The Trajectory Entropy of Continuous Stochastic Processes at Equilibrium

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Abstract

We propose to quantify the trajectory entropy of a dynamic system as the information content in excess of a free diffusion reference model. The space-time trajectory is now the dynamic variable and its path probability is given by the Onsager-Machlup action. For the time propagation of the over-damped Langevin equation, we solved the action path integral in the continuum limit and arrived at an exact analytical expression that emerged as a simple functional of the deterministic mean force and the stochastic diffusion. This work could have direct implications in chemical and phase equilibria, bond isomerization and conformational changes in biological macromolecules, as well transport problems in general.

A dynamic system subjected to both random fluctuations and variations in the energy surface explores its possible outcomes during the evolution over time. We see such examples in areas including physics, chemistry, biology, as well economics. It would therefore be of great interest to have a quantitative measure that elucidates the manner by which the deterministic and the stochastic forces acting on the system affect the dynamics.

The general features of the problem are as follows. Let x be some continuous observable that characterizes the outcome of a system that is under stochastic thermal agitation; for example, x could be the distance characterizing the conformational change of a protein, the angle of a chemical bond isomerization process, the reaction coordinate of a chemical equilibrium, the relative population of a phase equilibrium, or the spatial coordinate of an electron diffusing classically in a periodic potential, to name a few. Without loss of generality, here x is designated as the spatial coordinate in this Letter. The system with an initial condition x_0 at time zero will evolve to trace out a trajectory function $X(t)$ that gives a value of x_t at time t, with t going from 0 to the finite observation time of $t_{\rm obs}$. A trajectory thus records how the system changes as a function of time and contains the dynamics information as Fig. 1 illustrates. This figure shows four different trajectories with the respective initial conditions marked by filled circles on the left-most plane. The contours on the same plane mark the potential $V(x)$ of the mean force, $F(x) = -dV(x)/dx$, that drives the system deterministically. In this work, we non-dimensionalize the potential of mean force (PMF) by $k_{\rm B}T$, where $k_{\rm B}$ is the Boltzmann constant and T is the temperature. A rugged PMF, *e.g.*, a $V(x)$ with many local minima and maxima, will encode complicated features in the resulting trajectories that are composed of various dynamical processes such as waiting in different wells and making transitions between them.

In the presence of stochastic forces, the trajectories become even more complex to exhibit zigzags: One realization of the trajectory $X_1(t)$ will be different from the next, $X_2(t)$, even if the initial conditions are identical. The combined actions of both the deterministic and the stochastic forces thus power the system to explore a specific space-time volume (cf. Fig. 1) and both forces contribute to this apparent feature of trajectories. Due to the presence of stochastic forces, any description of the system dynamics needs to be statistical,[1] and the problem of quantitatively characterizing the dynamics becomes evaluating the statistics of the ensemble of all trajectories that can be realized by the system.

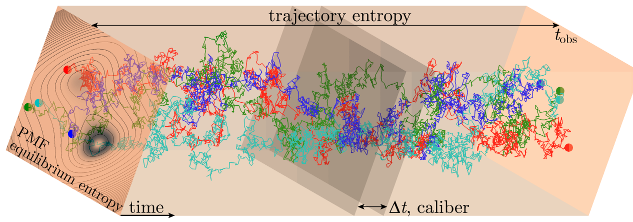

Figure 1: (color online) The space-time trajectories of a dynamic system under the influences of both deterministic and stochastic forces. The equilibrium entropy is determined by the potential of mean force (PMF, the left-most plane with contour lines) of the static distribution (the shaded gradients on the PMF plane). Jaynes's caliber evaluates the extent over which the system can explore over a slice of finite time width, Δt, such as betwen the two gray panes. The trajectory entropy focused in this work resolves both the static and dynamical contributions to the apparent variation in dynamics over the observation time from $t = 0$ to t_{obs}, and quantifies them analytically. This figure serves as a pictorial representation of space-time trajectories and does not correspond to the model systems studied later.

In this Letter, we use the entropy measure defined in Eq. (1),

$$\mathcal{S} \equiv - \int_0^{t_{obs}} \mathcal{D}X(t)\ \mathcal{P}[X(t)] \ln \frac{\mathcal{P}[X(t)]}{\mathcal{Q}[X(t)]}, \tag{1}$$

to quantitatively evaluate the trajectory ensemble, where $\mathcal{P}[X(t)]$ is the probability density of obtaining the trajectory $X(t)$, $\mathcal{Q}(X(t))$ is the probability density of obtaining the same trajectory but from a reference dynamics, and the integration over $\mathcal{D}X(t)$ is a path-integral over all realizable $X(t)$ from the dynamics. In one limiting case that only the deterministic forces are present, the initial condition sets the future and the dynamics is precisely known. In the other limiting case that the system is influenced by stochastic forces only, the time propagation is the purely diffusive Brownian dynamics (BD). In this work, the latter case is chosen to be the reference dynamics for determining $\mathcal{Q}(X(t))$. Therefore, if the system is solely influenced by random fluctuations, the trajectory entropy follows $\mathcal{S} = 0$. On the other hand, if the system is driven by deterministic forces without stochasticity, $\mathcal{S} \to -\infty$ for fully predictive trajectories. In general, the trajectory entropy will be bound by these two limiting cases.

As an illustration, we consider the three model PMFs shown in Fig. 2. Their equilibrium probability density functions, $p_{\rm eq}(x) = \exp\left(-V(x)\right)/Z_{\rm eq}$ and $Z_{\rm eq}$ the equilibrium partition function,[2] have identical values of the equilibrium entropy, $S_{\rm eq} = -\int dx p_{\rm eq}(x) \ln p_{\rm eq}(x) = -1.683$. However, visual inspection of the sample trajectories generated with identical diffusion coefficients shown in Fig. 2 indicates that their dynamics are obviously distinctive. Although Model 1 appears to be the most simplistic with a single minimum, the well is wider than those of Model 2 and 3 that have two and three minima, respectively. One can also tell that the space-time paths of the three models seem to carry specific information about the differences in time propagation, for which the equilibrium entropy is an irrelevant measure.[3–7] The trajectory entropy measure of Eq. (1), on the other hand, could in principle allow a quantitative understanding of the dynamical behaviors of different models. An immediate difficulty one encounters, however, is that a direct numerical integration of Eq. (1) leads to divergence. In this work, we illustrate that the physical origin of different dynamics in trajectories can be made transparent to clearly resolve the contributions from deterministic *vs.* stochastic forces. Our main result is an analytical expression of $\mathcal{S}$ for the over-damped Langevin dynamics, $dx_t = DF(x_t)dt + \sqrt{2D}dW_t$. D is the diffusion coefficient, and the Wiener process of stochastic forces, dW_t, satisfies $\langle dW_t dW_{t'} \rangle = \delta(t-t')dt$. The ergodic limit distribution of the Langevin equation is $p_{\rm eq}(x)$.[2]

We show that the trajectory entropy for this widely used model of dynamics is given analytically as the following functional:

$$\mathcal{S}[F(x), D] = S_{\rm eq} - \frac{t_{\rm obs}}{2}\left\langle DF^2(x)\right\rangle_{\rm eq} + \lim_{\Delta t \to 0^+} \frac{t_{\rm obs}}{\Delta t} \ln \sqrt{D}. \quad (2)$$

In Eq. (2), Δt is the time resolution for recording the trajectories, and the initial conditions of which are assumed to follow $p_{\rm eq}(x)$. In terms of the three models in Fig. 2, an important outcome of Eq. (2) is the explicit quantification of the physics underlying the intuition that

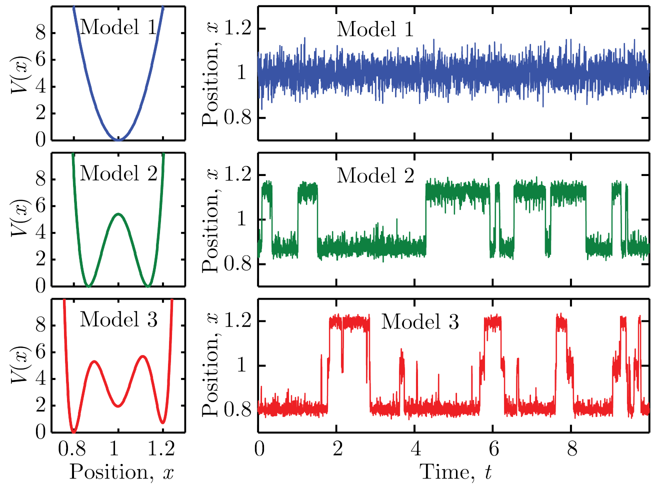

Figure 2: (color online) Three dynamic models have identical values of equilibrium entropy but different dynamics. (left) The potential of mean force, $V(x)$, of Model 1: $247.15(x-1)^2$, Model 2: $17302.265(x-1)^4 - 611.347(x-1)^2$, and Model 3: $\frac{1}{15.47}\left[\left(\frac{x-1}{13.9}\right)^6 - 15\left(\frac{x-1}{13.9}\right)^4 + 53\left(\frac{x-1}{13.9}\right)^2 + 2\left(\frac{x-1}{13.9}\right) - 15\right]$. Model 1, 2, and 3 have 1, 2, and 3 minima in $V(x)$, respectively. (right) A sample Langevin trajectory for each of the three models with $D = 1$ in the dimensionless unit.

the three sample trajectories differ in their dynamics. It is now clear how their differences come from the deterministic forces physically: Having more wells in the PMF would cause the time propagation to be more complex since $\mathcal{S}$ would take a lower value with the excess magnitude in force contributed as $\langle DF^2(x)\rangle_{\text{eq}}$. Eq. (2) also describes how stochastic diffusion contributes to the trajectory entropy by itself and relative to the deterministic mean forces. In the remainder of this Letter, we present the essential ideas and steps of deriving Eq. (2) followed by comparing the analytical expression with numerical calculations to further illustrate the underlying physical picture.

The trajectory entropy defined in Eq. (1) is the negative of the Kullback-Leibler (KL) divergence that measures the extra information required to encode a probability density, $\mathcal{P}(X(t))$, relative to the reference distribution of $\mathcal{Q}(X(t))$. Each trajectory in the integral is wighted by the equilibrium probability density $\mathcal{P}(X(t))$ of the system dynamics. $\mathcal{S}$ is thus negative and becomes zero only when the queried distribution is identical to that of the reference and is often used to characterize the relaxation of non-equilibrium states back to equilibrium and the entropy production involved.[8,9] The choice of reference dynamics is thus important to accentuate the information content in $\mathcal{P}(X(t))$ through the path integral of Eq. (1). Our strategy is to use the most structureless BD with zero force $F_{\rm ref}(x) = 0$. The diffusion coefficient $D_{\rm ref}$ for the reference BD is arbitrary and only contributes to a constant in $\mathcal{S}$. The procedure we designed for evaluating $\mathcal{S}$ can be understood as a two-step thermodynamic integration (1) along the mean force coordinate as the negative KL divergence between the trajectory probabilities for the Langevin dynamics and those for the BD at the same diffusion coefficient $D_{\rm ref} = D$ and (2) along the diffusion coefficient coordinate as the negative KL divergence of the BD with D to that of $D_{\rm ref}$:

$$\mathcal{S}[F(x), D; D_{\rm ref}] = \mathcal{S}_{F_{\rm ref}\to F(x)}(D) + \mathcal{S}_{D_{\rm ref}\to D}(F_{\rm ref} = 0). \tag{3}$$

This design allows us to separate out the deterministic and stochastic contributions, as will be seen shortly.

Path integral of the Onsager-Machlup (OM) action.—Here, our evaluation of the trajectory entropy begins with the probability density of a Langevin path of duration $t_{\rm obs}$ that is proportional to the OM action $E^{\rm OM}[X(t)]$ as:[10–12]

$$\mathcal{P}[X(t)] = e^{-V(x_0)}/Z_{\rm eq}\left(e^{-E^{\rm OM}[X(t)]}/\mathcal{Z}\right) \tag{4}$$

$$\mathcal{Z} = \int \mathcal{D}X(t) e^{-E^{\rm OM}[X(t)]} \tag{5}$$

$$\begin{aligned} E^{\rm OM}[X(t)] =& \frac{1}{2}\left(V(x_{t_{\rm obs}}) - V(x_0)\right) \\ &+ \frac{1}{4}\int_0^{t_{\rm obs}} dt\ \frac{\dot{x}_t^2}{D} + DF^2(x_t) + 2DF'(x_t) \end{aligned} \tag{6}$$

Applying Eqs. (4)–(6) to Eq. (1) with the BD reference and collecting terms lead to the following expression [1]:

$$\begin{aligned}\mathcal{S} = \frac{1}{2}\left\langle V(x_0) + V(x_{t_{\rm obs}})\right\rangle_{X(t)} - \frac{D}{4}\left\langle \int_0^{t_{\rm obs}} dt\, F^2(x_t)\right\rangle_{X(t)} \\ + \frac{1}{4}\left\langle \int_0^{t_{\rm obs}} dt\, \frac{\dot{x}_t^2}{D} - \frac{\dot{x}_t^2}{D_{\rm ref}}\right\rangle_{X(t)} + \ln Z_{\rm eq} + \ln\frac{\mathcal{Z}}{\mathcal{Z}_{\rm ref}}.\end{aligned} \tag{7}$$

The terms in Eq. (7) are taken over the distribution of trajectories of the system dynamics. For an arbitrary functional of $X(t)$, $\langle g[X(t)]\rangle_{X(t)} = \int \mathcal{D}X(t)\mathcal{P}[X(t)]g[X(t)]$. An important consequence of equilibrium dynamics is that the path-integral expectation of single-time functions can be obtained by switching the order of integrating over time $\int dt$ and path $\int \mathcal{D}X(t)$ such that $\langle \int dt g(x_t)\rangle_{X(t)}$ becomes $\int dt \int dx_t g(x_t) p_{\rm eq}(x_t) = t_{\rm obs}\langle g(x)\rangle_{\rm eq}$.[13] Applying this result together with the fact that $\langle V(x)\rangle_{\rm eq} + \ln Z_{\rm eq} = S_{\rm eq}$, Eq. (7) becomes:

$$\begin{aligned}\mathcal{S} = S_{\rm eq} - t_{\rm obs}\frac{D}{4}\left\langle F^2(x)\right\rangle_{\rm eq} \\ + \frac{1}{4}\left\langle \int_0^{t_{\rm obs}} dt\, \frac{\dot{x}_t^2}{D} - \frac{\dot{x}_t^2}{D_{\rm ref}}\right\rangle_{X(t)} + \ln\frac{\mathcal{Z}}{\mathcal{Z}_{\rm ref}}.\end{aligned} \tag{8}$$

The remaining terms can be obtained from the trajectory partition function defined in Eq. (5). Since the origin of stochastic forces of the Langevin equations is the same as that of random diffusion without the deterministic forces, the value of $\mathcal{Z}$ is identical to the result of Brownian dynamics:[14,15]

$$\mathcal{Z}(D) = (4\pi D\Delta t)^{t_{\rm obs}/2\Delta t}. \tag{9}$$

The exponent is the number of time steps used to discretize the trajectory and hence the dimensionality of the path integral in Eq. (1) and Eq. (5). The result of Eq. (9) can also be reached by taking the functional derivative of Eq. (5) with respect to $F(x)$ and observing that the result is zero.[16] Since $\mathcal{Z}$ is the cumulant generator of the OM action defined in

[1]For the $F_{\rm ref} = 0$ reference dynamics we have discarded $V_{\rm ref}$ and set $(Z_{\rm eq})_{\rm ref} = 1$ to ignore the unnecessary scalar offsets.

Eq. (6), the velocity-squared terms in Eq. (7) can be obtained by applying $d\ln(\mathcal{Z})/d(1/D)$ to Eq. (9) and imposing the definition of Eq. (6) to arrive the following expression:

$$\left\langle \dot{x}_t^2 \right\rangle_{X(t)} = \frac{2D}{\Delta t} - D^2 \left\langle F^2(x) \right\rangle_{\text{eq}} . \tag{10}$$

The non-differentiability of Langevin trajectories does cause the velocity-squared term to diverge in the continuum limit of $\Delta t \to 0^+$ as expected, but one immediately sees that the procedure of Eq. (3) removes the divergence with that of the BD reference.

Applying Eq. (10) to Eq. (8), the dependence of trajectory entropy on $F(x)$ reads:

$$\mathcal{S}_{F_{\text{ref}} \to F(x)} = S_{\text{eq}} + t_{\text{obs}} D \left[\frac{D}{4D_{\text{ref}}} - \frac{1}{2} \right] \left\langle F^2(x) \right\rangle_{\text{eq}} . \tag{11}$$

Along the diffusion coefficient coordinate, taking the ratio of trajectory partition functions and adding the $\sim 2D/\Delta t$ terms from the path integral of square velocity leads to the asymptote

$$\mathcal{S}_{D_{\text{ref}} \to D} = \lim_{\Delta t \to 0^+} \frac{t_{\text{obs}}}{2\Delta t} \left[\ln\left(\frac{D}{D_{\text{ref}}} \right) + 1 - \frac{D}{D_{\text{ref}}} \right] . \tag{12}$$

It ought be noted that extending the result of Eqs. (11) and (12) to multiple dimensions only requires a generalized path action and careful integration by parts to give the force expectation term $\langle \vec{F}(x) \cdot \vec{F}(x) \rangle_{\text{eq}}$. The arbitrariness of reference dynamics in the trajectory entropy functional derived above can in fact be eliminated by employing the most disordered dynamics of $F_{\text{ref}}(x) \to 0$ and $D_{\text{ref}} \to \infty$ as the reference model. Discarding the scalar constants irrelevant to $F(x)$ and D in Eqs. (12) and (11) gives the trajectory entropy functional presented in Eq. (2).

Numerical studies.—We next use Eq. (2) to illustrate how the three model PMFs shown earlier in Fig. 2 give rise to different levels of complexity in dynamics despite their identical values of $S_{\text{eq}} = -1.683$. The results of numerical calculations can also serve as an independent validation for the analytical expression derived earlier. In this regard, it is instructive to contrast our results with Jaynes's caliber that considers the statistics of dynamics according to the conditional propagator, $p(x_{\Delta t}|x_0)$ [17–19] with the trajectory entropy. The contours of $p(x_{\Delta t}|x_0)$ at an informative time lag for the three model systems listed in Fig. 2 are shown in Fig. 3. Caliber was originally defined for finite-state Markov models [20] and may be generalized to the continuous space as the conditional entropy for the propagator $p(x_{\Delta t}|x_0)$ at a time resolution Δt:

$$S(\Delta t) = -\int dx_0 dx_{\Delta t}\, p(x_{\Delta t}, x_0) \ln p(x_{\Delta t}|x_0). \tag{13}$$

The caliber thus quantifies both the static and the dynamical complexity of the system within a time slice of Δt (Fig. 1).

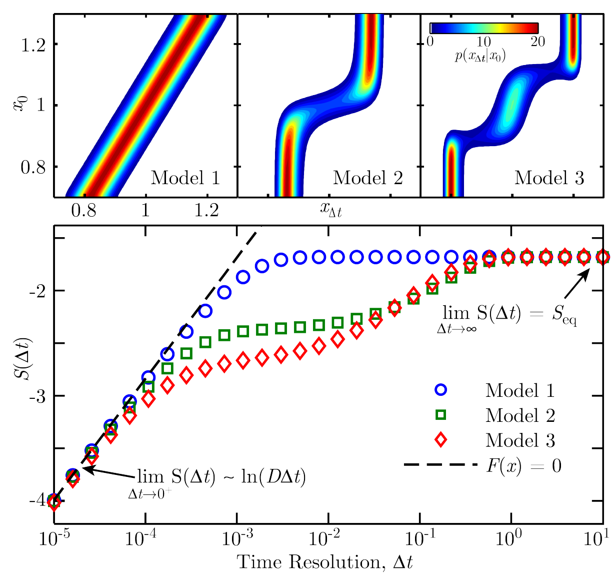

Figure 3: (color online) Conditional entropy of the time propagator. (top) The contours of the transition probability density $p(x_{\Delta t}|x_0)$ for the time propagation of Model 1, 2, and 3 with $\Delta t = 10^{-3}$. (bottom) The conditional entropy as a function of Δt for the 3 model systems. In all cases, $D = 1$ in the dimensionless unit.

At a specified value of Δt, Eq. (13) can be evaluated by solving the corresponding Fokker-Planck equation using standard numerical schemes or averaging over Langevin trajectories.[2] As shown in Fig. 3, variation of the caliber with Δt can be used to gain insight about the system dynamics. As $\Delta t \to \infty$, the conditional probability density converges to $p_{eq}(x)$

and the information about dynamics is lost. In the continuum limit of $\Delta t \to 0^+$, the conditional entropy diverges at a rate of $\sim \ln(D\Delta t)$ due to the non-differentiability of the Weiner process.[14,15] By scanning Δt, the caliber does reveal differences in the dynamical contents of the three distinct models at intermediate Δt. However, the relative contributions from the deterministic and stochastic forces to dynamics are obscure in the caliber integral.

Since the caliber represents a temporal slice of the trajectory entropy (cf. Fig. 1),[16,17,21] applying Eq. (11) indicates that the KL divergence of the caliber,

$$S_{\mathrm{KL}}(\Delta t) = -\int dx_0 dx_{\Delta t} p(x_{\Delta t}, x_0) \ln p(x_{\Delta t}|x_0)/q(x_{\Delta t}|x_0).$$

Here, $q(x_{\Delta t}|x_0)$ is the conditional probability density of the time propagation of BD, would follow $S_{\mathrm{KL}}(\Delta t)/\Delta t \to -D/4\,\langle F^2(x)\rangle_{\mathrm{eq}}$ in the continuum limit when $D = D_{\mathrm{ref}}$. Therefore, numerical calculations of $S_{\mathrm{KL}}(\Delta t)/\Delta t$ can be used to compare with the values given by Eq. (11) that constitutes the deterministic part of the trajectory entropy, and Fig. 4 illustrates the quantitative agreement as $\Delta t \to 0^+$. Table 1 summarizes this numerical validation of Eq. (11) for the three models shown in Fig. 2. The dynamics of Model 3 is approximately ten times more "complex" than that in Model 1 due to the greater mean forces in having two additional wells. It is clear that the trajectory entropy enables a direct and immediate identification for the origin of the differing complexity in dynamical trajectories.

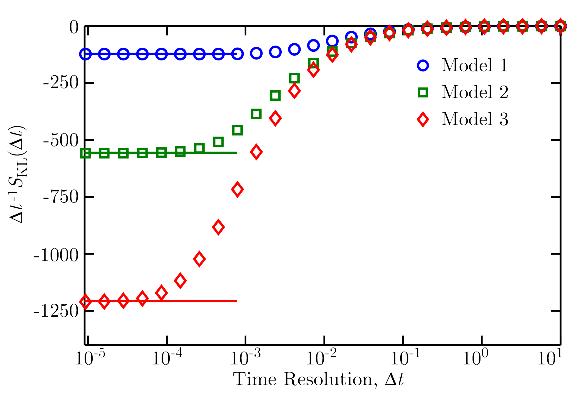

Figure 4: (color online) Comparison of numerical and analytical $S_{\mathrm{KL}}(\Delta t)$ for the three model systems at different levels of time resolution Δt. The horizontal lines indicate the analytic prediction of $-D/4\langle F^2(x)\rangle_{\mathrm{eq}}$ in the continuum limit. In this comparison, $D = D_{\mathrm{ref}}$.

Table 1: Numerical calculations of $S_{\mathrm{KL}}(\Delta t)$ for the three model systems discussed in this letter. $q(x_{\Delta t}|x_0)$ is the reference time propagator of BD with the same diffusion constant $D = 1$ in the dimensionless unit. When $D_{\mathrm{ref}}{=}D$, the relation between the trajectory entropy and $S_{\mathrm{KL}}(\Delta t)$ leads to $S_{\mathrm{KL}}(\Delta t)/\Delta t \to -D/4\,\langle F^2(x)\rangle_{\mathrm{eq}}$ in the continuum limit as discussed in the text.

Functionals	Model 1	Model 2	Model 3
$-\int dx p_{\mathrm{eq}}(x) \ln p_{\mathrm{eq}}(x)$	-1.683	-1.683	-1.683
[2] $\Delta t^{-1} S_{\mathrm{KL}}(\Delta t)$	-123.6	-558.6	-1210
[3] $-D/4\langle F^2(x)\rangle_{\mathrm{eq}}$	-123.5	-558.7	-1211

Concluding perspective.—This work illustrates how the path integral of the entire continuous stochastic trajectory ensemble can be compressed into an analytic functional. The results provide a foundation for understanding the dynamics due to fluctuations in systems that can be modeled by an over-damped Langevin equation. In addition to the examples noted in the introductory paragraph of this Letter, a potential application is using the expression of the trajectory entropy in design equations of information processing for dynamic systems. For systems that propagate quantum information, for example, the commonly employed modeling equations are isomorphic to the Langevin equation discussed here.[22] For future works generalizing the ideas to non-equilibrium cases and to more complex dynamics such as those with memory effects, the analytical result presented here—which is valid for an arbitrary potential of mean force—can serve as a general starting reference.

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