Analytical Mechanics in Stochastic Dynamics: Most Probable Path, Large-Deviation Rate Function and Hamilton-Jacobi Equation

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Abstract

Analytical (rational) mechanics is the mathematical structure of Newtonian deterministic dynamics developed by D’Alembert, Langrange, Hamilton, Jacobi, and many other luminaries of applied mathematics. Diffusion as a stochastic process of an overdamped individual particle immersed in a fluid, initiated by Einstein, Smoluchowski, Langevin and Wiener, has no momentum since its path is nowhere differentiable. In this exposition, we illustrate how analytical mechanics arises in stochastic dynamics from a randomly perturbed ordinary differential equation \( dX_t = b(X_t)dt + \epsilon dW_t \) where \( W_t \) is a Brownian motion. In the limit of vanishingly small \( \epsilon \), the solution to the stochastic differential equation other than \( \dot{x} = b(x) \) are all rare events. However, conditioned on an occurrence of such an event, the most probable trajectory of the stochastic motion is the solution to Lagrangian mechanics with \( L = \|\dot{q} - b(q)\|^2/4 \) and Hamiltonian equations with \( H(p, q) = \|p\|^2 + b(q) \cdot p \). Hamiltonian conservation law implies that the most probable trajectory for a “rare” event has a uniform “excess kinetic energy” along its path. Rare events can also be characterized by the principle of large deviations which expresses the probability density function for \( X_t \) as \( f(x, t) = e^{-u(x, t)/\epsilon} \), where \( u(x, t) \) is called a large-deviation rate function which satisfies the corresponding Hamilton-Jacobi equation. An irreversible diffusion process with \( \nabla \times b \neq 0 \) corresponds to a Newtonian system with a Lorentz force \( \ddot{q} = (\nabla \times b) \times \dot{q} + \frac{1}{2} \nabla \|b\|^2 \). The connection between stochastic motion and analytical mechanics can be explored in terms of various techniques of applied mathematics, for example, singular perturbations, viscosity solutions, and integrable systems.

1 Introduction

Dynamics as an analytical concept is one of the most important contributions of mathematics to modern thinking. Currently there are three fundamentally different types of dynamics: classical, quantum, and stochastic [1]. Quantum dynamics aside, classical dynamics in term of deterministic “trajectories” of a system, continuous or not, is still the dominant model in quantitative science and engineering. However, rapid development of quantitative biology in recent years, and the sustained interests in statistical physics, has pushed the third, stochastic dynamics, to the forefront of applied mathematics. For recent reviews on Darwinian dynamics and the Delbrück-Gillespie process
for cellular biochemical systems, see [1][2]. Novel and even non-orthodox stochastic dynamic approaches to quantum phenomena can be found in [3][4][5]. Describing the celestial mechanical system of a few interacting bodies, Newton’s equations of motion in terms of classical dynamics is one of the most successful mathematical models known to mankind. An in-depth study of the subject in terms of analytical mechanics exposes one to a wide range of applied mathematical theories and techniques: Hamiltonian systems, Lagrangian principle, and Hamilton-Jacobi equations are several shining jewels of the treasure box [6][7][8].

In this exposition, we shall illustrate that much of these classical, deterministic mathematics also emerge naturally in the theory of stochastic dynamics, when one is interested in the relationship between stochastic and deterministic dynamics. This is reminiscent of the semi-classical theory of quantum dynamics developed in the 1970s [9]. More importantly, not only are they useful as tools for solving problems, several quantities also acquired a strong probabilistic meaning, such as large deviation rate functions and most probable paths.

Even though stochastic dynamics is often described in terms of its probability distribution changing with time, we need to emphasize, at the onset, that neither the distribution perspective, nor a trajectory perspective, is a complete description of a stochastic process. The mathematical notion of a random variable, developed by A. Kolmogorov, can not rest solely on its distribution function, nor its realizations [10]. It is truly an independent new mathematical object with deep philosophical consequences.

### 2 Stochastic Dynamics in Terms of Stochastic Differential Equations and Diffusion Processes

One of the extensively studied problems that connect stochastic and deterministic dynamics is an ordinary differential equation with small random perturbations [11]. Let us consider a diffusion process $X_t$ with the stochastic differential equation

$$dX_t = b(X_t)dt + \sqrt{2\epsilon}dB_t,$$

and the corresponding Kolmogorov forward equation

$$\frac{\partial f(x,t)}{\partial t} = \epsilon \frac{\partial^2 f}{\partial x^2} - \frac{\partial}{\partial x} (b(x)f(x,t)).$$

In the limit of $\epsilon = 0$, (2) is formally reduced to the first-order partial differential equation (PDE):

$$\frac{\partial f(x,t)}{\partial t} = - \frac{\partial}{\partial x} (b(x)f(x,t)),$$

1Two issues immediately come to mind: (i) The mathematical theory of probability requires all possible outcomes being known a priori, in the very definition of a random variable. This makes the concept of a random variable only retrospective. In statistics, this is intimately related to the concept of a prior distribution; and in economics this distinguishes risk from uncertainty. (ii) Classical dynamics has trajectories but only singular distributions; quantum dynamics has distributions but no trajectories due to Heisenberg’s uncertainty principle; stochastic dynamics requires both perspectives.
which is equivalent to, according to Liouville’s theorem, a nonlinear ordinary differential equation (ODE)

\[
\frac{dx(t)}{dt} = b(x(t)). \tag{4}
\]

It is known that on any finite time interval \( t \in [0, T] \), the solution to Eq. (1) with initial value \( X_0 = x_0 \) approaches the solution of the ODE with probability 1 [11].

If we write \( f(x, t) = e^{u(x, t)} \), then the linear PDE (3) becomes

\[
\frac{\partial u(x, t)}{\partial t} = -b(x) \frac{\partial u(x, t)}{\partial x} - \frac{db(x)}{dx}, \tag{5}
\]
a linear, first-order partial differential equation.

Now for Eq. (2), let us assume \( f(x, t) = e^{-u_\epsilon(x, t)/\epsilon} \), widely known as the WKB ansatz. Then we have

\[
\frac{\partial u_\epsilon(x, t)}{\partial t} = - \left( \left( \frac{\partial u_\epsilon}{\partial x} \right)^2 + b(x) \frac{\partial u_\epsilon}{\partial x} \right) + \epsilon \left[ \frac{\partial^2 u_\epsilon}{\partial x^2} + \frac{db(x)}{dx} \right]. \tag{6}
\]

Therefore, to leading order, if \( \lim_{\epsilon \to 0} u_\epsilon(x, t) = u(x, t) \) exists and is differentiable, one has

\[
\frac{\partial u(x, t)}{\partial t} = - \left( \frac{\partial u(x, t)}{\partial x} \right)^2 - b(x) \frac{\partial u(x, t)}{\partial x}. \tag{7}
\]

Eq. (7) is widely called the Hamilton-Jacobi, or Eikonal, equation (HJE) [12, 13]. Note that this equation is different from Eq. (5): It is a nonlinear, first-order PDE. As we shall discuss below, the solution to (5) is the limit of equation (2) when \( \epsilon \to 0 \). The solution to (7) is the convergence rate of that limiting process. \( u(x, t) \) is called the large-deviation rate function.

To relate a continuous random variable \( X \) with probability density function \( f_X(x) \) to a deterministic quantity, the expected value \( E[X] \) and modal value \( x^* \), with \( f(x^*) \geq f(x) \), are often taken as the counterpart. Let us now consider a local minimum of the function \( u(x, t) \) located at \( x = x^*(t) \). How does the location and the value of the minimum change with time? According to Eq. (7):

\[
\frac{du^*(t)}{dt} = \left[ \frac{\partial u(x, t)}{\partial t} + \left( \frac{\partial u(x, t)}{\partial x} \right) \frac{dx^*(t)}{dt} \right]_{x=x^*(t)} \tag{8}
\]

\[
= \left[ - \left( \frac{\partial u(x, t)}{\partial x} \right)^2 - b(x) \frac{\partial u(x, t)}{\partial x} + \left( \frac{\partial u(x, t)}{\partial x} \right) \frac{dx^*(t)}{dt} \right]_{x=x^*(t)}
\]

\[
= 0.
\]

Also from Eq. (7) we have:

\[
0 = \frac{d}{dt} \left( \frac{\partial u(x^*(t), t)}{\partial x} \right) \left|_{x=x^*(t)} \right. = \left[ \frac{\partial^2 u(x, t)}{\partial x \partial t} + \frac{\partial^2 u(x, t)}{\partial x^2} \left( \frac{dx^*(t)}{dt} \right) \right]_{x=x^*(t)}. \tag{9}
\]
Therefore,

\[
\frac{dx^*(t)}{dt} = -\left[ \left( \frac{\partial^2 u(x, t)}{\partial x^2} \right)^{-1} \frac{\partial^2 u(x, t)}{\partial x \partial t} \right]_{x=x^*(t)}
\]

\[
= \left[ \left( \frac{\partial^2 u(x, t)}{\partial x^2} \right)^{-1} \left( 2 \frac{\partial u(x, t)}{\partial x} \frac{\partial^2 u(x, t)}{\partial x^2} + \frac{dB(x)}{dx} \frac{\partial u(x, t)}{\partial x} + b(x) \right) \frac{\partial^2 u(x, t)}{\partial x^2} \right]_{x=x^*(t)}
\]

\[
= b(x^*(t)).
\]  

(10)

So indeed, the modal values follow the ODE (4). For an ODE with multiple domains of attraction, they correspond to a multi-modal distribution. Furthermore,

\[
\frac{d}{dt} \left( \frac{\partial^2 u(x^*(t), t)}{\partial x^2} \right) = \left[ \frac{\partial^3 u(x, t)}{\partial x^2 \partial t} + \frac{\partial^3 u(x, t)}{\partial x^3} \left( \frac{dx^*(t)}{dt} \right) \right]_{x=x^*(t)}
\]

\[
= \left[ -\left( \frac{\partial u}{\partial x} \right) \left( 2 \frac{\partial^3 u}{\partial x^3} + \frac{dB(x)}{dx} \right) - 2 \left( \frac{\partial^2 u}{\partial x^2} \right)^2 \right.
\]

\[
\left. -2 \frac{dB(x)}{dx} \frac{\partial^2 u}{\partial x^2} + \left( \frac{dx^*(t)}{dt} - b(x) \right) \frac{\partial^3 u}{\partial x^3} \right]_{x=x^*(t)}
\]

\[
= -2 \left( \frac{dx^*(t)}{dx} + \frac{\partial^2 u(x^*(t), t)}{\partial x^2} \right) \frac{\partial^2 u(x^*(t), t)}{\partial x^2}.
\]  

(11)

Hence, the value \( u(x^*(t), t) \) does not change, and its location follows the ordinary differential equation \( \dot{x} = b(x) \). A local minimum of the function \( u(x, t) \) follows the corresponding deterministic ODE. Furthermore, the curvature about it follows Eq. (11).

Since \( u(x, t) \) is the rate of convergence of a normalized probability distribution for \( X_t \) when \( \epsilon \to 0 \), it is a non-negative function with its minima necessarily zero. In fact, except for the very critical condition known as phase transition, the minimum is unique. Eqs. (8) and (10) state that if an initial \( u(x, 0) \) is non-negative with a global minimum zero, \( u(x, t) \) will remain non-negative with global minimum zero. In other words, the properties of being a large-deviation rate function are preserved.

Finally, observing that the values of local minima are related to the probability associated with each “attractor”, Eq. (5) states that diffusion processes in different “attractors” are almost reducible in the limit of \( \epsilon \to 0 \). Generically speaking, besides the dominant attractor with the global minimum of \( u(x, t) \), the probability of each attractor with a local minimum vanishes. This results in the Law of Large Numbers.

However, conditioned upon being outside the dominant attractor, there will be another global attractor. These states are known as metastable in statistical physics.
3 The Probabilistic Interpretation of $u(x, t)$

We now give the precise meaning for $u(x, t)$. Let us denote the solution to Eq. (2), with initial condition $f(x, 0) = \delta(x - x_o)$. As the solution to (2), the transition probability $f_\epsilon(x, t|x_o)$ is the fundamental solution to the linear PDE. For fixed $x, t, \text{ and } x_o$, when $\epsilon \to 0$, one has

$$\lim_{\epsilon \to 0} f_\epsilon(x, t) = \delta (x - x_t),$$

where $x_t$ is the solution to the ODE $\dot{x}_t = b(x_t)$ with initial value $x_o$. Or in a more authentic probabilistic notation:

$$\lim_{\epsilon \to 0} \Pr \{|X_t(\epsilon; x_o) - x_t| > \epsilon\} = 0.$$  

(13)

We therefore can introduce the rate of convergence:

$$\lim_{\epsilon \to 0} -\epsilon \ln \Pr\{x < X_t(\epsilon; x_o) \leq x + dx\} = u(x, t; x_o).$$

(14)

3.1 Laws of large numbers, central limit theorem and theory of large deviations

Let us consider a sequence of iid (independent, identically distributed) $X_i$ and their mean value

$$Z_n = \frac{1}{n} \sum_{i=1}^{n} X_i.$$  

(15)

The weak law of large numbers (LLN) states that

$$\lim_{n \to \infty} Z_n = \mu^*, \quad \mu^* = E[X].$$

(16)

That is, the probability density function for a continuous random variable

$$\lim_{n \to \infty} f_{Z_n}(z) = \delta (z - \mu^*), \quad \mu^* = E[X].$$

(17)

Furthermore, the central limit theorem states that

$$\lim_{n \to \infty} \frac{1}{\sqrt{n}} f_{Z_n} \left( \frac{x}{\sqrt{n}} + \mu^* \right) = \frac{1}{\sqrt{2\pi \sigma^2}} e^{-x^2/(2\sigma^2)}, \quad \sigma^2 = Var[X].$$

(18)

We note that the result in Eq. (15) implies Eq. (17), which implies Eq. (16).

The large-deviation rate function for the LLN given in Eq. (16) is defined as

$$u(x) = \lim_{n \to \infty} -\frac{1}{n} \ln f_{Z_n}(x).$$

(19)

Note that the convergence of the probability distribution functions in Eq. (17) is always non-uniform. Asymptotics beyond all orders, therefore, necessarily enters the theory of large deviations.
According to Chernoff’s formula [14], \( u(x) \) is related to the cumulant generating function (CGF), \( \lambda(\theta) \), for the random variable \( X \):

\[
\lambda(\theta) = \ln E \left[ e^{-\theta X} \right],
\]

via the Fenchel-Legendre transform

\[
\lambda(\theta) = \sup_x \{ \theta x - u(x) \}.
\]

Furthermore, we know that the Fenchel-Legendre transform of \( \lambda(\theta) \),

\[
u^*(x) = \sup_{\theta} \{ x \theta - \lambda(\theta) \},
\]

is the affine regularization of \( u(x) \). \( u^*(x) \) is a convex function; it is identical to \( u(x) \) in the neighbourhood of the global minimum of \( u(x) \). Cumulant (or the Thiele semi-invariants) expansion has recently found applications in renormalization-group approach to singular perturbation [15].

From Eq. (22) and the basic properties of the Fenchel-Legendre transform, we have

\[
\min_x u^*(x) = -\lambda(0) = 0,
\]

\[
x \big|_{u^*(x) = 0} = \lambda'(\theta) \big|_{\theta = 0} = E[X] = \mu^*.
\]

\[
\frac{d^2}{dx^2} u^*(x) \big|_{x = \mu^*} = (\lambda''(\theta) \big|_{\theta = 0})^{-1} = (Var[X])^{-1} = \frac{1}{\sigma^2}.
\]

Therefore, we have in the neighbourhood of global minimum of \( u(x) \), \( x = \mu^* \):

\[
u(x) = u^*(x) = \frac{(x - \mu^*)^2}{2\sigma^2} + a_3(x - \mu^*)^3 + \cdots.
\]

While \( u^*(x) \) is convex, \( u(x) \) need not be. Hence, away from the global minimum \( x = \mu^* \), \( u(x) \) can have many local minima. Let us denote their locations as \( x_\ell \) and with corresponding local expansions

\[
u(x) = u(x_\ell) + \frac{a_\ell}{2} (x - x_\ell)^2 + \cdots, \quad \ell = 1, 2, \cdots
\]

in which \( u(x_\ell) > 0 \) and \( a_\ell > 0 \). The \( f_{Z_n}(x) \) then has an asymptotic expansion

\[
f_{Z_n}(x) = e^{-nu(x) + o(n)} = \sqrt{\frac{n}{2\pi\sigma^2}} e^{-nu(x) + o(n)}.
\]
Eq. (28) implies Eq. (18) in the following sense:

\[
\int_{-\infty}^{\infty} \left\| f_{Z_n}(x) - \sqrt{\frac{n}{2\pi \sigma^2}} e^{-\frac{n(x-\mu^*)^2}{2\sigma^2}} \right\| dx = \int_{-\infty}^{\infty} \left\| \sqrt{\frac{n}{2\pi \sigma^2}} e^{-\frac{n(x-\mu^*)^2}{2\sigma^2}} \right\| dx \approx \int_{-\infty}^{\infty} \left\| \sqrt{\frac{n}{2\pi \sigma^2}} e^{-\frac{n(x-\mu^*)^2}{2\sigma^2}} \right\| dx = \frac{1}{\sqrt{n}} \int_{-\infty}^{\infty} e^{-\frac{a_3 x^3}{\sqrt{n}}} + o\left(\frac{1}{\sqrt{n}}\right) \ dx.
\]

That is, the convergence of the distribution in Eq. (18) is in $L_1$ and it is of the order $\frac{1}{\sqrt{n}}$.

Note that the non-convex parts of $u(x)$, as given in Eq. (27), only contribute to terms on the order of

\[
e^{-nu(x)} \int_{-\infty}^{\infty} e^{-\frac{n u(x-x^*)^2}{2 a^2}} \ dx = \sqrt{\frac{2\pi}{na_\ell}} e^{-nu(x^*)}.
\]

It is exponentially small, i.e., beyond all orders.

### 3.2 Linear dynamics, Gaussian processes, and an exactly solvable HJE

We now consider the SDE in (1) with linear drift, i.e., a Gaussian process:

\[
dX_t = -bX_t \, dt + \sqrt{2\epsilon} \, dB_t.
\]

The corresponding Kolmogorov forward equation is

\[
\frac{\partial f(x,t)}{\partial t} = \epsilon \frac{\partial^2 f}{\partial x^2} + \frac{\partial}{\partial x} \left( bx f(x,t) \right),
\]

and the WKB ansatz leads to the PDE

\[
\frac{\partial u(x,t)}{\partial t} = - \left[ \left( \frac{\partial u(x)}{\partial x} \right)^2 - bx \frac{\partial u(x)}{\partial x} \right] + \epsilon \left[ \frac{\partial^2 u(x)}{\partial x^2} - b \right]
\]
for \( u_\epsilon(x, t) \). We can express
\[
  u_\epsilon(x, t) = a(t) + \frac{(x - \mu(t))^2}{2\sigma^2(t)}, \tag{33}
\]
then we have a set of nonlinear ODEs:
\[
  \frac{d}{dt}\sigma^2(t) = 2 \left( 1 - b\sigma^2(t) \right), \tag{34a}
\]
\[
  \frac{d\mu(t)}{dt} = -b\mu(t), \tag{34b}
\]
\[
  \frac{da(t)}{dt} = +\epsilon \left( \frac{1}{\sigma^2} - b \right). \tag{34c}
\]
Their explicit solution is
\[
  \sigma^2(t) = \frac{1}{b} + \left( \sigma^2(0) - \frac{1}{b} \right) e^{-2bt}, \tag{35a}
\]
\[
  \mu(t) = \mu(0)e^{-bt}, \tag{35b}
\]
\[
  a(t) = \frac{\epsilon}{2} \ln \left( \frac{\sigma^2(t)}{\sigma^2(0)} \right) + a(0). \tag{35c}
\]
Assembling these together, we have
\[
  e^{-u_\epsilon(x, t)/\epsilon} = \frac{A}{\sqrt{2\pi\epsilon\sigma^2(t)}} \exp \left\{ -\frac{(x - \mu(t))^2}{2\epsilon\sigma^2(t)} \right\}, \tag{36}
\]
where \( A = \sqrt{2\pi\epsilon\sigma^2(0)}e^{-a(0)/\epsilon} \) is a constant.

We note that in Eq. (34), the \( \epsilon \) term only contributes to \( a(t) \). This is a very surprising result: The diffusive behavior characterized by \( \sigma^2(t) \) actually is determined by a first-order nonlinear PDE (7)!

### 3.3 Large-deviation rate function on a circle

We now consider dynamics on a circle \( \theta \in S^1[0, 1] \) with periodic angular velocity \( \dot{\theta} = b(\theta) = b(\theta + 1) \). In general, a saddle-node bifurcation on the cycle gives rise to a counter-clockwise or clockwise cyclic motion when either \( b(\theta) > 0 \) or \( b(\theta) < 0 \) \( \forall \theta \in [0, 1] \). We have shown above that the corresponding large-deviation rate function \( u(\theta) \) has its minima and maxima corresponding to the stable and unstable fixed points. We now illustrate that corresponding to this cyclic motion, \( u(\theta) \) becomes a constant on the entire circle.

Without losing generality, we shall assume there is only one minimum and one maximum of \( u(x, t) \) and let \( x(t) \) and \( y(t) \) be the location of the minimum of \( u(\theta, t) \)
and the corresponding curvature. We are interested in how $x$ and $y$ behave in the infinitely long time limit. Following Eqs. (10) and (11) we have

\[
\begin{align*}
\frac{dx}{dt} &= b(x), \quad (37a) \\
\frac{dy}{dt} &= -2 \left(b'(x) + y\right) y. \quad (37b)
\end{align*}
\]

Fig. 1 graphically shows the occurrence of a Hopf bifurcation in this autonomous planar system in $\mathbb{R}^2$, corresponding to a saddle-node bifurcation of $b(\theta)$ on the circle $S^1$.

We now show for the case of $\dot{x} = b(x) > 0$ periodic solution as shown in Fig. 1B, with $y(t) \to 0$ asymptotically. Since $x(t)$ is a periodic function of $t$, $b'(x(t))$ is also periodic. Furthermore,

\[
\phi(t) = \int_0^t b' \left(x(s)\right) ds = \int_0^t \frac{b'(x(s))}{b(x(s))} \left(\frac{dx(s)}{ds}\right) ds = \ln b(x(t)) + \text{const.} \quad (38)
\]

is also a periodic function of time. Then

\[
\frac{dy}{dt} = -2 \left(\frac{d\phi(t)}{dt} + y\right) y. \quad (39)
\]

This equation can be re-written as

\[
\frac{d}{dt} \left(y(t)e^{2\phi(t)}\right) = -2 \left(y(t)e^{2\phi(t)}\right)^2 e^{-2\phi(t)}.
\]

The right-hand-side of Eq. (40) is $\leq 0$ and it is 0 iff $y(t) = 0$. Therefore, $y(t) \to 0$ if $y(0) > 0$. In other words, the curvature approaches zero. The large deviation function along a limit cycle is a constant [17].

4 A “Fictitious” Classical Newtonian Motion

Eq. (7) has the form of a Hamilton-Jacobi equation (HJE) for a classical Newtonian motion according to analytical mechanics [6, 7, 8].

4.1 A Hamiltonian system

In analytical mechanics, the solution $u(x, t)$ to the HJE, a nonlinear PDE like (7), is called a principal function. $u(x, t)$ furnishes the entire family of orbits, i.e., a flow, corresponding to an associated Hamiltonian dynamical system in terms of a system of nonlinear ODEs.

The Hamiltonian system, with time-independent Hamiltonian $^2$

\[
H(q, p) = p^2 + b(q)p, \quad (41)
\]

is a classical Newtonian motion. The Hamiltonian associated with a discrete birth-and-death process (B&DP) with birth and death rates $u_n$ and $w_n$, is $H(p, q) = u(q)e^p + w(q)e^{-p} - u(q) - w(q)$ where $u(q)$ and $w(q)$ are the continuous limits of $u_n$ and $w_n$. Note this $H(p, q)$ is reduced to Eq. (41) if $p \ll 1$. The B&DP and diffusion corresponding to very different forms of the HJE leads to the diffusion’s dilemma [18].
is a system of autonomous ODEs

\[
\begin{aligned}
\dot{q} &= \frac{\partial H}{\partial p} = 2p + b(q), \\
\dot{p} &= -\frac{\partial H}{\partial q} = -p \frac{db(q)}{dq}.
\end{aligned}
\]  
(42)

It is a re-formulation of a Newton’s “equation of motion”

\[
\frac{d^2q}{dt^2} = b(q) \frac{db(q)}{dq} = \frac{d}{dq} \left( \frac{b^2(q)}{2} \right).
\]  
(43)

This “fictitious” analytical mechanical system associated with stochastic dynamics has been identified and explored by Graham and Tel [19], and in the even earlier work of Martin-Siggia-Rose [20].

According to analytical mechanics, the Hamiltonian system also has a corresponding “Lagrangian”

\[
\mathcal{L} [q, \dot{q}] = [p \dot{q} - H(q, p)]_{p=\frac{1}{2} (q - b(q))} = \left( \frac{\dot{q} - b(q)}{2} \right)^2,
\]  
(44)

with the action functional,

\[
S_0 [q(t); (t_0, q(t_0)) \rightarrow (t, q(t))] = \int_{t_0}^{t} \frac{1}{4} \left[ \frac{dq(s)}{dt} - b(q(s)) \right]^2 ds.
\]  
(45)

In classical mechanics, the action has never had a “meaning” more than being a mathematical device which provides trajectories for a mechanical motion. In the present work, however, \(e^{-S_0/\epsilon}\) turns out to be exactly the probability of a path of the stochastic dynamics in [1] with vanishing \(\epsilon\). For finite \(\epsilon\), the generalized Onsager-Machlup functional is \(S_\epsilon = S_0 + (\epsilon/2) b'(q)\) [21, 22, 23, 24]. The action functional in Eq. (45) plays a central role in Freidlin-Wentzell’s theory of large deviations [11]. Also see [25] for a rigorous mathematical treatment and [26] for a monograph with an applied mathematical bend.

One should not confuse the present Hamiltonian system with a more involved Hamiltonian formulation associated with stochastic dynamics recently proposed in [27].

4.2 Path integral formalism for the probability of a diffusion process

We now show heuristically that the path integral in Eq. (45) represents the probability of a diffusion process according to Eq. (2). Statistical physicists have long used it as a useful mathematical tool, starting with Onsager and Machlup [21] for Gaussian processes and later by Haken, Hunt and Ross [22, 24] for the general diffusion process. See [28] for its application in the protein folding problem and [29] for a very recent study on nonequilibrium steady-state physics using this formalism.
First, let us consider the solution to a simple one-dimensional diffusion process defined by Eq. (1) with a linear drift $bx$. The corresponding Fokker-Planck equation has the fundamental solution

$$f(x, t + \Delta t | x', t) = \frac{1}{\sqrt{4\pi \epsilon \Delta t}} \exp \left[ -\frac{(x - x'e^{b\Delta t})^2}{2(\epsilon/b) (e^{2b\Delta t} - 1)} \right]$$

$$\approx \frac{1}{\sqrt{4\pi \epsilon \Delta t (1 + b \Delta t)}} \exp \left[ -\frac{(x - x' - bx' \Delta t)^2}{4\epsilon \Delta t} \right].$$

(46)

Now for the solution to the general Eq. (2) with drift $b(x)$, the probability density of a trajectory is approximately

$$f(x_n, n\Delta t; x_{n-1}, (n-1)\Delta t; \cdots; x_1, \Delta t|x_0, 0)$$

$$= \frac{1}{\sqrt{4\pi \epsilon \Delta t}} \prod_{i=1}^{n} \exp \left[ -\frac{(x_i - x_{i-1} - b(x_{i-1})\Delta t)^2}{4\epsilon \Delta t} - \frac{1}{2} \ln (1 + b'(x_i)\Delta t) \right]$$

$$\approx A \exp \left\{ -\frac{1}{4\epsilon} \int_0^t \left[ \left( \frac{dx(t)}{dt} - b(x(t)) \right)^2 + 2\epsilon b'(x(t)) \right] dt \right\} = Ae^{-\frac{1}{2} S[x(t)]},$$

(47)

where $t = n\Delta t$ and $A$ is an appropriate normalization factor. Note that according to Wiener’s theory of diffusion, the stochastic trajectory $x(t)$ is nowhere differentiable. Hence, the use of $dx(t)/dt$ in Eq. (47) is heuristic, and only becomes mathematically meaningful in the limit $\epsilon = 0$. See [25] and [11] for a rigorous treatment.

4.3 Conditional probability interpretation of “excess kinetic energy”

A Hamiltonian system has a conserved quantity: the $H(p(t), q(t))$, along each and every trajectory. If we re-arrange the first equation in (42), we obtain

$$p = (\dot{q} - b(q))/2.$$ 

Then,

$$H(p, q) = p(p + b(q)) = \frac{1}{4} (\dot{q} - b(q)) (\dot{q} + b(q)) = \frac{1}{4} \{\dot{q}^2 - b^2(q)\},$$

that is

$$\dot{q}^2 = b^2(q) + 4H,$$

(48)

in which $H$ is constant along a trajectory. Comparing this with the noiseless trajectory $\dot{q} = b(q)$ with $H = 0$, we see there is a constant $4H$ added to the $\dot{q}^2$. This result can be interpreted as follows.

We shall call the square of the velocity $\dot{q}^2$ the “kinetic energy”. A noiseless trajectory, i.e., the one with $H = 0$, follows the differential equation $\dot{q} = b(q)$. This means
that with starting time \( t = t_1 \) at position \( q_1 \), the noiseless trajectory will be precisely at \( q_2 \) at time \( t_2 \). Any other trajectories arriving at \( q_2 \) with a different time are impossible for deterministic dynamics, and are rare events when \( \epsilon \) is small. If, however, one observes such a rare event: motion from \( q_1 \) to \( q_2 \) with a time \( \hat{t}_2 \neq t_2 \), what will be the “most probable trajectory among all possible \( \hat{q}(t) \) with \( \hat{q}(t_1) = q_1 \) and \( \hat{q}(\hat{t}_2) = q_2 \)?

This is a problem of conditional probability. Among all the rare trajectories,

\[ \{ \hat{q}(t) | \hat{q}(t_1) = q_1, \hat{q}(\hat{t}_2) = q_2, \hat{t}_2 \neq t_2 \} \]

the most probable one follows a solution to the Hamiltonian system with an appropriate \( H \neq 0 \).

More explicitly, since \( \hat{q}(t) \) arrives at \( q_2 \) with a time different from \( t_2 \), say \( \hat{t}_2 < t_2 \), then it has to be speeded up compared to \( q(t) \). On the other hand, if \( \hat{t}_2 > t_2 \), it has to be slowed down. The solution to the Hamiltonian equation states that the most probable trajectory is the one having a constant amount of excess kinetic energy \((4H)\) added or reduced along the trajectory. In the theory of probability, this is a consequence of the van Campenhout-Cover theorem [31].

The fictitious Hamiltonian system, therefore, is the consequence of stochastic dynamics conditioned on the occurrence of a rare event. The kinetic energy exists “retrospectively” in some stochastic dynamics.

5 Solutions to the Hamilton-Jacobi Equation (HJE)

Since the HJE is a nonlinear PDE, there is no systematic method to obtain its solution for arbitrary initial data. Rather, there are classes of solutions one can obtain; exactly or approximately. Since this is a rather developed area of applied mathematics, we shall only touch upon some issues highly relevant to our mission.

5.1 A class of exact solutions

The standard way to solve a HJE is precisely by solving its corresponding Hamiltonian dynamics in terms of the ODEs. Since the Hamiltonian \( H(q,p) \) does not depend explicitly on time, one can verify that \( u(x,t) = u_0(x) - Et \) is a solution to HJE (7) if \( u_0(x) \) is a solution to

\[ H \left( \frac{du_0(x)}{dx}, x \right) = E. \quad (49) \]

Therefore,

\[ u(x,t) = \int_{x_0}^{x} p(q) dq - Et = \frac{1}{2} \int_{x_0}^{x} \left( -b(z) \pm \sqrt{b^2(z) + 4E} \right) dz - Et. \quad (50) \]

Initial data \( u_0(x) \) satisfying Eq. (49) is called characteristic initial data [32].

For \( E = 0 \), \( u(x,t) = u_0(x) \) \( \forall t \). Hence it is a stationary solution to the HJE. In this case, Eq. (49) yields

\[ u^{st}(x) = - \int_{0}^{x} b(z) dz \quad (51) \]
and a trivial solution \( u_0(x) \). The solution in Eq. (51) corresponding to \( E = 0 \) is the expected stationary solution.

5.2 Solutions via characteristics

The solutions given in Eq. (50) is in a special class. Certainly not any initial data \( u(x, 0) \) is characteristic. More importantly, the \( u(x, t) \) in (50) can not satisfy the basic properties of a large deviation rate function: It has to be non-negative with its minimum exactly being zero. Therefore, we need to look for other possible solutions to the HJE (7) corresponding to noncharacteristic initial data [32].

According to Evans [32], let

\[
\frac{\partial u}{\partial t} \rightarrow y, \quad \frac{\partial u}{\partial x} \rightarrow z, \quad u \rightarrow u, \quad t \rightarrow t, \quad x \rightarrow x.
\]

The the HJE (7) is in the form of

\[
F(y, z, u, t, x) = y + z^2 + zb(x) = 0,
\]

with

\[
\begin{align*}
\dot{y}(s) &= -F'_t = 0, \\
\dot{z}(s) &= -F'_x = -z \frac{db(x)}{dx}, \\
\dot{u}(s) &= F'_y y + F'_z z = y + (2z + b(x)) z, \\
\dot{t}(s) &= F'_y(y, z, t, x) = 1, \\
\dot{x}(s) &= F'_z(y, z, t, x) = 2z + b(x).
\end{align*}
\]

Note that \( y = -(z^2 + zb(x)) \) is the Hamiltonian \(-H(x, z)\). The pair of equations (52b) and (52e) are the Hamiltonian system in Eq. (42). \( \dot{u}(s) = \dot{x} z - H(x, z) \) is the corresponding "Lagrangian".

5.3 Phase portrait of characteristic lines of Hamiltonian system

In our case, Eq. (42) can be solved since \( p^2 + b(q)p = E \) is a constant of motion:

\[
\frac{dq}{dt} = \pm \sqrt{b^2(q) + 4E}, \quad \text{i.e.,} \quad \int \frac{dq}{\sqrt{b^2(q) + 4E}} = \pm t + \text{const.}
\]

When \( E = 0 \), this is precisely the solution to the ODE \( dq/dt = \pm b(q) \). Fig. 2 shows the phase portrait of the Hamiltonian dynamics.

The phase portrait in term of \( p \) as a function of \( q \) is

\[
p(q) = \frac{-b(q) \pm \sqrt{b^2(q) + 4E}}{2}.
\]
5.4 Solution to HJE with noncharacteristic initial value

As a large-deviation rate function, one appropriate initial condition for \( u(x,t) \) should be \( u(x,0) = 0 \). It is clear that \( u(x, t) = 0 \) is a solution to the HJE, but this is not a meaningful one. Therefore, one could be interested in the solution to the HJE with an infinitesimal initial data \( u(x, 0) \). Therefore, initially, one can linearize Eq. (6):

\[
\frac{\partial u_0(x,t)}{\partial t} = -b(x) \frac{\partial u_0}{\partial x} + \epsilon \left[ \frac{\partial^2 u_0}{\partial x^2} + \frac{db(x)}{dx} \right] + O(\epsilon^2) .
\] (55)

The exact result for a Gaussian process can provide some insights: Note that if \( \sigma^2(0) = \infty \), then the initial \( u(x, 0) = 0 \).

5.5 HJE on a circle

We again consider \( \theta \in S^1[0,1] \) with periodic angular velocity \( \dot{\theta} = b(\theta) \). The \( b(\theta) \) on a circle can be decomposed as

\[
b(\theta) = b_0 - \frac{dU(\theta)}{d\theta},
\] (56)

with a differentiable periodic potential \( U(\theta) = U(\theta + 1), \theta \in S^1 \). The corresponding Hamiltonian equation on a torus is

\[
\begin{cases}
\dot{\theta} &= 2\omega + b(\theta) = 2\omega + b_0 - \frac{dU(\theta)}{d\theta}, \\
\dot{\omega} &= -\omega \frac{db(\theta)}{d\theta} = -\omega \frac{d^2U(\theta)}{d\theta^2},
\end{cases}
\] (57)

with the Hamiltonian \( H(\theta, \omega) = \omega^2 + \omega b_0 - \omega U'(\theta); (\theta, \omega) \in S^2 \).

In general, there are two types of fixed points \( (\theta, \omega)^* \) in system (57): \( \omega^* = 0 \) and \( U''(\theta^*) = b_0 \), or \( U''(\theta^*) = 0 \) and \( \omega^* = (1/2)(U'(\theta^*) - b_0) \). These two types are the same for systems with \( b_0 = 0 \) (i.e., a gradient system on \( S^1 \)). For a rotational system with \( b(\theta) > 0 \) or \( < 0 \) on the entire \( S^1 \), the first type does not exist. Therefore, taking the index theory for a \( C^1 \)-vector in a plane into consideration [33], the occurrence of a cyclic motion in \( \dot{\theta} = b(\theta) \) with changing \( b_0 \) corresponds to an annihilation of two fixed points of the two types.

6 High Dimensional Cases: Momentum, Entropy Production and Nonequilibrium

From a standpoint of the theory of Markov processes, the one-dimensional system in [1] can only reach a time-reversible stationary process [34]. This result corresponds to the statement that an ODE on \( \mathbb{R}^1 \) is always a gradient system: \( \dot{x} = b(x) = -dU(x)/dx \) with \( U(x) = -\int b(x)dx \). For autonomous ODE systems in higher dimensions, a limit cycle can occur. This corresponds to a nonequilibrium phenomena in system [60] in dimension 2 or higher.
We now consider an \( N \)-dimensional diffusion process with the stochastic differential equation
\[
\frac{dX_t}{dt} = b(X_t) dt + \sqrt{2\epsilon} dB_t, \quad X_t \in \mathbb{R}^N,
\] (58)
and a corresponding Fokker-Planck equation for the probability density function \( f(x,t) dx \)
\[
\frac{\partial}{\partial t} f(x,t) = \epsilon \frac{\partial^2}{\partial x^2} f(x,t) - \frac{\partial}{\partial x} (b(x) f(x,t)).
\] (59)

### 6.1 HJE in two-dimensional systems

For a two-dimensional SDE:
\[
dX_t = b_x(X_t,Y_t) dt + \sqrt{2\epsilon} dB_t^{(1)}, \quad dY_t = b_y(X_t,Y_t) dt + \sqrt{2\epsilon} dB_t^{(2)},
\] (60)
the corresponding fictitious Hamiltonian is
\[
H(q_x,q_y,p_x,p_y) = p_x^2 + p_y^2 + b_x(q_x,q_y)p_x + b_y(q_x,q_y)p_y,
\] (61)
so the Hamiltonian dynamical system is
\[
\begin{align*}
\frac{d}{dt} q_x &= \frac{\partial H}{\partial p_x} = 2p_x + b_x(q_x,q_y), \\
\frac{d}{dt} q_y &= \frac{\partial H}{\partial p_y} = 2p_y + b_y(q_x,q_y), \\
\frac{d}{dt} p_x &= -\frac{\partial H}{\partial q_x} = -p_x \frac{\partial b_x}{\partial q_x} - p_y \frac{\partial b_y}{\partial q_x}, \\
\frac{d}{dt} p_y &= -\frac{\partial H}{\partial q_y} = -p_x \frac{\partial b_x}{\partial q_y} - p_y \frac{\partial b_y}{\partial q_y}.
\end{align*}
\] (62)

Its corresponding Lagrangian is
\[
\mathcal{L} [q_x,q_y,q_x',q_y'] = \left( \frac{\dot{q}_x - b_x}{2} \right)^2 + \left( \frac{\dot{q}_y - b_y}{2} \right)^2,
\] (63)
and the equations of motion are
\[
\begin{align*}
\ddot{q}_x &= \frac{\partial}{\partial q_x} \left( \frac{b_x^2 + b_y^2}{2} \right) - \left( \frac{\partial b_y}{\partial q_x} - \frac{\partial b_x}{\partial q_y} \right) q_y, \\
\ddot{q}_y &= \frac{\partial}{\partial q_y} \left( \frac{b_x^2 + b_y^2}{2} \right) + \left( \frac{\partial b_y}{\partial q_x} - \frac{\partial b_x}{\partial q_y} \right) q_x.
\end{align*}
\] (64)

In vector form Eq. (64) can be written as
\[
\frac{d^2}{dt^2} \vec{q}(t) = \left( \nabla \times \vec{b} \right) \times \frac{d}{dt} \vec{q}(t) + \frac{1}{2} \nabla \|\vec{b}\|^2.
\] (65)

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A Lorentz magnetic force like term arises if the vector field \( \vec{b}(q_x, q_y) \) is non-conservative. For a system of arbitrary dimension, the vector form Eq. (65) is still valid if one interprets
\[
(\nabla \times \vec{b}) \times \dot{\vec{q}}(t) \rightarrow \sum_j \left( \frac{\partial b_i}{\partial q_j} - \frac{\partial b_j}{\partial q_i} \right) \frac{dq_j(t)}{dt}.
\]

### 6.2 Force decomposition, momentum and entropy production

We now show an interesting relation between the non-gradient \( b(x) \) and the large deviation rate function \( u^{st}(x) \) for the stationary diffusion.

We consider the case of only a single attractive domain with only one stable fixed point at 0. Suppose the \( N \)-dimensional vector field \( b(x) \) admits an orthogonal decomposition [19]:
\[
b(x) = -\nabla U(x) + \ell(x),
\]
where the function \( U(x) \) is continuously differentiable, \( \nabla U(x) \neq 0 \) for \( x \neq 0 \), and the inner product in \( \mathbb{R}^N \), \( \ell(x) \cdot \nabla U(x) = 0 \). Then the large deviation rate function \( u^{st}(x) = U(x) + \text{const.} \), and the unique extreme of the action functional \( S_0[x(t) : (t_0, 0) \rightarrow (T, x^*)] \) is given by the equation
\[
\frac{dx}{dt} = \nabla U(x) + \ell(x),
\]
where \( t \in [t_0, T] \) and \( x(t_0) = 0, x(T) = x^* \).

Recall that \( u^{st}(x) \) is the stationary solution to the Hamiltonian-Jacobi equation
\[
\frac{\partial u(x, t)}{\partial t} = -\|\nabla u(x, t)\|^2 - b(x) \cdot \nabla u(x, t),
\]
associated with Hamiltonian \( H(q, p) = \|p\|^2 + b(q) \cdot p \).

Hence the Hamiltonian dynamics follow
\[
\begin{aligned}
\dot{q}_i &= \frac{\partial H}{\partial p_i} = 2p_i + b_i(q) \\
\dot{p}_i &= \frac{\partial H}{\partial q_i} = -p \cdot \frac{\partial b(q)}{\partial q_i}
\end{aligned}
\]

The action functional \( S_0 \) is just the path integration of the corresponding Lagrangian
\[
\mathcal{L}[\dot{q}, q] = \{p \dot{q} - H(q, p)\} = \sum_i \left( \frac{\dot{q}_i - b_i(q)}{2} \right)^2.
\]

It is easy to calculate that along the classical trajectory associated with \( dx/dt = \nabla U(x) + \ell(x) \), we have
\[
\begin{aligned}
p(t) &= -\nabla u^{st}(x(t)); \\
\dot{q}(t) &= \nabla U(q(t)) + \ell(q(t)).
\end{aligned}
\]
The Hamiltonian of this optimal dynamics is always zero, and the associated trajectories cross all the fixed points of the deterministic dynamic system (4).

In applied stochastic dynamics, the stationary solution $u^{st}(x)$ to Eq. (67) can be considered as a “landscape” for the dynamics (35) (38). Then Eq. (69) provides a very novel “meaning” for the conjugate momentum in the fictitious Hamiltonian system: It is the force associated with the landscape. Moreover, $(p(t), \ell(q(t)) = 0$, i.e., the Lorentz force $\ell(x)$ is perpendicular to the momentum.

For a multi-dimensional diffusion process (58) the entropy production rate for the stationary diffusion process is defined as (34):

$$e_p = \frac{1}{\epsilon} \int \| b(x) - \epsilon \nabla \log \pi(x; \epsilon) \|^2 \pi(x; \epsilon) dx,$$

(70)

in which $\pi(x; \epsilon)$ is the probability density function for the stationary process. Therefore, $e_p = 0$ if and only if $\ell(x) = 0$. $e_p \neq 0$ is widely considered to be a fundamental property of a nonequilibrium steady state; $e_p = 0$ implies that the stationary process $X_t$ is time reversible (34).

When $\epsilon$ tends to zero, if $\epsilon \nabla \log \pi(x; \epsilon)$ converges, then the $u^{st}(x)$ is related to the stationary probability density through a Boltzmann-like relation

$$\lim_{\epsilon \to 0} \epsilon \nabla \log \pi(x; \epsilon) = -\nabla u^{st}(x),$$

(71)

and then

$$\| b(x) - \epsilon \nabla \log \pi(x; \epsilon) \|^2 \to \| \ell(x) \|^2,$$

(72)

the left-hand-side of which is inside the integral in Eq. (70). Therefore, asymptotically we have

$$e_p \approx \frac{1}{\epsilon} \int \| \ell(x) \|^2 e^{-U(x)/\epsilon} dx.$$

(73)

Cases with multiple attractive domains are much more complex due to the problem of turning points and boundary layers in the limit of $\epsilon$ tending to zero (36) (37).

### 6.3 Processes with time-reversal

We now consider the diffusion process corresponding to Eqs. (58) and (59) with a time-reversal. The corresponding forward equation for the reversed process is

$$\frac{\partial}{\partial t} \bar{f}(x, t) = \epsilon \frac{\partial^2}{\partial x^2} \bar{f}(x, t) - \frac{\partial}{\partial x} \left[ \left( 2\epsilon \frac{\partial \ln \pi(x)}{\partial x} - b(x) \right) \bar{f}(x, t) \right],$$

(74)

where $\pi(x)$ is the stationary density for Eq. (59). In other words, the corresponding drift is

$$\tilde{b}(x) = 2\epsilon \frac{\partial \ln \pi(x)}{\partial x} - b(x).$$

(75)

In fact, both $b(x)$ and $\tilde{b}(x)$ can be written as

$$b(x) = \epsilon \frac{\partial \ln \pi(x)}{\partial x} + \ell(x), \quad \tilde{b}(x) = \epsilon \frac{\partial \ln \pi(x)}{\partial x} - \ell(x),$$

(76)
with
\[ \ell(x) = b(x) - \epsilon \frac{\partial \ln \pi(x)}{\partial x}. \] (77)

If we denote the stationary distribution
\[ \pi(x) = e^{-U(x)/\epsilon}, \] (78)
then \( b(x) = -\nabla U(x) + \ell(x) \) and \( \tilde{b}(x) = -\nabla U(x) - \ell(x) \). Their corresponding fictitious Hamiltonians are
\[ H(p,q) = p^2 + p (\nabla \cdot \ell(q)) \] (79)
and
\[ \tilde{H}(p,q) = p^2 + p (\nabla \cdot \ell(q)). \] (80)
The corresponding “equations of motion” are given by Eq. (65):
\[ \frac{d^2 \mathbf{q}(t)}{dt^2} = \pm \left( \nabla \times \ell(\mathbf{q}) \right) \times \frac{d}{dt} \mathbf{q}(t) + \frac{1}{2} \nabla \left( ||\nabla U(\mathbf{q})||^2 + ||\ell(\mathbf{q})||^2 \right). \] (81)

In the case of reversible processes, \( \ell(x) = 0 \) and \( \tilde{b}(x) = b(x) = -\nabla U(x) \).

## 7 Interpretive Remarks

Stochastic dynamics following trajectories defined by Eq. (58), with the time-evolution of the corresponding probability distribution characterized by Eq. (59), has a continuous but nowhere differentiable trajectory. Diffusion represents motions of a particle in a highly viscous medium in which inertia is completely lost instantaneously [38]. At any given position \( x \in \mathbb{R}^N \), the particle can move in any possible direction with any possible speed, but the mean velocity is \( \langle dx/dt \rangle = b(x) \). There is no momentum in the classical sense.

The analytical mechanical structure hidden in the stochastic dynamics discussed in the present review, however, is Newtonian. We note that the acceleration for deterministic dynamics
\[ \frac{dx}{dt} = b(x), \] (82)
is
\[ \frac{d^2 x_i}{dt^2} = \frac{d}{dt} b_i(x(t)) = \sum_{j=1}^{N} \frac{\partial b_i(x)}{\partial x_j} b_j(x) \]
\[ = \sum_{j=1}^{N} b_j(x) \left( \frac{\partial b_i(x)}{\partial x_j} - \frac{\partial b_j(x)}{\partial x_i} \right) + \sum_{j=1}^{N} b_j(x) \frac{\partial b_j(x)}{\partial x_i} \]
\[ = (\nabla \times b(x)) \times b(x) + \frac{1}{2} \nabla ||b(x)||^2. \] (83)
This is exactly Eq. (65). But how should one interpret the inertia and momentum in the fictitious Newtonian motion? How can we interpret the Hamiltonian as a conserved quantity in a stochastic trajectory?

**Mean dynamics and probability moment closure problem.** The mean behavior of nonlinear stochastic dynamics like (58), while being a deterministic function of time, can not be represented by a simple ordinary differential equation. For a stochastic process \( x(t) \):

\[
\frac{d}{dt} \langle x(t) \rangle = \langle b(x) \rangle \neq b\left( \langle x(t) \rangle \right).
\]

A traditional approach to resolve this problem is to introduce higher-order moments for the distribution of \( x(t) \), and to express the stochastic dynamics in terms of the mean, variance, third moments, etc. The method of moment closure was introduced to reduce this infinite hierarchy to approximately a finite system.

Such an approach encounters significant difficulties if a nonlinear \( b(x) \) has multiple domains of attraction. In this case, the mean dynamics reflects two fundamentally different behaviors on very different time scales: the intra-attractor dynamics and inter-attractor dynamics [2]. For a small \( \epsilon \), the latter are rare events.

**Kinetic energy without momentum.** The equations in (82) and (83) seem to suggest another line of hierarchical characterization of stochastic dynamics. The Hamiltonian dynamics corresponding to Eq. (83) yields Eq. (82) when \( H = 0 \). For all other dynamics with \( H \neq 0 \), they are impossible for Eq. (82), i.e., Eq. (58) with \( \epsilon = 0 \). However, they are the dynamics of a rare event when \( \epsilon \neq 0 \); because they are the most probable trajectory conditioned upon the rare event being observed. In fact, the \( H \) is the uniform amount of excess kinetic energy required, added or reduced, to lead a rare event to occur. The Hamiltonian dynamics, in this sense, has no forward predictive power based on given position and momentum; but it can predict detailed dynamical paths retrospectively, as in the Lagrangian formulation of classical mechanics and Fermat’s principle for optics.

It is easy to see from Eq. (83) that one conserved quantity in dynamics is \( q^2 - \|b(q)\|^2 \). Hence, such a solution has a “uniform excess kinetic energy” compared with Eq. (82). Conditioned on a given rare event, the problem of most probable ensemble is precisely the subject of Boltzmann-Gibbs’ statistical mechanics and the Gibbs conditioning in the theory of large deviations [39, 31].

**Evolution of the landscape.** The large-deviation rate function \( u^{st}(x) \), as the stationary solution to the HJE (67) or the “Boltzmann factor” for the stationary solution to Eq. (59):

\[
u^{st}(x) = \lim_{\epsilon \to 0} - \frac{1}{\epsilon} \ln f^{st}(x; \epsilon),
\]

has been known for a long time to have a Lyapunov property for the dynamics \( dx/dt = b(x) \):

\[
\frac{d}{dt} u^{st}(x(t)) = \nabla u^{st}(x) \cdot b(x) = -\|\nabla u^{st}(x)\|^2 \leq 0.
\]

This means the ergodic, stationary stochastic dynamics contains a great deal of information on the time-dependent behavior of the system. In physics and biology, there is a growing interest to use the function \( u^{st}(x) \) as an analytical visualization tool for
global behavior of complex dynamics: a landscape \[40, 19, 41, 35, 18\]. $u^x(x)$ can even exist for vector fields $b(x)$ which are non-conservative. The time-dependent HJE \[67\], therefore, can be interpreted as the evolution of the landscape.

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Figure 1: The local minimum and its dynamics of $u(\theta, t)$ on a circle. $x$ is the location of a minimum and $y$ its curvature, with their dynamics given in Eq. (37). When the dynamical system on the circle has a stable fixed point at $x^\dagger$, i.e., $b(x^\dagger) = 0$ and $b'(x^\dagger) < 0$, the local minimum will approach $x = x^\dagger$ and $y = -b''(x^\dagger)$. The black filled circle in (A) represent a stable fixed point of the $xy$ planar dynamics, the grey and open circles represent saddles and unstable node. However, when there is Hopf bifurcation as shown in (B), the $x(t)$ and $y(t)$ will be periodic functions of $t$. $u(\theta, t)$ will not reach stationarity. However, as shown in Eq. (40), infinite time $u(\theta, t)$ is a trivial periodic function with a constant value.
Figure 2: Phase portrait for Hamiltonian system (42): $\dot{q} = f(p,q), \dot{p} = g(p,q)$. The nullcline for $g(p,q) = 0$ are $p = 0$ and $q = q^*$ where $q^*$’s are where $\frac{db(q)}{dq} = 0$, shown in blue dashed lines. The nullcline for $f(p,q) = 0$ are $p = -b(q)/2$, shown in red dashed lines. The orange lines of $p = 0$ and $p = -b(q)$ are the contour for $H(q,p) = p^2 + b(q)p = 0$. The intersections between blue and red dashed lines are equilibrium points of the Hamiltonian system: Centers are by green open circles and saddles are in black filled circles. Trajectories in green have $H < 0$ and in pink have $H > 0$. 