^{3/2}). \quad (\text{C2})$$

Then, using the relation $N_{ik}N_{jk} = 2k_B T \Gamma_{ij}^s$ and Eq. (A8), we obtain

$$\begin{aligned} \frac{\det(\Gamma^s(\bar{A}_l^f))^{-1/2}}{\det(\Gamma^s(\bar{A}_l^r))^{-1/2}} &= \frac{|\det(\mathbf{N}^{-1}(\bar{A}_l^f))|}{|\det(\mathbf{N}^{-1}(\bar{A}_l^r))|} \\ &= \exp \left[- (2\alpha - 1) \left[(\mathbf{N}^{-1})_{jm} \frac{\partial N_{mj}}{\partial A_k} \right]_{\bar{\mathbf{A}}_l} dA_k(l) + \mathcal{O}(\epsilon^{3/2}) \right] \\ &= \exp \left[- \frac{2\alpha - 1}{2} \left[(\Gamma^{s-1})_{jm} \frac{\partial (\Gamma^s)_{mj}}{\partial A_k} \right]_{\bar{\mathbf{A}}_l} dA_k(l) + \mathcal{O}(\epsilon^{3/2}) \right]. \end{aligned} \quad (\text{C3})$$

In $\epsilon \rightarrow 0$ limit, dividing Eq. (A23) by Eq. (B4) first, and using the above equation and the relations given in Appendix D, we get

$$\begin{aligned} \frac{P}{P_r} &= \frac{p_0(\mathbf{A}_0)}{p_0(\mathbf{s} \circ \mathbf{A}_N)} \exp \left[- \frac{1}{k_B T} \sum_{l=1}^N (\mathcal{H}(\mathbf{A}_l) - \mathcal{H}(\mathbf{A}_{l-1})) + \mathcal{O}(\epsilon^{3/2}) \right] \\ &= \frac{p_0(\mathbf{A}(0))}{p_0(\mathbf{s} \circ \mathbf{A}(\tau))} \exp \left[- \frac{1}{k_B T} (\mathcal{H}(\mathbf{A}(\tau)) - \mathcal{H}(\mathbf{A}(0))) \right], \end{aligned} \quad (\text{C4})$$

where $\mathbf{A}(0) \equiv \mathbf{A}_0$ and $\mathbf{A}(\tau) \equiv \mathbf{A}_N$.

APPENDIX D: VARIOUS RELATIONS NEEDED FOR THE CALCULATION IN SEC. IIB

Recalling Eq. (10) of the main text,

$$dA_i(l) = \epsilon \mathcal{F}_i(\bar{A}_l^f) + \sqrt{\epsilon} N_{ij}(\bar{A}_l^f) \xi_j^l. \quad (\text{D1})$$

Note that the lowest order term in $dA_i(l)$ is a $\epsilon^{1/2}$ -term. Let us consider a function $G(\mathbf{A})$; expanding $G(\bar{A}_l^f)$ and $G(\bar{A}_l^r)$ around $\mathbf{A} = \bar{\mathbf{A}}_l \equiv (\mathbf{A}_l + \mathbf{A}_{l-1})/2$:

$$G(\bar{A}_l^f) = G\left(\bar{\mathbf{A}}_l + \frac{2\alpha - 1}{2} d\mathbf{A}_l\right) = G(\bar{\mathbf{A}}_l) + \frac{2\alpha - 1}{2} \left[\frac{\partial G}{\partial A_k} \right]_{\bar{\mathbf{A}}_l} dA_k(l) + \frac{1}{2} \left(\frac{2\alpha - 1}{2} \right)^2 \left[\frac{\partial^2 G}{\partial A_k \partial A_m} \right]_{\bar{\mathbf{A}}_l} dA_k(l) dA_m(l) + \mathcal{O}(\epsilon^{3/2}) \quad (\text{D2})$$

and

$$\begin{aligned} G(\bar{A}_l^r) &= G\left(\bar{\mathbf{A}}_l - \frac{2\alpha - 1}{2} d\mathbf{A}_l\right) \\ &= G(\bar{\mathbf{A}}_l) - \frac{2\alpha - 1}{2} \left[\frac{\partial G}{\partial A_k} \right]_{\bar{\mathbf{A}}_l} dA_k(l) + \frac{1}{2} \left(\frac{2\alpha - 1}{2} \right)^2 \left[\frac{\partial^2 G}{\partial A_k \partial A_m} \right]_{\bar{\mathbf{A}}_l} dA_k(l) dA_m(l) + \mathcal{O}(\epsilon^{3/2}), \end{aligned} \quad (\text{D3})$$

where $d\mathbf{A}_l = \mathbf{A}_l - \mathbf{A}_{l-1}$. Then

$$\begin{aligned} dA_i(l) dA_j(l) G(\bar{A}_l^f) &= dA_i(l) dA_j(l) G(\bar{\mathbf{A}}_l) + \frac{2\alpha - 1}{2} \left[\frac{\partial G}{\partial A_k} \right]_{\bar{\mathbf{A}}_l} dA_i(l) dA_j(l) dA_k(l) \\ &\quad + \frac{1}{2} \left(\frac{2\alpha - 1}{2} \right)^2 \left[\frac{\partial^2 G}{\partial A_k \partial A_m} \right]_{\bar{\mathbf{A}}_l} dA_i(l) dA_j(l) dA_k(l) dA_m(l) + \mathcal{O}(\epsilon^{5/2}). \end{aligned} \quad (\text{D4})$$

From Eq. (D1),

$$dA_i(l) dA_j(l) dA_k(l) = \xi_p^l \xi_q^l \xi_r^l N_{ip} N_{jq} N_{kr} \epsilon^{3/2} + (\xi_p^l \xi_q^l N_{ip} N_{jq} \mathcal{F}_k + \xi_p^l \xi_r^l N_{ip} N_{kr} \mathcal{F}_j + \xi_q^l \xi_r^l N_{jq} N_{kr} \mathcal{F}_i) \epsilon^2 + \mathcal{O}(\epsilon^{5/2}). \quad (\text{D5})$$

Our final expressions will be written in integral form, and since $\xi_j(t)$ is the time derivative of a Wiener process, we can write

$$\xi_p^l \xi_q^l \equiv \delta_{pq}, \quad (\text{D6})$$

$$\xi_p^l \xi_q^l \xi_r^l \equiv \delta_{pq} \xi_r^l + \delta_{pr} \xi_q^l + \delta_{rq} \xi_p^l, \quad (\text{D7})$$

$$\xi_p^l \xi_q^l \xi_r^l \xi_o^l \equiv \delta_{pq} \delta_{ro} + \delta_{pr} \delta_{qo} + \delta_{qr} \delta_{po}. \quad (\text{D8})$$

Using the above relations, Eq. (D1) and Eq. (6) ($N_{ik} N_{jk} = 2k_B T \Gamma_{ij}^s$), Eq. (D5) can be written as

$$dA_i(l) dA_j(l) dA_k(l) = 2k_B T (\Gamma_{ij}^s dA_k(l) + \Gamma_{jk}^s dA_i(l) + \Gamma_{ki}^s dA_j(l)) \epsilon + \mathcal{O}(\epsilon^{5/2}). \quad (\text{D9})$$

Similarly,

$$\begin{aligned} dA_i(l) dA_j(l) dA_k(l) dA_m(l) &= \xi_p^l \xi_q^l \xi_r^l \xi_o^l N_{ip} N_{jq} N_{kr} N_{mo} \epsilon^2 + \mathcal{O}(\epsilon^{5/2}) \\ &= (2k_B T)^2 (\Gamma_{ij}^s \Gamma_{km}^s + \Gamma_{ik}^s \Gamma_{jm}^s + \Gamma_{im}^s \Gamma_{jk}^s) \epsilon^2 + \mathcal{O}(\epsilon^{5/2}). \end{aligned} \quad (\text{D10})$$

Substituting Eqs. (D9) and (D10) into Eq. (D4), we obtain

$$\begin{aligned} dA_i(l) dA_j(l) G(\bar{\mathbf{A}}_l^f) &= dA_i(l) dA_j(l) G(\bar{\mathbf{A}}_l) + (2\alpha - 1) k_B T \left[\frac{\partial G}{\partial A_k} \right]_{\bar{\mathbf{A}}_l} (\Gamma_{ij}^s(\bar{\mathbf{A}}_l) dA_k(l) + \Gamma_{jk}^s(\bar{\mathbf{A}}_l) dA_i(l) + \Gamma_{ki}^s(\bar{\mathbf{A}}_l) dA_j(l)) \epsilon \\ &\quad + \frac{1}{2} [(2\alpha - 1) k_B T]^2 \left[\frac{\partial^2 G}{\partial A_k \partial A_m} (\Gamma_{ij}^s \Gamma_{km}^s + \Gamma_{ik}^s \Gamma_{jm}^s + \Gamma_{im}^s \Gamma_{jk}^s) \right]_{\bar{\mathbf{A}}_l} \epsilon^2 + \mathcal{O}(\epsilon^{5/2}). \end{aligned} \quad (\text{D11})$$

Similarly, from Eq. (D3), we readily obtain

$$\begin{aligned} dA_i(l) dA_j(l) G(\bar{\mathbf{A}}_l^r) &= dA_i(l) dA_j(l) G(\bar{\mathbf{A}}_l) - (2\alpha - 1) k_B T \left[\frac{\partial G}{\partial A_k} \right]_{\bar{\mathbf{A}}_l} (\Gamma_{ij}^s dA_k(l) + \Gamma_{jk}^s dA_i(l) + \Gamma_{ki}^s dA_j(l)) \epsilon \\ &\quad + \frac{1}{2} [(2\alpha - 1) k_B T]^2 \left[\frac{\partial^2 G}{\partial A_k \partial A_m} \right]_{\bar{\mathbf{A}}_l} (\Gamma_{ij}^s \Gamma_{km}^s + \Gamma_{ik}^s \Gamma_{jm}^s + \Gamma_{im}^s \Gamma_{jk}^s) \epsilon^2 + \mathcal{O}(\epsilon^{5/2}). \end{aligned} \quad (\text{D12})$$

Likewise, we can easily derive the following relations:

$$dA_i(l) G(\bar{\mathbf{A}}_l^f) = dA_i(l) G(\bar{\mathbf{A}}_l) + (2\alpha - 1) k_B T \epsilon \left[\Gamma_{ij}^s \frac{\partial G}{\partial A_j} \right]_{\bar{\mathbf{A}}_l} + \mathcal{O}(\epsilon^{3/2}), \quad (\text{D13})$$

$$dA_i(l) G(\bar{\mathbf{A}}_l^r) = dA_i(l) G(\bar{\mathbf{A}}_l) - (2\alpha - 1) k_B T \epsilon \left[\Gamma_{ij}^s \frac{\partial G}{\partial A_j} \right]_{\bar{\mathbf{A}}_l} + \mathcal{O}(\epsilon^{3/2}), \quad (\text{D14})$$

$$G(\bar{\mathbf{A}}_l^f) = G(\bar{\mathbf{A}}_l) + \mathcal{O}(\epsilon^{1/2}), \quad (\text{D15})$$

$$G(\bar{\mathbf{A}}_l^r) = G(\bar{\mathbf{A}}_l) + \mathcal{O}(\epsilon^{1/2}), \quad (\text{D16})$$

$$\left[\frac{\partial G}{\partial A_i} \right]_{\bar{\mathbf{A}}_l} dA_i(l) = G(\mathbf{A}_l) - G(\mathbf{A}_{l-1}) + \mathcal{O}(\epsilon^{3/2}). \quad (\text{D17})$$

APPENDIX E: THE RELATION BETWEEN ENTROPY PRODUCTION RATE AND \dot{s}

The free energy of the system at time t would be

$$\begin{aligned} F(t) &= \int \mathcal{H}(\mathbf{A}) p_t(\mathbf{A}) d\mathbf{A} - T \left[-k_B \int p_t(\mathbf{A}) \ln p_t(\mathbf{A}) d\mathbf{A} \right] \\ &= \langle [\mathcal{H}(\mathbf{A}) + k_B T \ln p_t(\mathbf{A})] \rangle, \end{aligned} \quad (\text{E1})$$

where $\langle \rangle$ stands for the ensemble average and $p_t(\mathbf{A})$ is the probability distribution of \mathbf{A} at time t . Let us define the free energy of a single trajectory of the system at time t as

$$f(t) = \mathcal{H}(\mathbf{A}(t)) + k_B T \ln p_t(\mathbf{A}(t)). \quad (\text{E2})$$

Then it is straightforward to show that

$$\frac{dF(t)}{dt} = \left\langle \frac{df(t)}{dt} \right\rangle. \quad (\text{E3})$$

1. For passive systems

From Eq. (32), we readily get

$$\left\langle \frac{df(t)}{dt} \right\rangle = -k_B T \langle \dot{s}(t) \rangle, \quad (\text{E4})$$

so from Eq. (E3)

$$\frac{dF(t)}{dt} = -k_B T \langle \dot{s}(t) \rangle. \quad (\text{E5})$$

Assuming that the system is always in metastable thermal equilibrium with the reservoir, the rate of change total entropy

of system and reservoir would be

$$\frac{dS(t)}{dt} = -\frac{1}{T} \frac{dF(t)}{dt} = k_B \langle \dot{s}(t) \rangle. \quad (\text{E6})$$

2. For active systems

For active systems, from Eq. (46), one can trivially prove that

$$\left\langle \frac{df(t)}{dt} \right\rangle = -k_B T \langle \dot{s}(t) \rangle + \langle w(t) \rangle, \quad (\text{E7})$$

where $\langle w(t) \rangle$ is average rate of the work performed by active forces. Hence, from Eq. (E3),

$$\frac{dF(t)}{dt} = -k_B T \langle \dot{s}(t) \rangle + \langle w(t) \rangle. \quad (\text{E8})$$

Therefore, the rate of total entropy production of the system and the reservoir is

$$\begin{aligned} \frac{dS(t)}{dt} &= -\frac{1}{T} \frac{dF(t)}{dt} + \frac{1}{T} \langle w(t) \rangle \\ &= k_B \langle \dot{s}(t) \rangle. \end{aligned} \quad (\text{E9})$$

APPENDIX F: THE DISSIPATION FUNCTION DEFINED BY SEIFERT *et al.* [5]

Seifert *et al.* [5] used the following form of the dissipation function:

$$\mathcal{S}_\tau = \ln \left[\frac{P}{P_r} \right], \quad (\text{F1})$$

where P is the probability density of a trajectory between $t = 0$ and $t = \tau$ which is given by Eq. (A12), and P_r is the probability density of the time-reversed trajectory, considering that the time-reversed trajectory starts at $t = \tau$, not at $t = 0$. Thus, the expression of \mathcal{S}_τ is readily obtained by replacing $p_0(s \circ A_N)$ with $p_t(s \circ A_N)$ in the expression of \mathcal{R}_τ [see Eq. (25)], that is

$$\mathcal{S}_\tau = \ln \frac{p_0(\mathbf{A}(0))}{p_\tau(s \circ \mathbf{A}(\tau))} - \frac{1}{k_B T} [\mathcal{H}(\mathbf{A}(\tau)) - \mathcal{H}(\mathbf{A}(0))]. \quad (\text{F2})$$

This dissipation function follows the fluctuation relation (24) in steady states only, not in general. However, as discussed by Ref. [5], it does always follow the integrated fluctuation relation (28) and therefore $\langle \mathcal{S}_\tau \rangle \geq 0$.

APPENDIX G: CALCULATION OF \dot{s} FOR THE ACTIVE SYSTEMS

Recalling equations of motion for the active systems

$$\frac{dA_i}{dt} = \mathcal{F}_i + \mathcal{X}_i + N_{ij} \xi_j(t), \quad (\text{G1})$$

where

$$\mathcal{F}_i \equiv -\Gamma_{ij} \frac{\partial \mathcal{H}}{\partial A_j} + k_B T \frac{\partial \Gamma_{ij}}{\partial A_j} - \alpha N_{ij} \frac{\partial N_{ij}}{\partial A_i}, \quad (\text{G2})$$

and \mathcal{X}_i is the active term. Writing \mathcal{X} as $\mathcal{X} = \mathcal{X}^s + \mathcal{X}^a$, where

$$\mathcal{X}^s(\mathbf{A}) = \frac{1}{2} (\mathcal{X}(\mathbf{A}) + s \circ \mathcal{X}(s \circ \mathbf{A})), \quad (\text{G3})$$

$$\mathcal{X}^a(\mathbf{A}) = \frac{1}{2} (\mathcal{X}(\mathbf{A}) - s \circ \mathcal{X}(s \circ \mathbf{A})) \quad (\text{G4})$$

follow the properties $\mathcal{X}^s(s \circ \mathbf{A}) = s \circ \mathcal{X}^s(\mathbf{A})$ and $\mathcal{X}^a(s \circ \mathbf{A}) = -s \circ \mathcal{X}^a(\mathbf{A})$. The Fokker-Planck equation for the probability density $p_t(\mathbf{A})$ of \mathbf{A} reads

$$\frac{\partial p_t(\mathbf{A})}{\partial t} = -\frac{\partial J_i(\mathbf{A}, t)}{\partial A_i}, \quad (\text{G5})$$

where

$$\begin{aligned} J_i(\mathbf{A}, t) &= \left(-\Gamma_{ij}^s(\mathbf{A}) \frac{\partial \mathcal{H}(\mathbf{A})}{\partial A_j} + \mathcal{Y}_i^a(\mathbf{A}) + \mathcal{X}_j^s(\mathbf{A}) \right) p_t(\mathbf{A}) \\ &\quad - k_B T \Gamma_{ij}^s(\mathbf{A}) \frac{\partial p_t(\mathbf{A})}{\partial A_j} \end{aligned} \quad (\text{G6})$$

is the probability current [23] and

$$\mathcal{Y}_i^a = \mathcal{X}_i^a + \frac{\partial \mathcal{H}}{\partial A_k} \Gamma_{ki}^a - k_B T \frac{\partial \Gamma_{ki}^a}{\partial A_k}. \quad (\text{G7})$$

Since $\mathcal{X}^a(s \circ \mathbf{A}) = -s \circ \mathcal{X}^a(\mathbf{A})$, using the relation $\Gamma_{ij}^a = -\Gamma_{ij}^a s_i s_j$ [Eq. (16)], it is easy to show that

$$\mathcal{Y}^a(s \circ \mathbf{A}) = -s \circ \mathcal{Y}^a(\mathbf{A}). \quad (\text{G8})$$

As Eq. (G5) has no term with N_{ij} , $p_t(\mathbf{A})$ would be independent of the choice of N_{ij} . Recalling Eq. (46)

$$\dot{s}(t) = w(t) - \frac{d}{dt'} \left(\ln p_t(\mathbf{A}(t')) + \frac{1}{k_B T} \mathcal{H}(\mathbf{A}(t')) \right) \Big|_{t'=t}, \quad (\text{G9})$$

where

$$\begin{aligned} w(t) &= \frac{\partial \mathcal{H}(\mathbf{A}(t))}{\partial A_i} \mathcal{X}_i^a(\mathbf{A}(t)) - k_B T \frac{\partial \mathcal{X}_i^a(\mathbf{A}(t))}{\partial A_i} \\ &\quad + (\Gamma^{s-1})_{ij}(\mathbf{A}(t)) \mathcal{X}_j^s(\mathbf{A}(t)) \left[\frac{dA_i}{dt} - \mathcal{Y}_i^a(\mathbf{A}(t)) \right]. \end{aligned} \quad (\text{G10})$$

Using Eqs. (G5) and (G6), one can write Eq. (46) in the following form:

$$\begin{aligned} \dot{s}(t) &= \frac{1}{k_B T} \left(\frac{J_i(\mathbf{A}, t)}{p_t(\mathbf{A})} - \mathcal{Y}_i^a(\mathbf{A}) \right) (\Gamma^{s-1})_{ij}(\mathbf{A}) \\ &\quad \times \left(\frac{J_j(\mathbf{A}, t)}{p_t(\mathbf{A})} - \mathcal{Y}_j^a(\mathbf{A}) \right) + R_s + R_0, \end{aligned} \quad (\text{G11})$$

where

$$R_s = -\frac{1}{p_t(\mathbf{A})} \frac{\partial}{\partial A_i} (p_t(\mathbf{A}) \mathcal{Y}_i^a(\mathbf{A})) \quad (\text{G12})$$

and

$$\begin{aligned} R_0 &= \left(\frac{dA_i}{dt} - \frac{J_i(\mathbf{A}, t)}{p_t(\mathbf{A})} \right) \left[\frac{1}{p_t(\mathbf{A})} \frac{\partial p_t(\mathbf{A})}{\partial A_i} \right. \\ &\quad \left. - \frac{1}{k_B T} \left((\Gamma^{s-1})_{ij}(\mathbf{A}) \mathcal{X}_j^s(\mathbf{A}) - \frac{\partial \mathcal{H}(\mathbf{A})}{\partial A_j} \right) \right]. \end{aligned} \quad (\text{G13})$$

The average of R_s reads

$$\begin{aligned} \langle R_s \rangle &= - \int \frac{1}{p_t(\mathbf{A})} \frac{\partial}{\partial A_i} (p_t(\mathbf{A}) \mathcal{Y}_i^a(\mathbf{A})) p_t(\mathbf{A}) d^n A \\ &= - \int \frac{\partial}{\partial A_i} (p_t(\mathbf{A}) \mathcal{Y}_i^a(\mathbf{A})) d^n A. \end{aligned} \quad (\text{G14})$$

The above expression can be written as a surface integral with the integrand $\mathbf{I}_s = -p_t(\mathbf{A})\mathcal{Y}^a(\mathbf{A})$. If the system is periodic in A_i (e.g., A_i is an angle), then the surface integral is already zero. If A_i lies in the infinite interval $(-\infty, \infty)$, then in $A_i \rightarrow \pm\infty$ limit, $p_t(\mathbf{A}) \rightarrow 0$, given that \mathbf{A} are physical variables. Assuming that $\|\mathbf{I}_s\|$ converges faster than $\|\mathbf{A}\|^{1-n}$, the surface integral is again zero. For $p_t(s \circ \mathbf{A}) = p_t(\mathbf{A})$ case, $\langle R_s \rangle$ is always zero as follows: setting $\mathbf{A} = s \circ \mathbf{A}'$ gives $d^n \mathbf{A} = d^n \mathbf{A}'$, then using Eq. (G8), we get

$$\begin{aligned} \langle R_s \rangle &= \int \frac{\partial}{\partial A'_i} (p_t(\mathbf{A}') \mathcal{Y}_i^a(\mathbf{A}')) d^n \mathbf{A}' \\ &= -\langle R_s \rangle, \end{aligned} \quad (\text{G15})$$

so $\langle R_s \rangle = 0$. Since the ensemble average of dA_i/dt for given \mathbf{A} and t is just $J_i(\mathbf{A}, t)/p_t(\mathbf{A})$, $\langle R_o \rangle = 0$. Therefore, the ensemble average of Eq. (G11) is given by

$$\begin{aligned} \langle \dot{s}(t) \rangle &= \frac{1}{k_B T} \left\langle \left(\frac{J_i(\mathbf{A}, t)}{p_t(\mathbf{A})} - \mathcal{Y}_i^a(\mathbf{A}) \right) (\Gamma^{s-1})_{ij}(\mathbf{A}) \right. \\ &\quad \left. \times \left(\frac{J_j(\mathbf{A}, t)}{p_t(\mathbf{A})} - \mathcal{Y}_j^a(\mathbf{A}) \right) \right\rangle. \end{aligned} \quad (\text{G16})$$

Similarly, $\langle w(t) \rangle$ given by Eq. (G10) can be written in the following form:

$$\begin{aligned} \langle w(t) \rangle &= \left\langle \left(\frac{dA_i}{dt} - \frac{\partial \mathcal{H}}{\partial A_k} \Gamma_{ki}^a + k_B T \frac{\partial \Gamma_{ki}^a}{\partial A_k} \right) (\Gamma^{s-1})_{ij} \mathcal{X}_j^s \right\rangle \\ &\quad - \left\langle \left(\frac{dA_i}{dt} - \mathcal{Y}_i^a \right) (\Gamma^{s-1})_{ij} \mathcal{X}_j^a \right\rangle. \end{aligned} \quad (\text{G17})$$

Here, if $p_t(s \circ \mathbf{A}) \neq p_t(\mathbf{A})$, then we must assume that $\|p_t(\mathbf{A})\mathcal{X}^a(\mathbf{A})\|$ converges faster than $\|\mathbf{A}\|^{1-n}$.

APPENDIX H: STATIONARY SOLUTION OF THE FOKKER-PLANCK EQUATION ASSOCIATED WITH EQ. (8)

The Fokker-Planck equation for the probability distribution $p_t(\mathbf{A})$ of the solution of Eq. (8) is given by

$$\frac{\partial p_t(\mathbf{A})}{\partial t} = -\frac{\partial J_i(\mathbf{A}, t)}{\partial A_i}; \quad (\text{H1})$$

the expression of the probability current $J_i(\mathbf{A}, t)$ reads [23]

$$\begin{aligned} J_i(\mathbf{A}, t) &= \left(-\Gamma_{ij}^s(\mathbf{A}) \frac{\partial \mathcal{H}(\mathbf{A})}{\partial A_j} + \frac{\partial \mathcal{H}}{\partial A_k} \Gamma_{ki}^a - k_B T \frac{\partial \Gamma_{ki}^a}{\partial A_k} \right) \\ &\quad \times p_t(\mathbf{A}) - k_B T \Gamma_{ij}^s(\mathbf{A}) \frac{\partial p_t(\mathbf{A})}{\partial A_j}. \end{aligned} \quad (\text{H2})$$

Undoubtedly, the dynamics of $p_t(\mathbf{A})$ is independent of the choice of N_{ij} and α . Since

$$\frac{\partial \mathcal{H}}{\partial A_k} \Gamma_{ki}^a - k_B T \frac{\partial \Gamma_{ki}^a}{\partial A_k}$$

is the Poisson bracket term, the stationary solution of the above equation is given by [25]

$$p_s(\mathbf{A}) = \frac{1}{\mathcal{Z}} \exp \left[-\frac{\mathcal{H}(\mathbf{A})}{k_B T} \right], \quad (\text{H3})$$

where \mathcal{Z} is the normalizing constant.

APPENDIX I: DEPENDENCE OF $\langle \mathcal{R}_\tau \rangle$ ON α FOR THE PASSIVE SYSTEMS

For the passive systems, \mathcal{R}_τ depends only on the initial and final states of the system \mathbf{A}_0 and \mathbf{A}_τ , so its average can be calculated using the formula [35]

$$\langle \mathcal{R}_\tau \rangle = \int \mathcal{R}_\tau p_0(\mathbf{A}_0) G(\mathbf{A}_0, \mathbf{A}_\tau; \tau) d^n \mathbf{A}_0 d^n \mathbf{A}_\tau, \quad (\text{I1})$$

where $p_0(\mathbf{A})$ is the probability distribution of \mathbf{A} at $t = 0$, and $G(\mathbf{A}, \mathbf{A}'; \tau)$ is the probability distribution of state \mathbf{A}' at $t = \tau$ given that the system was in the state \mathbf{A} at $t = 0$; it is the solution of Eq. (H1) with the initial condition $G(\mathbf{A}, \mathbf{A}'; \tau = 0) = \delta(\mathbf{A} - \mathbf{A}')$. As the solution of Eq. (H1) is independent of α , $\langle \mathcal{R}_\tau \rangle$ would be constant in α .

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