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Thèse de Doctorat

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par

Tongling Lin

pour l'obtention du grade de Docteur en Sciences

Path Probability and An Extension of Least Action Principle to Random Motion

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Abstract

The present thesis is devoted to the study of path probability of random motion on the basis of an extension of Hamiltonian/Lagrangian mechanics to stochastic dynamics. The path probability is first investigated by numerical simulation for Gaussian stochastic motion of non dissipative systems. This ideal dynamical model implies that, apart from the Gaussian random forces, the system is only subject to conservative forces. This model can be applied to underdamped real random motion in the presence of friction force when the dissipated energy is negligible with respect to the variation of the potential energy. We find that the path probability decreases exponentially with increasing action, i.e., $P(A) \sim e^{-\gamma A}$, where γ is a constant characterizing the sensitivity of the action dependence of the path probability, the action is given by $A = \int_0^T L dt$, a time integral of the Lagrangian $L = K - V$ over a fixed time period T , K is the kinetic energy and V is the potential energy. This result is a confirmation of the existence of a classical analogue of the Feynman factor $e^{iA/\hbar}$ for the path integral formalism of quantum mechanics of Hamiltonian systems.

The above result is then extended to real random motion with dissipation. For this purpose, the least action principle has to be generalized to damped motion of mechanical systems with a unique well defined Lagrangian function which must have the usual simple connection to Hamiltonian. This has been done with the help of the following Lagrangian $L = K - V - E_d$, where E_d is the dissipated energy. By variational calculus and numerical simulation, we proved that the action $A = \int_0^T L dt$ is stationary for the optimal paths determined by Newtonian equation. More precisely, the stationarity is a minimum for underdamped motion, a maximum for overdamped motion and an inflexion for the intermediate case. On this basis, we studied the path probability of Gaussian stochastic motion of dissipative systems. It is found that the path probability still depends exponentially on Lagrangian action for the underdamped motion, but depends exponentially on kinetic action $A = \int_0^T K dt$ for the overdamped motion.

Keywords: Path probability, Gaussian stochastic motion, Action,
Dissipative systems, Classical mechanics, Variational principle

Résumé

La présente thèse est consacrée à l'étude de la probabilité du chemin d'un mouvement aléatoire sur la base d'une extension de la mécanique Hamiltonienne/Lagrangienne à la dynamique stochastique. La probabilité d'un chemin est d'abord étudiée par simulation numérique dans le cas du mouvement stochastique Gaussien des systèmes non dissipatifs. Ce modèle dynamique idéal implique que, outre les forces aléatoires Gaussiennes, le système est seulement soumis à des forces conservatrices. Ce modèle peut être appliqué à un mouvement aléatoire réel de régime pseudo-périodique en présence d'une force de frottement lorsque l'énergie dissipée est négligeable par rapport à la variation de l'énergie potentielle. Nous constatons que la probabilité de chemin décroît exponentiellement lorsque son action augmente, c'est à dire, $P(A) \sim e^{-\gamma A}$, où γ est une constante caractérisant la sensibilité de la dépendance de l'action à la probabilité de chemin, l'action est calculée par la formule $A = \int_0^T L dt$, intégrale temporelle du Lagrangien. $L = K - V$ sur une période de temps fixe T , K est l'énergie cinétique et V est l'énergie potentielle. Ce résultat est une confirmation de l'existence d'un analogue classique du facteur de Feynman $e^{iA/\hbar}$ pour le formalisme intégral de chemin de la mécanique quantique des systèmes Hamiltoniens.

Le résultat ci-dessus est ensuite étendu au mouvement aléatoire réel avec dissipation. A cet effet, le principe de moindre action doit être généralisé au mouvement amorti de systèmes mécaniques ayant une fonction unique de Lagrange bien définie qui doit avoir la simple connexion habituelle au Hamiltonien. Cela a été fait avec l'aide du Lagrangien suivant $L = K - V - E_d$, où E_d est l'énergie dissipée. Par le calcul variationnel et la simulation numérique, nous avons prouvé que l'action $A = \int_0^T L dt$ est stationnaire pour les chemins optimaux déterminés par l'équation newtonienne. Plus précisément, la stationnarité est un minimum pour les mouvements de régime pseudo-périodique, un maximum pour les mouvements d'amortissement aperiodique et une inflexion dans le cas intermédiaire. Sur cette base, nous avons étudié la probabilité du chemin du mouvement stochastique Gaussien des systèmes dissipatifs. On constate que la probabilité du chemin dépend toujours de façon exponentielle de l'action Lagrangien pour les mouvements de régime pseudo-périodique, mais dépend toujours de façon exponentielle de l'action cinétique $A = \int_0^T K dt$ pour régime aperiodique.

Mots-clefs: Probabilité chemin, Mouvement stochastique Gaussien, Action, Systèmes dissipatifs, Mécanique classique, Principe variationnel

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Chapter 1

Introduction

1.1 Background

In physics, classical mechanics [1]-[6] is one of the two major sub-fields of mechanics, which is concerned with the set of physical laws describing the motion of bodies under the action of a system of forces. It is the most familiar of the theories of physics. The concepts it covers, such as mass, acceleration, and force, are commonly used and known. The initial stage in the development of classical mechanics is often referred to as Newtonian mechanics, and is associated with the physical concepts employed by and the mathematical methods invented by Newton himself, in parallel with Leibniz, and others. Later, more abstract and general methods were developed, leading to reformulations of classical mechanics known as Lagrangian mechanics and Hamiltonian mechanics [7]. These advances were largely made in the 18th and 19th centuries, and they extend substantially beyond Newton's work, particularly through their use of analytical mechanics [8, 9, 10, 11]. Ultimately, the mathematics developed for these were central to the creation of quantum mechanics [12, 13, 14].

Classical mechanics is capable of generating either completely regular motion, completely chaotic motion, or an arbitrarily complicated mixture of the two [15]. A path (trajectory) of regular motion of classical mechanics system always has probability one once it is determined by the equation of motion and the boundary condition, while a random motion may have many possible paths under the same condition, as can be easily verified with any stochastic process including Brownian motion [16]-[24]. The path of stochastic dynamics in mechanics has much richer physics content than that

of the regular or deterministic motion. For a given process between two given configuration points with given durations, each of those potential paths has some probability to be taken by the motion. The path probability is a very important quantity for the understanding and the characterization of random dynamics because it contains all the information about the physics: the characteristics of the stochasticity, the degree of randomness, the dynamical uncertainty, the equations of motion and so forth. Some theoretical works have been devoted to the study of this probability, such as the Wiener path measure [16], large deviation theory [26, 25], path probability method [27] and most probable path [28, 29].

When talking about the path probability of mechanical random motion, one naturally think of the Feynman factor $e^{iA/\hbar}$ of the path integral formulation of quantum mechanics [12]. Although this factor is not the path probability, it characterizes the likelihood for a Hamiltonian system to take given configuration path from one state to another in quantum motion. A question we may answer here about the classical path probability is whether it is possible to relate it to the action in a homologous manner to the Feynman factor. This question, among some others relative to the polemics on the kinship between mechanics and thermodynamics [30]-[35], has led to a possible extension of Hamiltonian and Lagrangian mechanics to a stochastic formalism [36, 37]. This theoretical frame [36, 37] was suggested to study the path probability in relation with the action of Hamiltonian system (non dissipation). The basis of the theory is an extended least action principle [1, 9, 10, 11] containing a path information [38, 39] depending on the path probability. For a special case of path information given by the Shannon formula [40], it was predicted that the probability that a path is taken was exponentially proportional to the action defined by $A = \int_{t_a}^{t_b} L dt$ along that path, where $L = K - V$ is the Lagrangian, K is the kinetic energy, V is the potential one, t_a is the time moment when the system is at the initial point a and t_b is the time moment when the system is at the final point b . To our knowledge, less experimental work or numerical experiment has been made to measure the path probability. This is certainly related to, among many reasons, the difficulty of experimental observation of a large number of stochastic motions. This large number is necessary to determine correctly the path probability.

For Hamiltonian systems, any real trajectory between two given configuration points must satisfy the least action principle given by a vanishing first variation due to tiny deformation of the trajectory, i.e., $\delta A = \delta \int_0^T L dt = \int_0^T \delta L dt = 0$ (suppose $t_a = 0$ and

$t_b = T$ from now on). One of the important results of this variational calculus is the Euler-Lagrange equation given by $\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{x}} \right) - \frac{\partial L}{\partial x} = 0$ (on the coordinate x), where \dot{x} is the velocity. In many cases when Hamiltonian H and Lagrangian L do not depend on time explicitly, a Hamiltonian system is energy conservative. For damped motion with friction force f_d , the above equation becomes $\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{x}} \right) - \frac{\partial L}{\partial x} = f_d$ which is equivalent to write $\int_0^T (\delta L + f_d \delta x) dt = 0$ [41]. Despite this vanishing equality, it is impossible to calculate and optimize an action integral with the above single Lagrangian function satisfying the Euler-Lagrange equation. This difficulty leads to the disappearance of least action principle in dissipative systems.

There has been a longstanding effort to formulate least action principle for nonconservative or dissipative system [42, 43, 44]. As far as we know, the first proposition was made by Rayleigh [45] who introduced a dissipative function, $D = \frac{1}{2}m\zeta\dot{x}^2$, to write $\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{x}} \right) + \frac{\partial D}{\partial \dot{x}} - \frac{\partial L}{\partial x} = 0$, where $\zeta = \gamma/m$, γ is the viscous drag coefficient in the Stokes' law $\vec{f}_d = -m\zeta\vec{\dot{x}}$ and m the mass of the damped body. Although the equation of motion is kept in a similar form as Lagrangian equation, the least action principle is not recovered since there is no single Lagrangian for defining an action which satisfies $\delta A = 0$. Other major propositions include the Bateman approach [46] to introduce complementary variables and equations, the definition of dissipative Lagrangian by multiplying the non dissipative one with an exponential factor $\exp(\zeta t)$ [47] where t is the time, the fractional derivative formulation [48], the pseudo-Hamiltonian mechanics [49] where a parameter was introduced to characterize the degree of dissipation, the formalism that incorporates dissipative forces into quantum mechanics [50, 51] and the variational formulation for the maximum energy dissipation principle in chemical thermodynamics [52]-[55]. The reader is referred to the reviews in Refs. [42]-[55] about the details of these propositions.

In general, the Lagrangian in these solutions is not unique and has no energy connection like $L = K - V$ (see for instance the quasi-Lagrangian $L = e^{\zeta t}(K - V)$ and the corresponding quasi-Hamiltonian $H = e^{-\zeta t}K + e^{\zeta t}V$ for damped harmonic oscillator [47]). The use of this action approach to stochastic motion with friction needs an extension of the least action principle or the variational action approach of Hamiltonian/Lagrangian mechanics to dissipative system including friction, that is, to find an action which has direct energy connection and whose variational calculus gives rise to Newtonian equation of motion in such a way that the unique trajectory still has the least or stationary action. The extension of least action principle to classical

dissipative motion is one of our effort in progress [56].

1.2 Research purpose

Based on the theoretical extension of Hamiltonian/Lagrangian mechanics to a stochastic formalism [36, 37] which predicts that path probability depending exponentially on action is possible for stochastic dynamics of classical mechanics systems without dissipation, we made numerical experiments to see whether or not the path probability, or its density, estimated with the help of the Wiener measure, has something to do with the action of classical mechanics. This work concerns only non dissipative or quasi-Hamiltonian system, meaning that, apart from the random forces and energy fluctuation, the systems contain only conservative forces without energy dissipation. The average energy of the system can or can not change during the entire period of the motion. In other cases where the dissipation is associated with fluctuation, we consider only weakly damped motion during which the energy dissipated is negligible compared to the variation of potential energy, i.e., the conservative force is much larger than friction force.

Since the least action principle was formulated only for Hamiltonian system (no dissipation), a question we may ask whether the path probability still depends exponentially on action for dissipative system? In order to answer this question, we established a least action principle of dissipative system that recovers the energy connection and the uniqueness of a single Lagrangian function, its relation with a conservative Hamiltonian, as well as the three formulations of analytical mechanics, i.e., the Hamiltonian, Lagrangian and the Hamilton-Jacobi equations. This work based on the model of a conservative system composed of the moving body and its environment coupled by friction. It was shown that this system with “internal dissipation” satisfies both Lagrangian and Hamiltonian mechanics, leading to correct equation of damped motion in a general way.

However a mathematical uncertainties persists about the pertinence of the variational calculus and the nature (maxima, minima and inflection) of the possible stationarity of action. By variational calculus and numerical simulation, we calculated the actions along the optimal path and many variational paths created with tiny random deformations in the vicinity of the optimal one. By the comparison of these actions, we

proved that the action is stationary for the optimal paths determined by Newtonian equation. More precisely, the stationarity is a minimum for the underdamped motion, a maximum for the overdamped motion and an inflexion for the intermediate case. On this basis, we studied the path probability of Gaussian stochastic motion of dissipative systems.

These above mentioned works are the ingredients of the present thesis, of which an overview is presented hereafter.

1.3 Overview of the thesis

The present thesis is devoted to the study of path probability of random motion on the basis of an extension of Hamiltonian/Lagrangian mechanics to stochastic dynamics. The main results are the following. The path probability of stochastic motion of dissipative systems depends exponentially on Lagrangian action for the underdamped motion, but plays exponentially with kinetic action for the overdamped motion, i.e., $P(A) \sim e^{-\gamma A}$, where γ is a constant characterizing the sensitivity of the action dependence of the path probability, the Lagrangian action is given by $A_L = \int_0^T L dt$ a time integral of the Lagrangian $L = K - V - E_d$ over a fixed time period T , K is the kinetic energy and V is the potential energy, E_d is the dissipated energy and the kinetic action is given by $A_K = \int_0^T K dt$. For the underdamped motion, the dissipative energy is negligible, the most probable path is the least Lagrangian action path; for the overdamped motion, the dissipative energy is strong, the most probable path is the maximum Lagrangian action path.

Each chapter will contain a detailed description of its own. The general structure and content of the document is as follows.

In the second chapter, we briefly provide an introduction of the fundamental principles including least action principle and virtual work principle. These principles led to the development of the Lagrangian and Hamiltonian formulations of classical mechanics. In the following, we consider a system where the randomness comes from either the intrinsic noise of the dynamics or from the external perturbation or the random uncontrollable perturbations. There is no external dissipative forces (such as friction force) in the system. We give a derivation from virtual work principle for random dynamics to stochastic action principle, which was postulated as a hypothesis. After that,

we introduce a Shannon information as a path information. If the path entropy takes the Shannon form, the stochastic action principle yields an exponential probability distribution of action. Finally, three schemas of a random dynamics are illustrated in phase space. This chapter is the theoretical extension of Hamiltonian and Lagrangian mechanics to a stochastic formalism in non dissipative systems.

In the third chapter, the path probability of stochastic motion of non dissipative or quasi-Hamiltonian systems is first investigated by numerical experiment. The simulation model generates ideal one-dimensional motion of particles subject only to conservative forces in addition to Gaussian distributed random displacements. In the presence of dissipative forces, application of this ideal model requires that the dissipated energy is small with respect to the variation of the conservative forces. The sample paths are sufficiently smooth space-time tubes with suitable width allowing correct evaluation of position, velocity, energy and action of each tube. It is found that the path probability decays exponentially with increasing action of the sample paths. i.e., $P(A) \sim e^{-\gamma A}$, where γ is a constant characterizing the sensitivity of the action dependence of the path probability, the action is given by $A = \int_0^T L dt$, a time integral of the Lagrangian $L = K - V$ over a fixed time period T , K is the kinetic energy and V is the potential energy. The decay rate increases with decreasing Gaussian randomness. This result is a confirmation of the existence of a classical analogue of the Feynman factor $e^{iA/\hbar}$ for the path integral formalism of quantum mechanics of Hamiltonian systems.

In the fourth chapter, the least action principle has to be generalized to damped motion of mechanical systems with a unique well defined Lagrangian function which must have the usual simple connection to Hamiltonian. We consider a whole isolated conservative system containing a damped body and its environment, coupled to each other by friction. The Lagrangian is $L = K - V - E_d$ with an effective conservative Hamiltonian $H = K + V + E_d$ where K is kinetic energy of the damped body, V its potential energy and E_d is the negative work of the friction force. We formulated a possible answer to a longstanding question of classical mechanics about the least action principle for damped motion, in keeping all the four conventional formulations of mechanics, i.e., Newtonian, Lagrangian, Hamiltonian and Hamilton-Jacobi equations.

This least action principle can also be derived from the virtual work principle. It is shown that, within this formulation, the least action principle can be equivalent to a least dissipation principle for the case of Stokes damping or, more generally, for

overdamped motion with more kinds of damping. By variational calculus and numerical simulation, we proved that the action $A = \int_0^T L dt$ is stationary for the optimal paths determined by Newtonian equation. The model of the simulation is a small ball subject to constant force combined with Stokes' drag force. It turns out that the extrema of action do exist and shift from a minimum to a maximum as the motion duration and the damping coefficient increase, i.e., with increasing dissipative energy. From this point of view, similar transition of extrema of action can be expected for other friction and conservative forces. We have made same simulations as above with constant friction $f_d = m\zeta$ and the quadratic friction $f_d = m\zeta x^2$, as well as harmonic oscillator damped by Stokes' drag.

In the fifth chapter, based on the extension of least action principle to random motion, we make the numerical experiments of stochastic motion of dissipative systems in order to calculate the path probability and to investigate its dependence the conventional mechanical quantities. The model of the simulation is small silica (SiO_2) particles subject to conservative forces, friction force and Gaussian noise. It is found that the path probability still depends exponentially on Lagrangian action for the underdamped motion, but plays exponentially with kinetic action $A = \int_0^T K dt$ for the overdamped motion. The difference from the non dissipative motion is that, for the underdamped motion, the most probable path is the least Lagrangian action path; for the overdamped motion, the most probable path is the maximum Lagrangian action path.

Finally, we sum up the conclusions of this work and give some perspectives in the last chapter.

Chapter 2

Stochastic action principle and path probability distribution

2.1 Stochastic action principle

2.1.1 Principle of least action

In physics, the principle of least action [1, 9, 10, 11] or, more accurately, the principle of stationary action is a variational principle that, when applied to the action of a mechanical system, can be used to obtain the equations of motion for that system. The principle led to the development of the Lagrangian and Hamiltonian formulations of classical mechanics.

2.1.1.1 Statements of action principles

In classical mechanics, there are two major versions of the action [57]-[70], due to Hamilton and Maupertuis, and two corresponding action principles. Hamilton action A and Maupertuis action A_m have the same dimensions, i.e. energy \times time, or angular momentum, these differ from each other (they are related by a Legendre transformation [9]). The Hamilton's action principle is nowadays the most used. The Hamilton action A is defined as an integral along an actual or virtual (trial) space-time trajectory $q(t)$ connecting two specified space-time events, initial event $a \equiv (q_a, t_a = 0)$ and final event

$b \equiv (q_b, t_b = T)$,

$$A = \int_0^T L(q, \dot{q}) dt, \quad (2.1)$$

where $L(q, \dot{q})$ is the Lagrangian, and $\dot{q} = dq/dt$. For most of what follows we will assume the simplest case where $L = K - V$, where K and V are the kinetic and potential energies, respectively. In general, q stands for the complete set of independent generalized coordinates, q_1, q_2, \dots, q_n , where n is the number of degrees of freedom. Hamilton's principle states that among all conceivable trajectories $q(t)$ that could connect the given end points q_a and q_b in the given time T , the true trajectories are those that make A stationary. Hamilton's least action principle states:

$$(\delta A)_T = 0, \quad (2.2)$$

where the constraint of fixed time T is written explicitly, and the constraint of fixed end-positions q_a and q_b is left implicit. It is clear from Eq. (2.1) that A is a functional of the trial trajectory $q(t)$, and in Eq. (2.2) δA denotes the first-order variation in A corresponding to the small variation $\delta q(t)$ in the trial trajectory. The Hamilton's least action principle means that, given the stated constraints, the variation of the action δA vanishes for any small trajectory variation $\delta q(t)$ around a true trajectory.

The second major version of the action is Maupertuis action A_m ,

$$A_m = \int_{q_a}^{q_b} p dq = \int_0^T 2K dt, \quad (2.3)$$

where the first (time-independent) form is the general definition, with $p = \partial L / \partial \dot{q}$ the canonical momentum, and $p dq$ stands for $p_1 dq_1 + p_2 dq_2 + \dots + p_f dq_f$ in general. The second (time-dependent) form for A_m in Eq. (2.3) is valid for normal systems in which the kinetic energy K is quadratic in the velocity components $\dot{q}_1, \dot{q}_2, \dots, \dot{q}_f$. The Maupertuis' least action principle states that for true trajectories A_m is stationary on trial trajectories with fixed end positions q_a and q_b and fixed energy H :

$$(\delta A_m)_H = 0, \quad (2.4)$$

Note that H is fixed but T is not in Eq. (2.4), the reverse of the conditions in Eq. (2.2).

2.1.1.2 Euler-Lagrange equation

As noted above, the requirement that the action integral be stationary under small perturbations of the evolution is equivalent to a set of differential equations (called the

Euler-Lagrange equations) that may be determined using the calculus of variations. We illustrate this derivation here using only one coordinate, x ; the extension to multiple coordinates is straightforward [2, 8].

Adopting Hamilton's least action principle, we assume that the Lagrangian L (the integrand of the action integral) depends only on the coordinate $x(t)$ and its time derivative $dx(t)/dt$, and may also depend explicitly on time. In that case, the action integral can be written

$$A = \int_0^T L(x, \dot{x}, t) dt, \quad (2.5)$$

where the initial and final times (0 and T) and the final and initial positions are specified in advance as $x_0 = x(0)$ and $x_T = x(T)$. Let $x_{true}(t)$ represent the true evolution that we seek, and let $x_{per}(t)$ be a slightly perturbed version of it, albeit with the same endpoints, $x_{per}(0) = x_0$ and $x_{per}(T) = x_T$. The difference between these two evolutions, which we will call $\epsilon(t)$, is infinitesimally small at all times $\epsilon(t) = x_{per}(t) - x_{true}(t)$. At the endpoints, the difference vanishes, i.e., $\epsilon(0) = \epsilon(T) = 0$.

Expanded to first order, the difference between the actions integrals for the two evolutions is

$$\begin{aligned} \delta A &= \int_0^T [L(x_{per} + \epsilon_{per}, \dot{x}_{per} + \dot{\epsilon}_{per}, t) - L(x_{true}, \dot{x}_{true}, t)] dt \\ &= \int_0^T \left(\epsilon \frac{\partial L}{\partial x} + \dot{\epsilon} \frac{\partial L}{\partial \dot{x}} \right) dt, \end{aligned} \quad (2.6)$$

Integration by parts of the last term, together with the boundary conditions $\epsilon(0) = \epsilon(T) = 0$, yields the equation

$$\delta A = \int_0^T \left[\frac{\partial L}{\partial x} - \frac{d}{dt} \left(\frac{\partial L}{\partial \dot{x}} \right) \right] \epsilon dt \quad (2.7)$$

The requirement A that be stationary implies that the first-order change must be zero for any possible perturbation $\epsilon(t)$ about the true evolution (Principle of least action)

$$\delta A = 0 \quad (2.8)$$

This can be true only if

$$\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{x}} \right) - \frac{\partial L}{\partial x} = 0 \quad (2.9)$$

is just the Euler-Lagrange equation. The quantity $\frac{\partial L}{\partial \dot{x}}$ is called the conjugate momentum for the coordinate x . An important consequence of the Euler-Lagrange equations is

that if L does not explicitly contain coordinate x , i.e., if $\frac{\partial L}{\partial x} = 0$, then $\frac{\partial L}{\partial \dot{x}}$ is constant in time. In such cases, the coordinate x is called a cyclic coordinate, and its conjugate momentum is conserved.

2.1.2 Principle of virtual work

Virtual work arises in the application of the principle of least action to the study of forces and movement of a mechanical system. Historically, virtual work and the associated calculus of variations were formulated to analyze systems of rigid bodies [9], but they have also been developed for the study of the mechanics of deformable bodies [71, 72].

2.1.2.1 Basic definitions

If a force acts on a particle as it moves from point a to point b , then, for each possible trajectory that the particle may take, it is possible to compute the total work done by the force along the path. The principle of virtual work, which is the form of the principle of least action applied to these systems, states that the path actually followed by the particle is the one for which the difference between the work along this path and other nearby paths is zero. The formal procedure for computing the difference of functions evaluated on nearby paths is a generalization of the derivative known from differential calculus, and is termed the calculus of variations.

Let the function $\mathbf{r}(t)$ define the path followed by a point. A nearby path can then be defined by adding the function $\delta\mathbf{r}(t)$ to the original path, so that the new path is given by $\mathbf{r}(t) + \delta\mathbf{r}(t)$. The function $\delta\mathbf{r}(t)$ is called the variation of the original path, and each of the components of $\delta\mathbf{r} = (\delta x, \delta y, \delta z)$ is called a virtual displacement. This can be generalized to an arbitrary mechanical system defined by the generalized coordinates $q_i, i = 1, \dots, n$. In which case, the variation of the trajectory $q_i(t)$ is defined by the virtual displacements $\delta q_i, i = 1, \dots, n$.

Virtual work can now be described as the work done by the applied forces and the inertial forces of a mechanical system as it moves through a set of virtual displacements. Consider a particle that moves along a trajectory $\mathbf{r}(t)$ from a point a to a point b , while

a force F is applied to it, then the work done by the force is given by the integral

$$W = \int_{\mathbf{r}(0)=a}^{\mathbf{r}(T)=b} \mathbf{F} \cdot d\mathbf{r} = \int_0^T \mathbf{F} \cdot \mathbf{v} dt, \quad (2.10)$$

where $d\mathbf{r}$ is the differential element along the curve that is the trajectory of the particle, and \mathbf{v} is its velocity. It is important to notice that the value of the work W depends on the trajectory $\mathbf{r}(t)$.

Now consider the work done by the same force on the same particle again moving from point a to point b , but this time moving along the nearby trajectory that differs from $\mathbf{r}(t)$ by the variation $\delta\mathbf{r}(t) = \epsilon\mathbf{h}(t)$, where ϵ is a scaling constant that can be made as small as desired and $\mathbf{h}(t)$ is an arbitrary function that satisfies $\mathbf{h}(0) = \mathbf{h}(T) = 0$,

$$\bar{W} = \int_a^b \mathbf{F} \cdot d(\mathbf{r} + \epsilon\mathbf{h}) = \int_0^T \mathbf{F} \cdot (\mathbf{v} + \epsilon\dot{\mathbf{h}}) dt, \quad (2.11)$$

The variation of the work δW associated with this nearby path, known as the virtual work, can be computed to be

$$\delta W = W - \bar{W} = \int_0^T \mathbf{F} \cdot \epsilon\dot{\mathbf{h}} dt, \quad (2.12)$$

Now assume that $\mathbf{r}(t)$ and $\mathbf{h}(t)$ depend on the generalized coordinates $q_i, i = 1, \dots, n$, then the derivative of the variation $\delta\mathbf{r}(t) = \epsilon\mathbf{h}(t)$ is given by

$$\frac{d}{dt}\delta\mathbf{r} = \epsilon\dot{\mathbf{h}} = \epsilon \left(\frac{\partial\mathbf{h}}{\partial q_1} \dot{q}_1 + \dots + \frac{\partial\mathbf{h}}{\partial q_n} \dot{q}_n \right), \quad (2.13)$$

then we have

$$\begin{aligned} \delta W &= \int_0^T \left(\mathbf{F} \cdot \frac{\partial\mathbf{h}}{\partial q_1} \epsilon\dot{q}_1 + \dots + \mathbf{F} \cdot \frac{\partial\mathbf{h}}{\partial q_n} \epsilon\dot{q}_n \right) dt \\ &= \int_0^T \mathbf{F} \cdot \frac{\partial\mathbf{h}}{\partial q_1} \epsilon\dot{q}_1 dt + \dots + \int_0^T \mathbf{F} \cdot \frac{\partial\mathbf{h}}{\partial q_n} \epsilon\dot{q}_n dt. \end{aligned} \quad (2.14)$$

The requirement that the virtual work be zero for an arbitrary variation $\delta\mathbf{r}(t) = \epsilon\mathbf{h}(t)$ is equivalent to the set of requirements

$$F_i = \mathbf{F} \cdot \frac{\partial\mathbf{h}}{\partial q_i} = 0 \quad i = 1, \dots, n \quad (2.15)$$

The terms F_i are called the generalized forces associated with the virtual displacement $\delta\mathbf{r}$.

2.1.2.2 Static equilibrium

Static equilibrium is the condition in which the applied forces and constraint forces on a mechanical system balance such that the system does not move. The principle of virtual work states that the virtual work of the applied forces is zero for all virtual movements of the system from static equilibrium, that is, $\delta W = 0$ for any variation $\delta \mathbf{r}$ [45]. This is equivalent to the requirement that the generalized forces for any virtual displacement are zero, that is $F_i = 0$.

Let the forces on the system be $\mathbf{F}_j, j = 1, \dots, N$ and let the virtual displacement of each point of application of these forces be $\delta \mathbf{r}_j, j = 1, \dots, N$, then the virtual work generated by a virtual displacement of these forces from the equilibrium position is given by

$$\delta W = \sum_{j=1}^N \mathbf{F}_j \cdot \delta \mathbf{r}_j, \quad (2.16)$$

Now assume that each $\delta \mathbf{r}_j$ depends on the generalized coordinates $q_i, i = 1, \dots, n$, then

$$\delta \mathbf{r}_j = \frac{\partial \mathbf{r}_j}{\partial q_1} \delta q_1 + \dots + \frac{\partial \mathbf{r}_j}{\partial q_n} \delta q_n, \quad (2.17)$$

and

$$\delta W = \left(\sum_{j=1}^N \mathbf{F}_j \cdot \frac{\partial \mathbf{r}_j}{\partial q_1} \right) \delta q_1 + \dots + \left(\sum_{j=1}^N \mathbf{F}_j \cdot \frac{\partial \mathbf{r}_j}{\partial q_n} \right) \delta q_n. \quad (2.18)$$

The n terms

$$F_i = \sum_{j=1}^N \mathbf{F}_j \cdot \frac{\partial \mathbf{r}_j}{\partial q_i}, \quad i = 1, \dots, n \quad (2.19)$$

are the generalized forces acting on the system. Kane [73] shows that these generalized forces can also be formulated in terms of the ratio of time derivatives. In order for the virtual work to be zero for an arbitrary virtual displacement, each of the generalized forces must be zero, that is

$$\delta W = 0 \quad \Rightarrow \quad F_i = 0, \quad i = 1, \dots, n. \quad (2.20)$$

This principle for static equilibrium problem was extended to “dynamical equilibrium” by d’Alembert [74] who added the inertial force $-m_j \mathbf{a}_j$ on each point of the system in motion

$$\delta W = \sum_{i=1}^N (\mathbf{F}_j - m_i \mathbf{a}_j) \cdot \delta \mathbf{r}_j, \quad (2.21)$$

where m_j is the mass of the point j and \mathbf{a}_j its acceleration. From this principle, we can not only derive Newtonian equation of dynamics, but also other fundamental principles such as least action principle. The deterministic character and the uniqueness of trajectory of the dynamics dictated by these two principles can be illustrated in both configuration and phase spaces as shown in Fig. 2.1 which tells us that a motion from a point a in configuration space must arrive at point b when the duration of motion $T = t_b - t_a$ is given. Equivalently in phase space, once the initial point (condition) a is given, the path is then determined, meaning that the unique destination after $T = t_b - t_a$ is b .

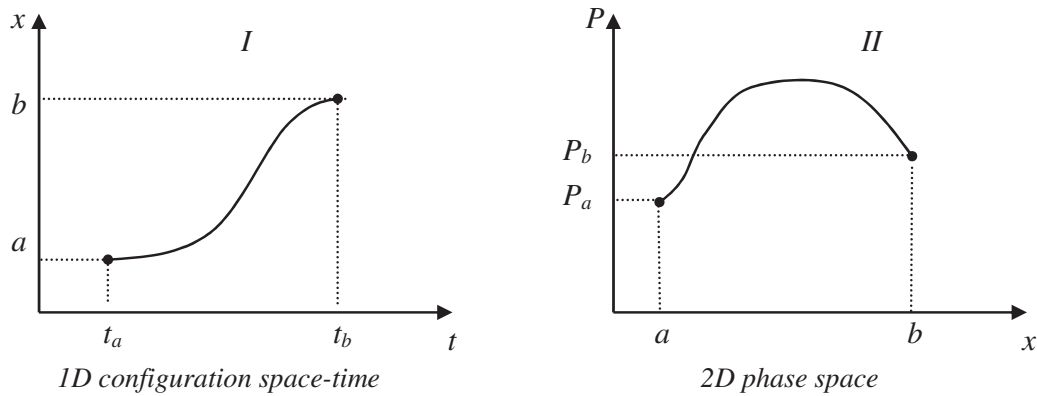


Fig. 2.1: Illustration of a least action path of regular motion of Hamiltonian system between two points a and b in configuration space (I) and in phase space (II). The virtual work on each point of this path is zero according to Eq. (2.21). The duration of motion $T = t_b - t_a$ for the path in configuration space is given, while for the phase space path the duration of motion is not specified since it is hinted in the initial or final conditions (positions and velocities). The meaning of this is that a motion from a given phase point a must have a single destination b .

2.1.3 Stochastic action principle

2.1.3.1 Random motion

The above mentioned principles hold whenever the motion is regular. In other words, we can refer to any motion which can be described analytically and explicitly by Newtonian laws as regular motion.

On the contrary, we define an irregular or random motion as a dynamics which

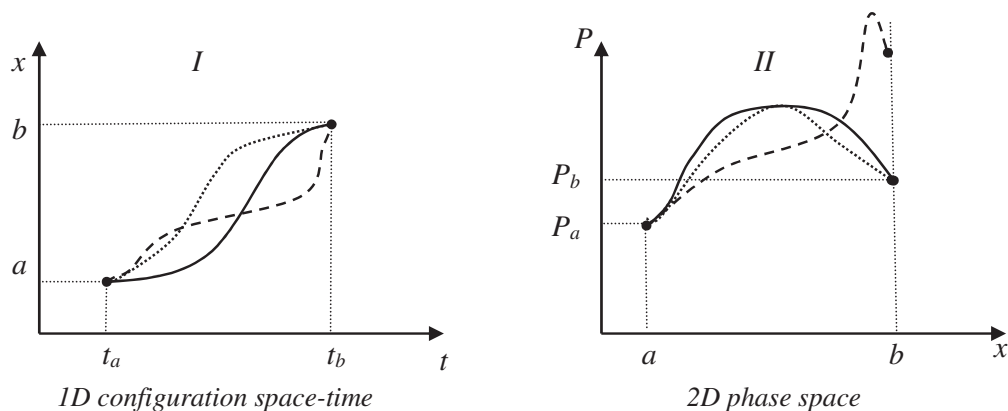


Fig. 2.2: An illustration of the non uniqueness of trajectory of random dynamics. Notice that the three path examples between a and b in configuration space may have different end points in phase space even if they have the same initial state.

violates the above paradigms. One of the most remarkable characteristics of random motions is the non uniqueness of paths between two given points in configuration space as well as in phase space. This behavior implies the occurrence of multiple paths to different destinations from a given phase point, which is illustrated in Fig. 2.2.

The cause of the randomness is without any doubt the noises or random forces in and around the observed system. Here we do not run into the study of the origin of the noises. We only look into the effects, i.e., the multiplicity of paths mentioned above for a motion during a time period, or the multiplicity of states for a given moment of time of the motion.

Since in the present approach the effect of noises is represented by the multiplicity of paths and states, the quantities such as the Hamiltonian H , the Lagrangian L , the action A and the virtual work δW will be calculated without considering the random forces which are actually impossible to be introduced into the calculation of these quantities due to their random nature. In this approach, it is obvious that among all the paths between two points, there must be a thin bundle of paths around the geodesic determined by $\delta A = 0$ or $\delta W = 0$. Other paths must have $\delta A \neq 0$ and $\delta W \neq 0$.

In what follows, we introduce the extension of the above fundamental principles to random dynamics by considering a very common case: the descent of a body from an inclined smooth but irregular long surface. The friction can be neglected although the surface is somewhat rugged [75].

2.1.3.2 Stochastic least action principle

The least action principle [10, 11] was formulated for regular dynamics of mechanical system. One naturally asks the question about its fate when the system is subject to noise making the dynamics irregular. In order to answer this question, a stochastic action principle (SAP)

$$\overline{\delta A} = 0 \tag{2.22}$$

has been developed in [36, 37] where δA is a variation of the Lagrange action A and the average is carried out over all possible paths between two given points in configuration space. Eq. (2.22) was postulated as a hypothesis in the previous work [36]. Here we give a derivation from the virtual work principle for random dynamics [76, 77].

We consider a statistical ensemble of mechanical systems out of equilibrium and its trajectories in configuration space. Each system is composed of N particles moving in the $3N$ dimensional space starting from a point a . If the motion was regular, all the systems in the ensemble would follow a single $3N$ -dimensional trajectory from a to a given point b according to the least action principle. In random dynamics, every system can take different paths from a to b as discussed in previous.

Now let us look at the random dynamics of a single system following a trajectory, say, k , from a to b . At a given time T , the total force on a particle i in the system is denoted by \mathbf{F}_i and the acceleration by \mathbf{a}_i with an inertial force $-m_i\mathbf{a}_i$ where m_i is its mass. The virtual work at this moment on a virtual displacement $\delta\mathbf{r}_{ik}$ of all the particle on the trajectory k reads

$$\delta W_k = \sum_{i=1}^N (\mathbf{F}_i - m_i\mathbf{a}_i)_k \cdot \delta\mathbf{r}_{ik}. \tag{2.23}$$

and the average virtual work can be shown as

$$\overline{\delta W} = \sum_{k=1}^w p_k \delta W_k = 0 \tag{2.24}$$

where we considered discrete paths denoted by $k = 1, 2 \dots w$ (if the variation of path is continuous, the sum over k must be replaced by path integral between a and b [12]), and p_k is the probability that the path k is taken. Eq. (2.24) is used as the new virtual work principle for random dynamics. It can be stipulated as: The statistical mean of the total virtual work done by all the forces acting on a system (equilibrium or not) in

random motion must be zero, where the means is taken over all the possible positions or states of the system at a given moment of time [75].

Now let us establish the relationship between virtual work and action variation (for one dimensional case, x is the position in the configuration space). For a given path k , the action variation is given by

$$\begin{aligned}
\delta A_k &= \sum_{i=1}^N \int_a^b \delta L_{ik} dt \\
&= \sum_{i=1}^N \int_a^b \left(\frac{\partial L}{\partial x_i} \delta x_i + \frac{\partial L}{\partial \dot{x}_i} \delta \dot{x}_i \right)_k dt \\
&= \sum_{i=1}^N \int_a^b \left(-\frac{\partial H_i}{\partial x_i} - \dot{P}_{xi} \right)_k \delta x_{ik} dt \\
&= \int_a^b \sum_{i=1}^N (F_{x_i} - m\ddot{x}_i)_k \delta x_{ik} dt = \int_a^b \delta W_k dt
\end{aligned} \tag{2.25}$$

where we used, for the particle i with Hamiltonian H_i and Lagrangian L_i , $F_{x_i} = -\frac{\partial H_i}{\partial x_i} = \frac{\partial L_i}{\partial x_i}$, $m\ddot{x}_i = \dot{P}_{xi} = \frac{\partial}{\partial t} \left(\frac{\partial L_i}{\partial \dot{x}_i} \right)$ and $\int_a^b \frac{\partial}{\partial t} (\delta x_i \frac{\partial L_i}{\partial \dot{x}_i}) dt = (\delta x_i \frac{\partial L_i}{\partial \dot{x}_i}) \Big|_a^b$ because of the zero variation at a and b .

The average action variation being $\overline{\delta A} = \sum_{k=1}^w p_k \delta A_k = \int_a^b \overline{\delta W} dt$, the virtual work principle Eq. (2.24) yields Eq. (2.22), i.e., $\overline{\delta A} = 0$. This SAP implies an varentropy variational approach. To see this, we calculate

$$\overline{\delta A} = \delta \sum_{k=1}^w p_k A_k - \sum_{k=1}^w \delta p_k A_k = \delta \overline{A}_{ab} - \delta Q_{ab} \tag{2.26}$$

where $\overline{A}_{ab} = \sum_{k=1}^w p_k A_k$ is the ensemble mean of action A_k between a and b , and δQ_{ab} can be written as

$$\delta Q_{ab} = \delta \overline{A}_{ab} - \overline{\delta A} = \sum_{k=1}^w A_k \delta p_k. \tag{2.27}$$

which is a varentropy measuring the uncertainty in the choice of trajectories by the system. We can introduce a path entropy S_{ab} such that

$$\delta Q_{ab} = \frac{\delta S_{ab}}{\gamma}. \tag{2.28}$$

Then Eqs. (2.22), (2.26) and (2.28) yield

$$\delta(S_{ab} - \gamma \overline{A}_{ab}) = 0. \tag{2.29}$$

If the normalization condition is added as a constraint of variational calculus, Eq. (2.29) becomes

$$\delta(S_{ab} - \gamma \sum_{k=1}^w p_k A_k + \alpha \sum_{k=1}^w p_k) = 0. \quad (2.30)$$

This is a maximum path entropy with two Lagrange multipliers α and γ , an approach originally proposed in the Ref. [36].

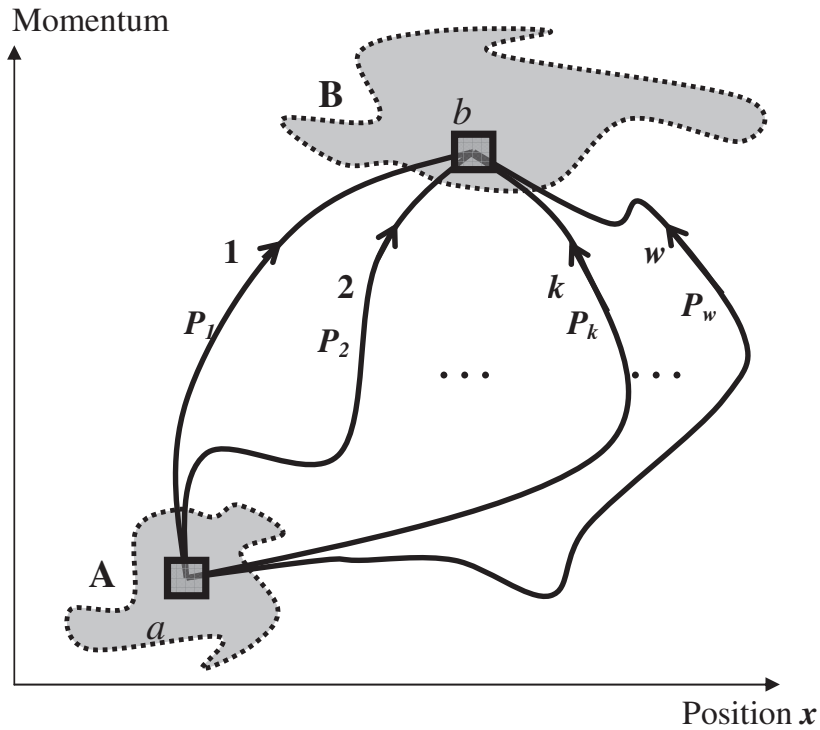


Fig. 2.3: Illustration of the 3 schemas of a random dynamics in phase space. **A** is the initial volume at time t_a and a is any point in **A**. **B** is the final volume at time t_b and b is any point in **A**. The directed schema means the system, leaving from a certain a , must arrive at a fixed b in **B**. The panoramic schema means the system, leaving from certain a , arrives at any arbitrary point b in **B**. The initial condition schema adds the uncertainty in the initial condition, meaning that the system, arriving at certain point b in **B**, can come from any arbitrary point a in **A**.

2.2 A path probability distribution

According to Shannon [40], the information can be measured by the formula $S = -\sum_i p_i \ln p_i$ where p_i is certain probability attributed to the situation i . We usually ask $\sum_i p_i = 1$ with a summation over all the possible situations. For the ensemble of w possible paths, a Shannon information can be defined as follows [36, 78]:

$$S_{ab} = -\sum_{k=1}^w p_k \ln p_k. \quad (2.31)$$

S_{ab} is a path information and should be interpreted as the missing information necessary for predicting which path a system of the ensemble takes from a to b .

2.2.1 Directed schema

If the path entropy takes the Shannon form, the SAP or Eq. (2.29) yields an exponential probability distribution of action

$$p_k(a, b) = \frac{1}{Z_{ab}} e^{-\gamma A_k(a, b)}. \quad (2.32)$$

where $Z_{ab} = \sum_{k=1}^w e^{-\gamma A_k(a, b)}$, meaning that this distribution describes a motion directed from a fixed point a to a fixed point b (see Fig. 2.3). The path entropy can be calculated by

$$S_{ab} = \ln Z_{ab} + \gamma \bar{A}_{ab}. \quad (2.33)$$

where $\bar{A}_{ab} = \sum_{k=1}^w p_k(a, b) A_k = -\frac{\partial}{\partial \gamma} \ln Z_{ab}$ is the average action between these two fixed points.

2.2.2 Panoramic schema

The above description is not complete for the dynamics since a real motion from an initial point a does not necessarily arrive at b . The system moves around and can reach any point in the final volume, say, B . Hence a complete description of the dynamics requires unfixed point b in B . The probability $p_k(a, B)$ for the system to go from a fixed point a to a unfixed b through a certain path k (depending on a and b) is given by

$$p_k(a, B) = \frac{1}{Z_a} e^{-\gamma A_k(a, b)}. \quad (2.34)$$

where $Z_a = \sum_{b,k} e^{-\gamma A_k(a,b)} = \sum_b Z_{ab}$, Hence the path entropy for this case is given by

$$S_{aB} = \ln Z_a + \gamma \bar{A}_a. \quad (2.35)$$

where $\bar{A}_a = \sum_b \sum_k p_k(a, B) A_k(a, b) = -\frac{\partial}{\partial \gamma} \ln Z_a$ is the average action over all the paths between a fixed point a to all the points in the final volume B . We have the following relationship $\bar{A}_a = \sum_b \sum_k p_k(a, B) A_k(a, b) = \sum_b \frac{Z_{ab}}{Z_a} \bar{A}_{ab} = \sum_b \frac{\exp(\ln Z_{ab})}{Z_a} \bar{A}_{ab} = \sum_b \frac{\exp(S_{ab} - \gamma \bar{A}_{ab})}{Z_a} \bar{A}_{ab}$. The function $p(a, B) = \exp(S_{ab} - \gamma \bar{A}_{ab})$ is the probability from the point a to an arbitrary point b in the final volume B no matter what path the process may take.

2.2.3 Initial condition schema

In order to include the contribution of the initial conditions to the dynamic uncertainty, we extend still the path probability to the schema in which a is also relaxed in the initial volume A . The transition probability from A to B through a certain path k is

$$p_k(A, B) = \frac{1}{Z} e^{-\gamma A_k(a,b)}. \quad (2.36)$$

where $Z = \sum_{a,b,k} e^{-\gamma A_k(a,b)} = \sum_a Z_a$. The total path entropy between A and B reads

$$S_{AB} = \ln Z + \gamma \bar{A}. \quad (2.37)$$

Here $\bar{A}_a = \sum_a \sum_b \sum_k p_k(A, B) A_k(a, b) = -\frac{\partial}{\partial \gamma} \ln Z$ is the average action of the process from A to B .

The total transition probability $p(A, B)$ between an arbitrary point a in A to an arbitrary point b in B through whatever paths is given by

$$p(A, B) = \frac{1}{Z} \exp(S_{ab} - \gamma \bar{A}_{ab}). \quad (2.38)$$

Using a Legendre transformation $F_{ab} = \bar{A}_{ab} - S_{ab}/\gamma = \frac{1}{\gamma} \ln Z_{ab}$ which can be called free action mimicking the free energy of thermodynamics, we can write $p(A, B) = \frac{1}{Z} \exp(-\gamma F_{ab})$.

This section provides a series of path probability distributions in exponential of action describing the likelihood of each path to be chosen by the motion. It is clear that if the constant γ is positive, the most probable path will be least action path. This implies that if the randomness of motion is vanishing, all the paths will collapse onto the

bundle of least action ones, which is accordance with the least action principle of regular motion. A more mathematical discussion can be found in Ref. [36, 37]. This formalism is to some extent a classical version of the idea of M. Gell-Mann [79, 80] to characterize, in superstring theory, the likelihoods of different solutions of the fundamental equation by quantized and Euclidean action.

Chapter 3

The path probability of stochastic motion of non dissipative systems

3.1 Introduction

The path (trajectory) of stochastic dynamics in mechanics has much richer physics content than that of the regular or deterministic motion. A path of regular motion always has probability one once it is determined by the equation of motion and the boundary condition, while a random motion may have many possible paths under the same condition, as can be easily verified with any stochastic process [16]. For a given process between two given states (or configuration points with given durations), each of those potential paths has some chance (probability) to be taken by the motion. The path probability is a very important quantity for the understanding and the characterization of random dynamics because it contains all the information about the physics: the characteristics of the stochasticity, the degree of randomness, the dynamical uncertainty, the equations of motion and so forth. Consideration of paths has long been regarded as a powerful approach to non equilibrium thermodynamics [81]-[90]. A key question in this approach is what are the random variables which determine the probability. The Onsager-Machlup type action [23, 24], is one of the answers for Gaussian irreversible process close to equilibrium where the path probability is an exponentially decreasing function of the action calculated along thermodynamic paths in general. This action has been extended to Cartesian space in Ref. [90]. The large deviation theory [25, 26] suggests a rate function to characterize an exponential path probability. There are

other suggestions by the consideration of the energy along the paths [91, 92]. For a Markovian process with Gaussian noises, the Wiener path measure [93, 94] provides a good description of the path likelihood with the product of Gaussian distributions of the random variables.

The reflexions behind this work are the following: suppose a mechanical random motion is trackable, i.e., the mechanical quantities of the motion under consideration such as position, velocity, mechanical energy and so on can be calculated with certain precision along the paths, is it possible to use the usual mechanical quantities to characterize the path probability of that motion? Possible answers are given in Refs. [91, 92]. The author of Ref. [91] suggests that the path probability decreases exponentially with increasing average energy along the paths [91]. This theory risks a conflict with the regular mechanical motion in the limit of vanishing randomness because the surviving path would be the path of least average energy, while it is actually the path of least action. The proposition of Ref. [92] is a path probability decreasing exponentially with the sum of the successive energy differences, which risks the similar conflicts with regular mechanics mentioned above.

In view of the imperative that the Newtonian path of regular motion should be recovered for vanishing randomness, we have thought about the possibility to relate the path probability to action, the only key quantity for determining paths of Hamiltonian systems in classical mechanics. Precisely, we want to know whether, in what case and under what conditions there can be a probability function analogous to the Feynman factor $e^{iA/\hbar}$ of quantum mechanics [12], i.e., a path probability decreasing exponentially with increasing action. As well known, the Feynman factor is not a probability, but here, in the presence of the quantum randomness, the action indeed characterizes the way the system evolves along the configuration paths from one quantum state to another [95]. At the same time, the systems remains Hamiltonian in spite of the quantum mechanical randomness. The classical mechanical paths will be recovered when the quantum randomness is vanishing with respect to the magnitude of the action (Planck constant \hbar tends to zero). Since action is well defined only for Hamiltonian (often energy conservative) systems [9, 43], in this work we will focus on nondissipative systems. The strongly damped motions will not be considered. From the previous results [81]-[92], it is evident that the paths of those random damped motions do not simply depend on the usual action, in general.

Hence the basic model of this work is an ideal mechanical motion, a random motion without dissipation. It can be described by the Langevin equation

$$m \frac{d^2x}{dt^2} = -\frac{dV(x)}{dx} - m\zeta \frac{dx}{dt} + R \quad (3.1)$$

with the zero friction limit (friction coefficient $\zeta \rightarrow 0$), where x is the position, t is the time, $V(x)$ is the potential energy and R is the Gaussian distributed random force. The Hamiltonian of these systems still makes sense in a statistical way. An approximate counterpart of this ideal model among real motions is the weakly damped random motion with negligible energy dissipation compared to the variation of potential energy, i.e., the conservative force is much larger than the friction force. In other words, the system is (statistically) governed by the conservative forces. These motions are frequently observed in Nature. We can imagine, e.g., a falling motion of a particle which is sufficiently heavy to fall in a medium with acceleration approximately determined by the conservative force at least during a limited time period, but not too heavy in order to undergo observable randomness due to the collision from the molecules around it or to other sources of randomness. In this case, Eq. (3.1) can still offer a good description. Other counterparts include the frequently used ideal models of thermodynamic processes, such as the free expansion of isolated ideal gas and the heat conduction within a perfectly isolated system which conserves energy in spite of the thermal fluctuation.

In what follows, we address only the motion prescribed by Eq. (3.1) in the zero friction limit. For this motion, a stochastic Hamiltonian/Lagrangian mechanics has been formulated in Ref. [36, 37] where the path probability is an exponentially decreasing function of action when the path entropy (a measure of the dynamic randomness or uncertainty of path probability) is given by the Shannon formula. The present work is a numerical simulation of this motion to verify this theoretical prediction. The method can be summarized as follows. We track the motion of a large number of particles subject to a conservative force and a Gaussian random force. The number of particles from one given position to another through some sample paths is counted. When the total number of particles are sufficiently large, the probability (or its density) of a given path is calculated by dividing the number of particles counted along this path by the total number of particles arriving at the end point through all the sample paths. The correlation of this probability distribution with two mechanical quantities, the action and the time integral of Hamiltonian calculated along the sample paths, is analyzed.

In what follows, we first give a detailed description of the simulation, followed by the analysis of the results and the conclusion.

3.2 Technical details of numerical computation

The numerical model of the random motion can be outlined as follows. A particle is subject to a conservative force and a Gaussian noise (random displacements χ , see Eq. (3.3) below) and moves along the axis x from an initial point a (position x_0) to a final point b (x_n) over a given period of time ndt where n is the total number of discrete steps and $dt = t_i - t_{i-1}$ the time increments of a step i which is the same for every step and $i=1,2,\dots,n$. Many different paths are possible, each one being a sequence of random positions $\{x_0, x_1, x_2 \cdots x_{n-1}, x_n\}$, where x_i is the position at time t_i and generated from a discrete time solution of Eq. (3.1) :

$$x_i = x_{i-1} + \chi_i + f(t_i) - f(t_{i-1}), \quad (3.2)$$

which is a superposition of a Gaussian random displacement χ_i and a regular motion $y_i = f(t_i)$, the solution of the Newtonian equation $m \frac{d^2x}{dt^2} = -\frac{dV(x)}{dx}$ corresponding to the least action path (a justification of this superposition is given below).

For each simulation, we select about 100 sample paths randomly created around the least action path $y = f(t)$. The magnitude of the Gaussian random displacements is controlled to ensure that all the sample paths are sufficiently smooth but sufficiently different from each other to give distinct values of action and energy integral. Each sample path is in fact a smooth tube of width δ whose axial line is a sequence of positions $\{z_0, z_1, z_2 \cdots z_{n-1}, z_n\}$. δ is sufficiently large in order to include a considerable number of trajectories in each tube for the calculation of reliable path probability, but sufficiently small in order that the positions z_i and the instantaneous velocities v_i determined along an axial line be representative of all the trajectories in a tube. If δ is too small, there will be few particles going through each tube, making the calculated probability too uncertain. If it is too large, z_i and v_i , as well as the energy and action of the axial line will not be enough representative of all the trajectories in the tube. The δ used in this work is chosen to be 1/2 of the standard deviation σ of the Gaussian distribution of random displacements. The left panels of Figs. 3.1-3.5 illustrate the axial lines of the sample paths.

For each sample path, the instantaneous velocity at the step i is calculated by $v_i = \frac{z_i - z_{i-1}}{t_i - t_{i-1}}$ along the axial line. This velocity can be approximately considered as the average velocity of all the trajectories passing through the tube, i.e., the trajectories satisfying $z_i - \delta/2 \leq x_i \leq z_i + \delta/2$ for every step i . The kinetic energy is given by $K_i = \frac{1}{2}mv_i^2$, the action by $A_L = \sum_{i=1}^{10} [\frac{1}{2}mv_i^2 - V(x_i)] \cdot dt$, called Lagrangian action from now on in order to compare with the time integral of Hamiltonian $A_H = \sum_{i=1}^{10} [\frac{1}{2}mv_i^2 + V(x_i)] \cdot dt$ referred to as Hamiltonian action. The magnitude of the random displacements and the conservative forces are chosen such that the kinetic and potential energy are of the same order of magnitude. This allows to clearly distinguish the two actions along a same path.

The probability that the path k is taken is determined by $P_k = N_k/N$ where N is the total number of particles moving from a to b through all the sample paths and N_k the number of particles moving along a given sample path k from a to b . Then these probabilities will be plotted versus A_L and A_H as shown in the Figs. 3.1-3.5. P_k can also be regarded as the probability for a particle to pass through a tube k when it is driven by Gaussian process.

In order to simulate a Gaussian process close to a realistic situation, we chose a spherical particle of 1- μm -diameter and of mass $m = 1.39 \times 10^{-15}$ kg. Its random displacement at the step i is produced with the Gaussian distribution

$$p(\chi_i, t_i - t_{i-1}) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{\chi_i^2}{2\sigma^2}}, \quad (3.3)$$

where χ_i is the Gaussian displacement at the step i , $\sigma = \sqrt{2D(t_i - t_{i-1})} = \sqrt{2Ddt}$ the standard deviation, $D = \frac{k_B T}{6\pi r \eta}$ the diffusion constant, k_B the Boltzmann constant, T the absolute temperature, and $r = 0.5 \mu\text{m}$ the radius of the particle. For the viscosity η , we choose the value 8.5×10^{-4} *Pas* of water at room temperature¹. In this case, $D \approx 4.3 \times 10^{-13}$ m^2/s and $\sigma \approx 3 \times 10^{-9}$ m with $dt = 10^{-5}$ s . The relaxation time is close to 10^{-7} s . With this reference, the simulations were made with different time increments dt ranging from 10^{-7} to 10^{-3} s . Due to the limited computation time, we have chosen $n = 10$.

We would like to emphasize that the simulation result should be independent of the choice of the particle size, mass, and water viscosity etc. For instance, if a larger body

¹Note that this viscosity is chosen to create a realistic noise felt by the particle as if it was in water. But this viscosity and the concomitant friction do not enter into the equation of motion Eq. (3.2).

is chosen, the magnitude (σ) of the random displacements and the time duration of each step, will be proportionally increased in order that the paths between two given points are sufficiently different from each other.

In what follows, we will describe the results of the numerical experiments performed with 5 potential energies: free particles with $V(x) = 0$, constant force with $V(x) = mgx$, harmonic force with $V(x) = \frac{1}{2}kx^2$ and two other higher order potentials $V(x) = \frac{1}{3}Cx^3$ and $V(x) = \frac{1}{4}Cx^4$ ($C > 0$) to check the generality of the results. These two last potentials yield nonlinear Newtonian equation of motion and may invalidate the superposition property in Eq. (3.2). Nevertheless we kept them in this work since linear equation is sufficient but not necessary for superposition. The reader will find that the results are similar to those from linear equations and that the superposition seems to work well. We think that this may be attributed to two favorable elements : 1) most of the random displacements per step are small (Gaussian) compared to the regular displacement; 2) the symmetrical nature of these random displacements may statistically cancel the nonlinear deviation from superposition property.

3.3 View path probability à la Wiener

Eq. (3.2) implies that the Gaussian distributed displacement is initialized at each step and the Gaussian bell of each step is centered on the position of the previous step. The probability of a given sample path k of width δ is just [16]

$$P_k = \prod_{i=1}^n \int_{z_i-\delta/2}^{z_i+\delta/2} p(\chi_i) dx_i = \frac{1}{\sqrt{2\pi}\sigma} \prod_{i=1}^n \int_{z_i-\delta/2}^{z_i+\delta/2} e^{-\frac{\chi_i^2}{2\sigma^2}} dx_i. \quad (3.4)$$

Substituting Eq. (3.2) for χ_i , one obtains

$$P_k = \frac{1}{\sqrt{2\pi}\sigma} \prod_{i=1}^n \int_{z_i-\delta/2}^{z_i+\delta/2} \exp\left\{-\frac{[x_i - x_{i-1} - f(t_i) + f(t_{i-1})]^2}{2\sigma^2}\right\} dx_i. \quad (3.5)$$

From this expression, it is not obvious to show the dependence of P_k on action without making approximation in the limit $dt \rightarrow 0$. We have calculated the path probability from Wiener measure in the special case where $V(x)$ is linear (see Appendix A for details). Exponential distribution of action is derived only for constant force. The calculation could not be solved for more complicated potentials. This is one of the motivations for doing numerical experiment to see what happens in reality.

3.4 Path probability distribution by numerical simulation

In each numerical experiment, we launch 10^9 particles from the initial point a . Several thousands N arrive, passing by all the sample paths, at the destination point b in the interval $z_b - \delta/2 \leq x_b \leq z_b + \delta/2$. The output of the simulation is N and N_k for every sample path whose actions have been already calculated. Once the path probability is determined by $P_k = N_k/N$, its correlation with the Lagrangian or Hamiltonian action of the sample paths can be found by drawing the probability values against the two actions. With 10^9 particles launched at point a , the calculated probability values are quite reliable, in the sense that more particles and longer computation time do not produce remarkable improvement of the probability distribution of action. The results presented below for each potential were obtained with $dt = 10^{-5}$ s.

3.4.1 Free particles

Free particles have zero potential energy and constant $f(t)$. So there is no difference between the Lagrangian and Hamiltonian actions. As expected from Eq. (3.5), the right panel of Fig. 3.1 shows a path probability of the form

$$P_k(A) = \frac{1}{Z} e^{-\gamma A_k}, \quad (3.6)$$

where A_k is either the Lagrangian or Hamiltonian action of the path k . The slope is $\gamma \approx 6.7 \times 10^{26} \text{ J}^{-1} \text{ s}^{-1}$. The normalization function Z can be analytically determined by the path integral technique [12]

$$\prod_{i=1}^{n-1} \int_{-\infty}^{\infty} \frac{dx_i}{\delta} P_k(A) = 1 \quad (3.7)$$

with fixed x_a and x_b , or numerically by the value of $\ln P(A=0)$ which can be found with the distribution curves in the figures.

3.4.2 Particles under constant force

To distinguish the dependences of the path probability on Lagrangian and Hamiltonian actions, it is necessary to random motion under conservative forces. The first force we

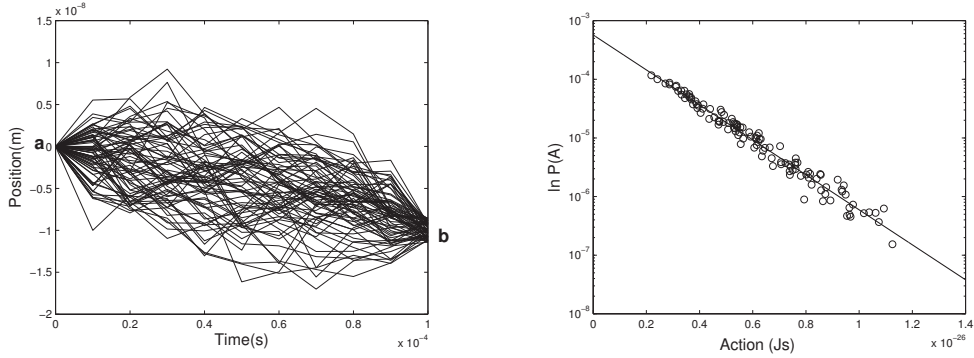


Fig. 3.1: The result for free particles. The left panel shows the axial lines of the sample paths between the given points a and b . The right panel shows the path probability distribution against the Lagrangian and Hamiltonian actions which are equal here as $V(x) = 0$ for free particles. The straight line is a best fit of the points with a slope of about $\gamma \approx 6.7 \times 10^{26} J^{-1}s^{-1}$.

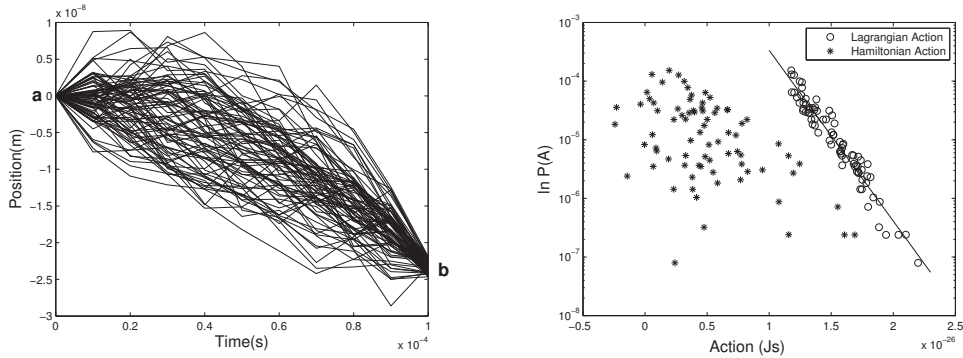


Fig. 3.2: The result for particles under constant force with potential $V(x) = mgx$. The left panel shows the axial lines of sample paths. The right panel shows the path probability distribution against the Lagrangian (circles) and Hamiltonian (stars) actions. The straight line is a best fit of the points. It implies an exponential dependence on the Lagrangian action with negative slope $\gamma \approx 6.4 \times 10^{26} J^{-1}s^{-1}$ in Eq. (3.6). There seems no correlation between the path probability and the Hamiltonian action.

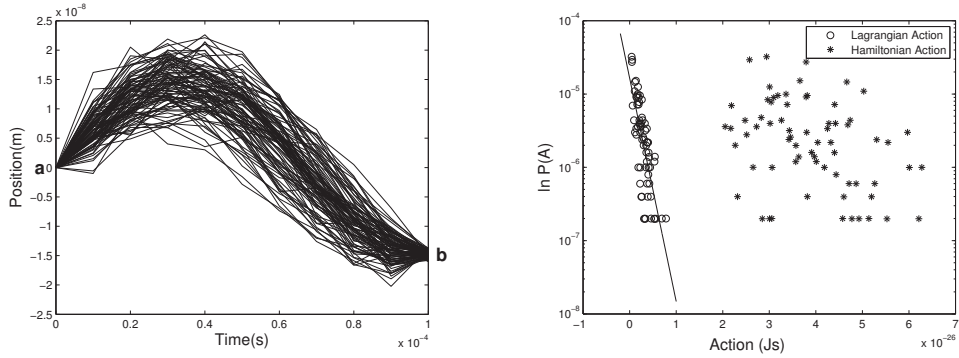


Fig. 3.3: The result for particles subject to a harmonic force with $V(x) = \frac{1}{2}kx^2$. The left panel shows the axial lines of sample paths. The right panel shows the path probability distribution against Lagrangian (circles) and Hamiltonian (stars) actions. The straight line is a best fit of the points whose negative slope $\gamma \approx 7 \times 10^{26} J^{-1}s^{-1}$ in Eq.(3.6).

studied is the constant force obtained from the potential $V(x) = mgx$. The regular motion is described by $f(t) = -\frac{1}{2}gt^2$, where the parameter $g = 10m/s^2$. The results are shown in the right panel of Fig. 3.2. Eq. (3.6) still holds with $\gamma \approx 6.4 \times 10^{26} J^{-1}s^{-1}$. There is no correlation between path probability and Hamiltonian action.

3.4.3 Particles under harmonic force

The potential of the harmonic force is $V(x) = \frac{1}{2}kx^2$ giving a regular motion $f(t) = A \sin(\omega t)$, where $A = 1.5 \times 10^{-8} m$ and $\omega = \sqrt{k/m} = 4.7 \times 10^4 s^{-1}$. The right panel of Fig. 3.3 shows the path probability distribution against actions. As for constant force, the path probability distribution decreases exponentially with increasing Lagrangian action with a slope of the straight line $\gamma \approx 7 \times 10^{26} J^{-1}s^{-1}$. No correlation with the Hamiltonian action is found.

3.4.4 Particles in cubic potential

To our opinion, the above results with 3 potentials are sufficiently convincing for the claim that the path probability decreases exponentially with increasing the Lagrangian action instead of the Hamiltonian one. But by curiosity, we also tried two other higher order potentials. The first one is $V(x) = \frac{1}{3}Cx^3$ giving a regular motion $f(t) = -\frac{6m}{C(t_0+t)^2}$ ($t_0 = 3 \times 10^{-5}$, $C = 200$). The path probability distributions against the two actions

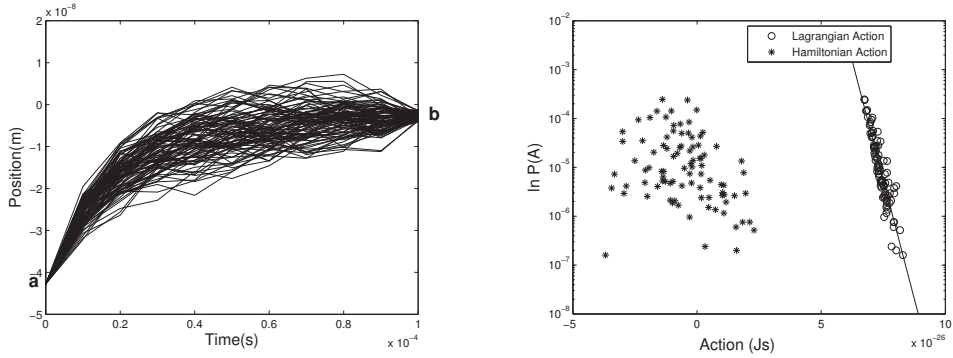


Fig. 3.4: The result for particles in a cubic potential $V(x) = \frac{1}{3}Cx^3$. The left panel shows that the axial lines of sample paths. The right panel shows the path probability distribution against Lagrangian (circles) and Hamiltonian (stars) actions. The straight line is a best fit of the points whose slope gives $\gamma \approx 4.5 \times 10^{26} J^{-1}s^{-1}$ for Eq. (3.6).

are shown in Fig. 3.4. Eq. (3.6) holds for the Lagrangian action with the coefficient $\gamma \approx 4.5 \times 10^{26} J^{-1}s^{-1}$.

3.4.5 Particles in quartic potential

For the one-dimensional quartic oscillator [58, 59, 60], the potential has the form $V(x) = \frac{1}{4}Cx^4$, with an approximate motion equation $f(t) \approx A \sin(\omega t)$. Unlike the harmonic potential, the frequency ω depends on the amplitude A , giving $\omega = \frac{2\pi}{T} \approx (\frac{3C}{4m})^{1/2}A = 2 \times 10^4 s^{-1}$ [58], where T is the complete cycle period (in the simulation, we have chosen $A = 1 \times 10^{-8} m$). The path probability distributions against the two actions are shown in Fig. 3.5. The distribution Eq. (3.6) with the Lagrangian action is still confirmed with $\gamma \approx 7.8 \times 10^{26} J^{-1}s^{-1}$.

3.5 Correlation between path probability and action

The path probability distributions depicted in Figs. 3.1-3.5 qualitatively confirm an exponential dependence on the Lagrangian action. To our opinion, the reliability of the result are rather remarkable taking into account the mediocre condition of simulation due to the limited computation time which restricts the number of steps of the motion

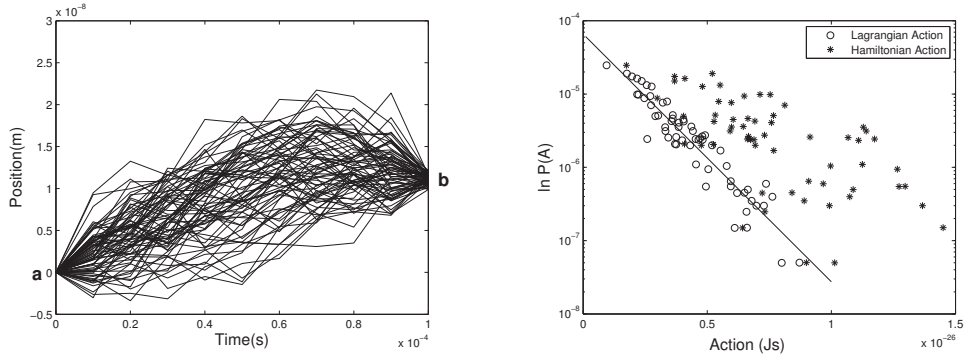


Fig. 3.5: The result for particles subject to a quartic potential. The left panel shows the axial lines of different sample paths. The right panel shows the path probability distribution against Lagrangian (circles) and Hamiltonian (stars) actions. The straight line is a best fit of the points whose slope gives $\gamma \approx 7.8 \times 10^{26} J^{-1}s^{-1}$ for Eq. (3.6).

and the minimum thickness of the sample paths. Larger number of steps would make the paths smoother and the calculation of velocity and action more reliable. Smaller thickness of the sample paths would reduce the uncertainty of the probability calculation for given action evaluated along the axial line of a sample path. But larger number of steps and smaller thickness of sample paths will reduce enormously the number of particles arriving at the end point and hence amplifies the uncertainty of the probability calculation. The choice of these two parameters must be optimized according to the computer power.

The quality of the computation of the probability distribution can be quantitatively estimated by using the correlation function $c(A)$ between A (A_L or A_H) and $-\ln P(A)$. This function is given by

$$c(A) = \frac{\sum_{i=1}^n (A_i - \langle A_i \rangle) [-\ln P(A_i) + \langle \ln P(A_i) \rangle]}{\sqrt{[\sum_{i=1}^n (A_i - \langle A_i \rangle)^2][\sum_{i=1}^n (-\ln P(A_i) + \langle \ln P(A_i) \rangle)^2]}}, \quad (3.8)$$

where $\langle A_i \rangle$ and $\langle \ln P(A_i) \rangle$ are the means of action A and $-\ln P(A)$ respectively. $|c(A)| \approx 1$ would indicate that A and $-\ln P(A)$ are linearly correlated. The results obtained from the numerical experiments are shown in Table 3.1.

The values of $c(A_L)$ close to unity confirms a linear correlation between $-\ln P(A)$ and A_L . It should be noticed that $c(A_H)$ and $c(A_L)$ are equal for free particles due to zero potential energy, and that $c(A_L)$ for different potentials are close to that for

Table 3.1: Values of the correlation function $c(A)$ between the path probability $-\ln P(A)$ and the Lagrangian action A_L in comparison with the Hamiltonian one A_H for the 5 considered potentials $V(x)$. The values of $c(A_L)$ close to unity confirms a linear correlation between $-\ln P(A)$ and A_L . The values of $c(A_H)$ are calculated for comparison. $c(A_H)$ is equal to $c(A_L)$ for free particles due to zero (or constant) potential energy. The fact that the addition of potentials does not significantly change $c(A_L)$ but considerably changes $c(A_H)$ with respect to the free particle values is another element advocating for the universal A_L dependence of the path probability.

$V(x)$	$c(A_L)$	$c(A_H)$
0	0.9865	0.9865
mgx	0.9686	0.4206
$\frac{1}{2}kx^2$	0.9473	0.3504
$\frac{1}{3}Cx^3$	0.9162	0.2302
$\frac{1}{4}Cx^4$	0.9397	0.5635

free particles while $c(A_H)$ for different potentials are quite different. This fact (the addition of different potentials does not significantly change $c(A_L)$ but considerably changes $c(A_H)$ with respect to the free particle result) is another proof of the A_L dependence of the path probability.

It has been also noticed that $c(A)$ is independent from the time scale dt (from 10^{-7} to 10^{-3} s).

3.6 Sensitivity of path probability to action

The decay rate of path probability with increasing action or its sensitivity to action is characterized by γ . The numerical experiments being performed with different time interval dt of each step, we noticed that γ is independent from the time increment dt . Logically, it should depend on the randomness of the Gaussian noise. For free particle, it is easy to show that $\gamma = \frac{1}{2mD}$ [36, 37, 96] which is not necessarily true with other potentials. Analysis of the probability distributions reveals that the ratio $\gamma/(1/D) \approx 3.2 \times 10^{14} \text{ kg}^{-1}$ for free particles, $\gamma/(1/D) \approx 3.1 \times 10^{14} \text{ kg}^{-1}$ for particles

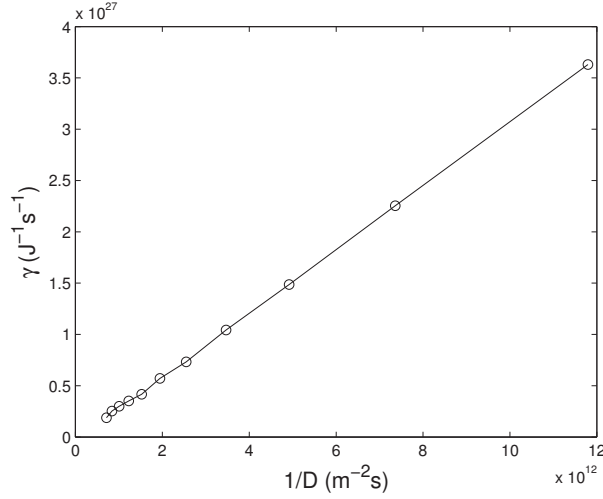


Fig. 3.6: $1/D$ dependence of the decay rate γ of path probability with action. The increase of γ with increasing $1/D$ implies that the stochastic motion is more dispersed around the least action path with more diffusivity. The slope or the ratio $\gamma/(1/D)$ is about $3.1 \times 10^{14} \text{ kg}^{-1}$.

subject to constant force, and $\gamma/(1/D) \approx 1.7 \times 10^{14} \text{ kg}^{-1}$ with harmonic force. Fig. 3.6 shows the $1/D$ dependence of γ for constant force as example. It was noticed that the ratio $\gamma/(1/D)$ of free particles is smaller than the theoretical value $1/2m = 3.6 \times 10^{14} \text{ kg}^{-1}$. This implies that, for given Gaussian noise, the numerically determined path probability decays less rapidly with increasing action than theoretical prediction. Two origins of this deviation are possible: the probability and the actions are either over-estimated by simulation for the paths far from the least action one, or under estimated for the paths close to the least action one. We think that the former origin is more probable. Further investigation is in progress to clarify this point.

As expected, γ increases with increasing $1/D$, i.e., the stochastic motion is more widely dispersed around the least action path with increasing diffusivity. This property can also be seen with the uncertainty relation of action given by the standard deviation $\sigma_A \geq \frac{1}{\sqrt{2\gamma}}$ [96]. For instance, when $\gamma = 3 \times 10^{27} \text{ (Js)}^{-1}$, $\sigma_A \geq 2.4 \times 10^{-28} \text{ Js}$. Finally, it is worth noticing the linear dependence of γ on $1/D$, at least in the range studied here. From theoretical point of view, γ should tends to infinity for vanishing D .

3.7 Conclusions

To summarize, by numerical simulation of Gaussian stochastic motion of non dissipative or weakly dissipative systems, we have shown the evidence of a classical homologue of the Feynman factor of quantum propagator. In spite of the uncertainty due to the limited computation time, the computation of the mechanical quantities and the path probability is rigorous and reliable. We hope that this result can be improved by more precise computation. Confirmation by experiment with weakly damped motion can also be expected. To our opinion, this result reveals a striking similarity between classical stochastic motion and quantum motion, and provides a new angle to view the classical random motion which can then benefit fully from the approach of path integral developed for quantum mechanics. An example of this tool borrowing is shown in Ref. [96] for the discussion of possible classical uncertainty relations. This probabilistic view of mechanical motion can possibly open a way to review some aspects of the relationship between mechanics and thermodynamics.

Unlike the Feynman factor $e^{iA/\hbar}$ which is just a mathematical object, $e^{-\gamma A}$ is a real function characterizing the path probability. This exponential form and the positivity of γ imply that the most probable path is just the least action path of classical mechanics, and that when the noise diminishes, more and more paths will shrink into the bundle of least action paths. In the limit case of vanishing noise, all paths will collapse on the least action path, the motion recovers the Newtonian dynamics.

The present result does not mean that the probability for single trajectory necessarily exists. Each path we considered is a tube of thickness δ and is sufficiently smooth and thin for the instantaneous position and velocity determined along its axial line to be representative for all the trajectories in it. The probability of such a path should tends to zero when $\delta \rightarrow 0$. However, the density of path probability should have a sense and can be defined by $\rho_k = \lim_{\delta \rightarrow 0} \frac{P_k}{\delta^n}$ for any finite n , the number of steps of a discrete random process.

Again, we would like to stress that the result of present work does not apply to the usual Brownian like motions studied with Langevin, Fokker-Planck, Kolmogorov equations [97]-[101] which include important dissipation due to friction. But it does not deny them neither. This work is not at odds with these well established approaches. This is a different angle to address stochastic dynamics. It is our hope that it will be applied to real stochastic dissipative motion. This application needs, first of all, a

fundamental extension of the least action principle to dissipative regular motion within classical mechanics. It is unimaginable that the action, being no more a characteristic variable of the paths of regular motion, can come into play when the same motion is perturbed by noise. This extension is another long story, and has been the objective of unremitting efforts of physicists till now [9, 43, 56, 102].

Chapter 4

Extended least action principle to dissipative mechanical systems

4.1 Introduction

The least action principle (LAP) is one of the most valuable heritages from the classical mechanics [10, 11, 103]. The fact that the formulation of the whole classical physics as well as of the quantum theory in its path integral formalism [12] could be based on or related to this single mathematical rule gives to LAP a fundamental priority to all other visibly different principles, empirical laws and differential equations in different branches of physics. This priority of LAP has nourished two major hopes or ambitions of physicists. The first one is the (rather controversial) effort to deepen the understanding of nature through this principle and to search for the fundamental meaning of its exceptional universality in physics [9, 103, 104, 105]. The second one is to extend it to more domains such as thermodynamics and statistical mechanics (with the pioneer effort of Boltzmann, Helmholtz and Hertz [30]), stochastic dynamics (e.g., large deviation theory [26] and stochastic mechanics [106, 107, 108]), and dissipative mechanical systems [43, 42, 44]. This chapter is following this last effort to formulate LAP for dissipative or nonconservative mechanical systems.

LAP was originally formulated only for Hamiltonian system [10], i.e., the sum $H = K + V$ of kinetic energy K and potential energy V of the considered system satisfies the Hamiltonian equations. For Hamiltonian systems, any real trajectory between two given configuration points must satisfy the LAP given by a vanishing first

variation δA due to tiny deformation of the trajectory [9, 10]

$$\delta A = \delta \int_0^T L dt = \int_0^T \delta L dt = 0 \quad (4.1)$$

where the action $A = \int_0^T L dt$ is a time integral of the Lagrangian $L = K - V$ on the trajectory from a point a to a point b over a fixed time period T (suppose $t_a = 0$ and $t_b = T$ from now on). One of the important results of this variational calculus is the Euler-Lagrange equation given by [9] (for one freedom x)

$$\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{x}} \right) - \frac{\partial L}{\partial x} = 0 \quad (4.2)$$

where \dot{x} is the velocity. In many cases when H and L do not depend on time explicitly, a Hamiltonian system is energy conservative. For damped motion with friction force f_d , the above equation becomes $\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{x}} \right) - \frac{\partial L}{\partial x} = f_d$ which is equivalent to write $\int_0^T (\delta L + f_d \delta x) dt = 0$ [41]. Despite this vanishing equality, it is impossible to calculate and optimize an action integral like A above with a single (Lagrangian) function satisfying Eq. (4.2). This difficulty leads to the disappearance of LAP in dissipative systems.

There has been a longstanding effort to formulate LAP for nonconservative or dissipative system [42]. As far as we know, the first proposition was made by Rayleigh [45] who introduced a dissipative function, $D = \frac{1}{2} m \zeta \dot{x}^2$, to write $\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{x}} \right) + \frac{\partial D}{\partial \dot{x}} - \frac{\partial L}{\partial x} = 0$, where $\zeta = \gamma/m$, γ is the viscous drag coefficient in the Stokes' law $\vec{f}_d = -m\zeta\vec{\dot{x}}$ and m the mass of the damped body. Although the equation of motion is kept in a similar form as Lagrangian equation, LAP is not recovered since there is no single Lagrangian for defining an action which satisfies Eq. (4.1). Other major propositions include the Bateman approach [46] to introduce complementary variables and equations, the definition of dissipative Lagrangian by multiplying the non dissipative one with an exponential factor $\exp(\zeta t)$ [47] where t is the time, the fractional derivative formulation [48], and the pseudo-Hamiltonian mechanics [49] where a parameter was introduced to characterize the degree of dissipation. The reader is referred to the reviews in [42, 43, 48, 49, 57] about the details of these propositions. In general, the Lagrangian in these solutions is not unique and has no energy connection like $L = K - V$ (see for instance the quasi-Lagrangian $L = e^{\zeta t}(K - V)$ and the corresponding quasi-Hamiltonian $H = e^{-\zeta t}K + e^{\zeta t}V$ for damped harmonic oscillator [47]). Hence no variational or optimal calculus was possible in general form [42, 43, 57].

A common character of these works is that the damped body is the only object taken into account in the calculations as if it was isolated. However, a dissipative system is always coupled to an environment and loses energy into the latter, an integral part of the motion. As far as this lost energy is not considered, the quasi-Lagrangian function of the damped body inevitably loses energy connection and generic optimal characters [42, 43] as mentioned above.

The aim of this chapter is to establish a LAP of dissipative system that recovers the energy connection and the uniqueness of a single Lagrangian function, its relation with a conservative Hamiltonian (Legendre transform), as well as the four formulations of analytical mechanics, i.e., the Newtonian equation of motion, the Lagrangian equations, the Hamiltonian equations and the Hamilton-Jacobi equation. However, as is shown below, the nonlocal character of the dissipative energy makes the Hamiltonian and Lagrangian non local in space and time. The variational calculus is thus more subtle than with instantaneous and local Lagrangian. Non local Lagrangian possibly gives to to the derived equation of motion non local character. A consequence of the non locality of the Lagrangian is that, by the consideration of different physical constraints, different variational calculus are possible. The problem is that some seemingly correct calculus does not lead to the correct equation of motion. This means that either this calculus is correct but the action is bad, or the action is good but the calculus has problem. Another open question concerning the dissipative LAP is about the nature (maximum, minimum or inflection) of the possible stationarity of action. If the action of the optimal path is a minimum when there is no friction, does this minimum survive with energy dissipation? If not, when is the optimal action a maximum and when an inflection (saddle) point? In what follows, we will present the different variational calculus and numerical simulations of damped motion. The purpose of this simulation is to calculate the actions along the optimal path and many variational paths created with tiny random deformations in the vicinity of the optimal one. By the comparison of these actions, we will have an idea about the existence of the stationarity $\delta A = 0$ for the optimal paths and its nature, in order to answer, at least partially, the above questions.

4.2 Least action principle for dissipative systems

4.2.1 The conservative Hamiltonian

The idea is to consider the damped moving body and its environment, coupled to each other by dissipative force, as a whole conservative system to which LAP can be a priori applied. The total Hamiltonian includes the instantaneous kinetic energy and the potential energy of the body, as well as the mechanical energy that is lost from the beginning of the motion and transformed into heat or other forms of kinetic and potential energy (noises, vibration etc) in the environment. Concretely, we construct a total system composed of a one dimensional large moving body (system 1) along the axis x and its environment (system 2) which includes all the parts coupled to system 1 by friction and receiving the dissipated mechanical energy. The total Hamiltonian can be given by $H = K + V + H_i + H_e$ where $K = \frac{1}{2}m\dot{x}^2$ is the kinetic energy, V is the potential of a conservative force acting only on system 1, H_i is the interaction energy between system 1 and system 2, $H_e = H_0 + E_d$ is the total energy of the environment, H_0 is its energy at the initial moment of the motion hence a constant independent of the motion, and E_d is the negative work of the friction force $\vec{f}_d = -f_d\vec{k}$ from $x_a = x(0)$ to a position $x(t)$ along a given path $s = s(t)$ ($0 \leq t \leq T$) where f_d is the magnitude of \vec{f}_d and \vec{k} is a unitary vector indicating the direction of the motion at a point $x(t)$. For simplicity, suppose that the energy of interaction H_i does not change in the course of the motion and system 2 does not move as a whole, hence the macroscopic moving paths of the whole system are just the paths of system 1. This allows to calculate the action of the whole system along the paths $s = x(t)$ of system 1 moving between two configuration points x_a and x_b during the time period T . The amount of energy E_d dissipated from system 1 to system 2 is given by:

$$\begin{aligned} E_d[x(0, t)] &= - \int_{x_a}^{x(t)} \vec{f}_d \cdot d\vec{s}(\tau) = \int_0^{x(t)} f_d \vec{k} \cdot ds(\tau) \vec{k} \\ &= \int_0^{x(t)} f_d ds(\tau) = \int_0^t f_d(\tau) \dot{x}(\tau) d\tau \end{aligned} \tag{4.3}$$

where τ is any time moment between $t_a = 0$ and t , $d\vec{s} = d\vec{x} = \dot{\vec{x}}d\tau$ is a small displacement along s . $E_d[x(0, t)]$ means that the dissipated energy depends on both the past trajectory $x_a = x(0)$ to the present instantaneous position $x(t)$. The magnitude of friction force f_d can be any function of time, position and velocity.

On the other hand, during the motion, the energy of system 2 at time t can be written as $H_e = H_0 + E_d$ where H_0 is its energy (a constant) at t_a and can be dropped from the variational calculus of the action. Finally we will consider only the following effective Hamiltonian for the motion: $H = K + V + E_d$. This effective Hamiltonian is formally nonlocal due to the space-time non locality of the integral of E_d in Eq. (4.3). E_d is dissipated part of H_e , its non-locality comes from its expression on the coordinates x of the damped body. But H_e is actually a local function of the motion and can be expressed by the instantaneous energy of the N constituent particles of the environment at the moment t , i.e., $H_e = \sum_{i=1}^N (k_i + v_i)$ where k_i and v_i is respectively the instantaneous kinetic and potential energy of the particle i .

Anyway, this non-locality of the Hamiltonian can have some influence on the variational calculus. It will be shown later that this influence can be avoided by the consideration of the principle of locality or of the energy conservation. The instantaneous increment of E_d is compensated by the simultaneous equal decrement of $K + V$, assuring a constant H in time and space for the isolated whole system.

Before proceeding with Lagrangian function and LAP, we stress that the impact of the thermal fluctuation in system 2 on system 1 should be neglected in order to have a smooth and deterministic motion of the latter. This is not difficult for a body which is much larger than the constituents of system 2 and has much larger energy variation during the motion than the energy fluctuation of the thermal motion in system 2. The reason for this approximation is that LAP for stochastic motion is still an unsolved problem to date. LAP in its conventional form is not compatible with random dynamics. It is also for this reason that, in this work aiming at extending LAP, expressing E_d in terms of the coordinates and velocities of the microscopic constituents of system 2 will not help because of their random motion related to heat, an inevitable effect of friction. Fortunately, no matter how the particles in system 2 move and whatever is their state of randomness, their unique relevant effect on the motion of system 1 is the friction. Thanks to the conservation law of energy, the dissipated energy E_d , i.e., the increment of the sum of the kinetic and potential energies of all the particles in system 2 expressed in terms of their coordinates and velocities, whatever is the form, can be mapped onto the coordinates of the system 1 through the work of the friction forces.

4.2.2 A dissipative Lagrangian function

The first difficulty for writing the Lagrangian is the impossibility to separate E_d into kinetic and potential parts relative to the coordinate x of interest. The second difficulty can be explained as follows. Suppose the simple case where E_d is only kinetic energy (heat in an ideal gas for example), we are inclined to write $L = K - V + E_d$ according to the convention. Unfortunately, it is straightforward to show that this will lead to an incorrect equation of motion when this L is introduced into Eq. (4.2).

In what follows, we consider the fact that E_d , after the integration in Eq. (4.3) over a certain trajectory from $x(0)$ to the instantaneous position $x(t)$ which is changing in time, implying that the integral of Eq. (4.3) is an indefinite one. According to the second fundamental theorem of calculus [109], the friction force at time t can be calculated from E_d by $f_d = \frac{\partial E_d}{\partial x}$ in a similar way as the conservative force is derived from a potential. Obviously E_d is not a potential since it depends not only on $x(t)$, but also on the past trajectory along which the integral Eq. (4.3) has been carried out (in practice, a trajectory $s = s(t)$ can be introduced in the calculation of E_d by writing $ds = \dot{s}(\tau)d\tau$). Moreover, it is impossible, contrary to potential energy, to recover E_d (an increasing function of time) as mechanical energy of system 1 just by moving the latter backwards. However, E_d has a common character with potential energy: its instantaneous increase yields the resistance force through the instantaneous displacement of the body; in other words, the infinitesimal increase dE_d at time t is equal to the negative work done by the friction force over an instantaneous displacement $dx(t)$, i.e., $dE_d = -\vec{f}_d \cdot d\vec{x} = f_d dx$ (for more than one dimension, this means $dE_d = -\vec{f}_d \cdot d\vec{r}$ or $\vec{f}_d = -\nabla_{\vec{r}(t)} E_d$). We think that the above arguments are sufficient, from the energetic point of view, for considering E_d as a pseudo-potential and writing $L = K - V - E_d$ as an effective Lagrangian. The effective action of the whole system on a given path between a and b is then given by

$$A = \int_0^T (K - V - E_d) dt. \quad (4.4)$$

Due to the space-time non locality of E_d , both H and L defined above are non local. This makes it possible to use different variational calculus from different physics points of view. In what follows, we will present briefly these variational techniques and the concomitant equations of motion for the sake of reflection about the technique of variation.

4.3 Variational formulation

4.3.1 The “global” variational calculus

Fig. 4.1 illustrates a variation operation over the entire optimal path (thick line) from the point a to the end point b . Let $\delta(t)$ be the variation on the position at time t , with $\delta(a) = \delta(b) = 0$. In the conventional previous calculus, thanks to the time locality of the Lagrangian, the variation of action A was only produced by the position variation $\delta x(t)$ in the Lagrangian, i.e., $\delta A = \int_0^T [L(x + \delta x(t), \dot{x} + \delta \dot{x}(t), t) - L(x, \dot{x}, t)] dt$. The effect of the variation over the whole path on the action is naturally taken into account through the time integral of the action. Now with the action of Eq. (4.4), the question arises about the variation at the moment τ before the moment t . The following calculus takes into account the variation $\delta x(\tau)$.

$$\delta A = \int_0^T \delta(K - V - E_d) dt. \quad (4.5)$$

The part $\int_0^T \delta(K - V) dt$ is $\int_0^T \left[\frac{d}{dt} \left(\frac{\partial(K-V)}{\partial \dot{x}} \right) - \frac{\partial(K-V)}{\partial x} \right] \delta x(t) dt$, while the part $\int_0^T \delta E_d dt$, with $E_d = \int_0^t f(\tau) d\tau$ and $f = f_d(\tau) \dot{x}(\tau)$ turns out to be (see Appendix B for details)

$$\int_0^T \left[\frac{\partial f}{\partial \dot{x}} + (T - t) \left(\frac{\partial f}{\partial x} - \frac{d}{dt} \left(\frac{\partial f}{\partial \dot{x}} \right) \right) \right] \delta x(t) dt.$$

Finally, the LAP $\delta A = 0$ gives

$$\frac{\partial(K - V)}{\partial x} - \frac{d}{dt} \left(\frac{\partial(K - V)}{\partial \dot{x}} \right) - \frac{\partial f}{\partial \dot{x}} - (T - t) \left(\frac{\partial f}{\partial x} - \frac{d}{dt} \left(\frac{\partial f}{\partial \dot{x}} \right) \right) = 0. \quad (4.6)$$

This equation is not the expected one (see Eq. 4.8 below) unless $f_d = \frac{\partial f}{\partial \dot{x}} + (T - t) \left(\frac{\partial f}{\partial x} - \frac{d}{dt} \left(\frac{\partial f}{\partial \dot{x}} \right) \right)$.

4.3.2 The “forward” variational calculus

It should be noticed that this extra term comes from the consideration of the variation of x at time τ before the moment t . Mathematically, this consideration is equivalent to considering the effect of the dissipative energy on the posterior motion, But physically, it is equivalent to considering the effect of the dissipative energy of the anterior motion on the present motion and violates the principle of locality of classical mechanics. The energy dissipated has been already absorbed irreversibly into the surroundings

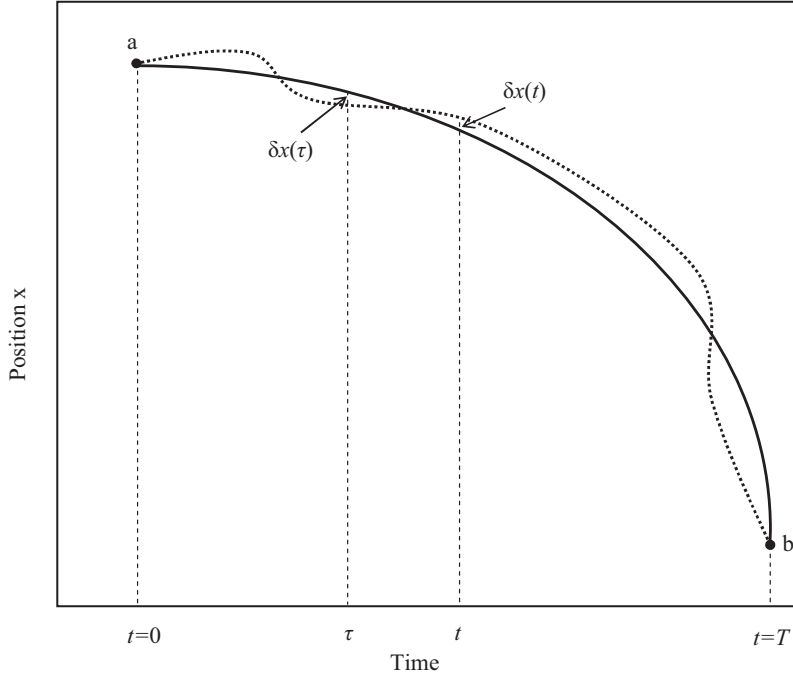


Fig. 4.1: Illustration of an exaggerated variation operation over the entire optimal path (thick line) from the point a to the end point b .

and should not affect the mechanical motion of the body any more if the thermal fluctuation of the environment is neglected as mentioned above. Hence we propose the following forward variational calculus which means that the variation $\delta x(\tau)$ will not be considered. This does not mean that the part of the path before t is not deformed. The variation of the path is the same as shown in Fig. 4.1, the deformation of the whole path is taken into account through the time integral over t . The usual variational calculus [9, 10]

$$\delta A = \int_0^T \delta L dt = \int_0^T \left[\frac{\partial L}{\partial x(t)} \delta x(t) + \frac{\partial L}{\partial \dot{x}(t)} \delta \dot{x}(t) \right] dt, \quad (4.7)$$

which becomes $\delta A = \int_0^T \left[\frac{\partial L}{\partial x(t)} - \frac{d}{dt} \left(\frac{\partial L}{\partial \dot{x}(t)} \right) \right] \delta x(t) dt$ after the time integral by part of $\delta \dot{x}$. Considering the condition $\delta x(t_a) = \delta x(t_b) = 0$, the vanishing first variation $\delta A = 0$ yields the Euler-Lagrangian equation Eq. (4.2) and the Newtonian equation of damped motion [56]:

$$m\ddot{x} = -\frac{\partial V}{\partial x} - f_d, \quad (4.8)$$

where we used the expression $f_d = \frac{\partial E_d}{\partial x}$.

In the above calculus, we considered the principle of locality of classical mechanics

in order to avoid the influence of earlier states on the present motion. This help from another principle to the variational calculus is in fact not necessary if we consider the differential version of LAP. The argument is the following. If A is a minimum over the entire optimal trajectory between a and b , the same must be true over any segment of the trajectory, i.e., the time integral of L over a segment Δx must be a minimum whatever its length is. If not, we can always play with this segment to make A smaller than its minimal value along the optimal path. Now if ΔA is the action over this small segment around the time moment t' , from Eq. (4.4), we have

$$\Delta A = \int_{t'}^{t'+\Delta t} \left[\frac{1}{2}m\dot{x}^2 - V - m\zeta \int_0^{x(t)} \dot{x}(\tau)dx(\tau) \right] dt. \quad (4.9)$$

The variation of the first two terms in the integrand is the same as in Eq. (4.7). The variation of the third term, i.e., of E_d , is

$$\delta E_d = m\zeta \int_0^{x(t)+\delta x(t)} \dot{x}(\tau)dx(\tau) - m\zeta \int_0^{x(t)} \dot{x}(\tau)dx(\tau) = \frac{\partial E_d}{\partial x(t)}\delta x(t).$$

Put this back into the variation of ΔA , we get

$$\begin{aligned} \delta \Delta A &= \int_{t'}^{t'+\Delta t} \frac{d}{dt} \left[\frac{\partial L}{\partial \dot{x}(t)} \delta x(t) \right] dt + \int_{t'}^{t'+\Delta t} \left[\frac{\partial L}{\partial x(t)} - \frac{d}{dt} \left(\frac{\partial L}{\partial \dot{x}(t)} \right) \right] \delta x(t) dt \\ &= \left[\frac{\partial L(t'+\Delta t)}{\partial \dot{x}(t'+\Delta t)} \delta x(t'+\Delta t) - \frac{\partial L(t')}{\partial \dot{x}(t')} \delta x(t') \right] \\ &\quad + \int_{t'}^{t'+\Delta t} \frac{d}{dt} \left[\frac{\partial L}{\partial x(t)} - \frac{d}{dt} \left(\frac{\partial L}{\partial \dot{x}(t)} \right) \right] \delta x(t) dt \end{aligned} \quad (4.10)$$

Since the variational path must join the optimal path before and after the small $\Delta x(t)$, hence $\delta x(t'+\Delta t) = \delta x(t') = 0$. The Euler-Lagrangian equation Eq. (4.2) will be a necessary consequence of the vanishing first variation $\delta \Delta A = 0$. This confirms the LAP by the variation of whole path aided by the principle of locality.

4.3.3 Derivation from virtual work principle

The above LAP can also be derived from other fundamental principles as has been done in analytical mechanics by using virtual work principle of d'Alembert [10, 74]. This latter principle is valid in the presence of friction force. For 1-dimensional moving body, it reads:

$$\delta W = (f - f_d - m\ddot{x})\delta x. \quad (4.11)$$

where $f = -\frac{\partial V}{\partial x}$ is the conservative force. This expression implies that system 2 has been involved in the motion since $E_d = \int_0^{x(t)} f dx(\tau)$ is a part of its energy. Using $\ddot{x}\delta x = \frac{d}{dt}(\dot{x}\delta x) - \dot{x}\delta\dot{x} = \frac{d}{dt}(\dot{x}\delta x) - \frac{\partial(K/m)}{\partial \dot{x}}\delta\dot{x}$, then integrating Eq. (4.11) over time from $t_a = 0$ to $t_b = T$, we get

$$\int_0^T \left[\frac{\partial K}{\partial \dot{x}}\delta\dot{x} - \frac{\partial(V + E_d)}{\partial x} \right] dt = \int_0^T \left(\frac{\partial L}{\partial \dot{x}}\delta\dot{x} + \frac{\partial L}{\partial x}\delta x \right) dt = \int_0^T \delta L dt = \delta A = 0 \quad (4.12)$$

where we used $\delta x(t_a) = \delta x(t_b) = 0$, $L = K - V - E_d$ and $A = \int_0^T L dt$.

Within this formalism, it is easy to verify that the Legendre transformation $H = p\dot{x} - L$ is still valid, where p is the momentum of system 1. With the usual method [9] using Euler-Lagrange equation Eq. (4.2), the Hamiltonian equations can be derived:

$$\dot{p} = -\frac{\partial H}{\partial x}, \quad \dot{x} = \frac{\partial H}{\partial p}. \quad (4.13)$$

The Hamilton-Jacobi equation also holds. To see this, we relax T in the integral Eq.(4.4) or consider the integral as indefinite, and compute $L = \frac{dA}{dt}$. Thanks to Eq. (4.2) and the above Legendre transformation, we can get $p = \frac{\partial A}{\partial x}$ and the Hamilton-Jacobi equation:

$$\frac{\partial A}{\partial x} + H = 0. \quad (4.14)$$

or $\frac{\partial A}{\partial x} = -\frac{1}{2m}(\frac{\partial A}{\partial x})^2 - V - E_d$ to show the dissipative character of this equation for the whole system (damped body + environment).

4.3.4 Application of Maupertuis' principle

It is worth mentioning that, if the conservation of the total Hamiltonian H is considered as a constraint of variation, the mathematical trouble of whole variation with the non locality of the expression of E_d can be easily avoided. The constraint of constant H for the total isolated system is reasonable because any conceivable motion (even virtual) should not violate this universal law. With this in mind, the non locality of Lagrangian disappears if we consider the Legendre transformation $L = p\dot{x} - H$ since L varies in the same way as $p\dot{x}$ if H is constant. Hence the optimization of L is equivalent to that of the function $p\dot{x}$. This remind us of the Maupertuis' LAP with the action defined by $A_m = \int_{x_a}^{x_b} m\dot{x}dx$ [11]. It is well known [57] that the Maupertuis' LAP $\delta A_m = 0$ is equivalent to the Hamilton's LAP $\delta A = 0$ stipulating with the conditions of fixed

points a and b as well as fixed time T instead of fixed total energy H . The calculus is

$$\delta A_m = \delta \int_{x_a}^{x_b} P dx = \int_{x_a}^{x_b} (\delta P dx + P \delta dx). \quad (4.15)$$

Considering $dx = \dot{x} dt$ in the two terms, the first term becomes $\delta(\frac{P^2}{2m}) dt$. Then making integration by part of $\delta \dot{x}$ in the second term, considering $\delta x(a) = \delta x(b) = 0$, this term becomes $-m \ddot{x} \delta x dt$. The total energy conservation $\delta H = 0$ means $\delta(\frac{P^2}{2m}) = -\frac{\partial V}{\partial x} \delta x - \frac{\partial E_d}{\partial x} \delta x$. Finally, we have

$$\delta A_m = \int_0^T \left[-\frac{\partial V}{\partial x} - \frac{\partial E_d}{\partial x} - m \ddot{x} \right] \delta x dt, \quad (4.16)$$

which implies that the Maupertuis' principle $\delta A_m = 0$ necessarily and sufficiently leads to the Euler-Lagrange equation Eq. (4.2) and to Eq. (4.8) as well.

4.3.5 The variational calculus with local Lagrangian

If the conservation of the total Hamiltonian $H = K + V + H_i + H_e$ or $H = K + V + H_e$ (with constant H_i) is considered, it is then possible to express H_e by the instantaneous energy of the N constituent particles of the environment at the moment t , i.e., $H_e = \sum_{i=1}^N (k_i + v_i)$ where k_i and v_i is respectively the kinetic and potential energy of the particle i . The Lagrangian can be written as $L' = K - V + K_e - V_e$ where $K_e = \sum_{i=1}^N k_i$ and $V_e = \sum_{i=1}^N v_i$, or $L' = K - V + 2K_e - H_e$. The action is given by $A = \int_0^T L dt$. Its variation due to $\delta x(t)$ is

$$\delta A = \int_a^b [\delta(K - V) + 2\delta K_e - \delta H_e] dt. \quad (4.17)$$

δK_e should vanish because K_e is not explicit function of x and \dot{x} . H_e should also be independent from \dot{x} . It is however x dependent if we keep of the energy conservation $\delta H = 0$ as a constraint of the variation, implying that $\delta H_e = -\delta(K + V) = \delta E_d = \frac{\partial E_d}{\partial x} \delta x$. Put this into Eq. (4.17), Newtonian equation Eq. (4.8) will follows.

It should be notice that the Lagrangian L' is equivalent to L defined previously if we consider the fact that K_e is not affected by the variation $\delta x(t)$ and that the affected part of H_e is just E_d , leading to effective Hamiltonian $H = K + V + E_d$ and Lagrangian $L = K - V - E_d$, as is explained before.

Summarizing the above application of variational calculus, the first global variational calculus seems inevitable from mathematical point of view although it is suspected of taking into account the same variation twice. This may be the origin of the

incorrect equation of motion. On the other hand, the second “forward” variation leads to correct equation but the argument of the irreversible motion for the rejection of $\delta x(\tau)$ may be accused of artificial choice. Regarding the Maupertuis’ version of LAP and the calculus with the local Lagrangian, the conservation of energy is needed to restrain the variation of the optimal paths, while in Hamiltonian/Lagrangian mechanics, the Hamilton version of LAP (with fixed duration of motion) does not have this constraint. From purely operational point of view, to fix the duration of motion is much easier than to fix the energy when numerically simulating the motion and the variational calculus.

Before this uncertainty, we decided to make numerical calculation and comparison of actions along the optimal path given by Newtonian equation and many other deformed paths around the optimal one. Since the deformation is created arbitrarily without constraint on the Hamiltonian, the dissipative action defined with $L = K - V - E_d$ is used. The aim is to see whether or not it is likely for this action to have extrema and what would be the nature (maximum, minimum or inflection). The techniques and the results will be presented below.

4.4 The optimal path and action with constant force and Stokes’ drag

The first case we consider is a small particle of mass $m = 1.39 \times 10^{-6}$ kg subject to a constant force $f = mg$ where $g = 10 \text{ ms}^{-2}$. The friction is given by the Stokes’ drag, i.e., $f_d = m\zeta\dot{x}$. The optimal path corresponding to $\delta A = 0$ or given by Eq. (4.8) is $x(t) = \frac{g}{\zeta^2}(1 - e^{-\zeta t}) - \frac{g}{\zeta}t$ for $x(0) = 0$ and $\dot{x}(0) = 0$. The optimal action $A_{op} = \int_0^T (\frac{m}{2}\dot{x}^2 - mgx - m\zeta \int_0^t \dot{x}^2 d\tau) dt$ can be calculated analytically and given by

$$A_{op} = \frac{mg^2}{\zeta^2} \left(-\frac{1}{2\zeta} e^{-2\zeta T} + \frac{2}{\zeta} e^{-\zeta T} - \frac{3}{2\zeta} + T \right) \quad (4.18)$$

whose ζ and T dependence are shown in Figs. 4.2 and 4.3, respectively. When ζ and T are sufficiently small, so that the dissipative part of the action $A_d = \int_0^T E_d dt = m\zeta \int_0^T \int_0^t \dot{x}^2 d\tau dt$ can be negligible, $A_{op} \approx \int_0^T (\frac{m}{2}\dot{x}^2 - mgx) dt = \frac{1}{3}mg^2T^3 = A_0(\zeta = 0)$ where A_0 denotes the usual action defined by $A_0 = \int_0^T (\frac{m}{2}\dot{x}^2 - mgx) dt$ or

$$A_0 = \frac{mg^2}{\zeta^2} \left(-\frac{1}{4\zeta} e^{-2\zeta T} + \frac{1}{4\zeta} - \frac{1}{2}T + \frac{1}{2}\zeta T^2 \right). \quad (4.19)$$

For $\zeta = 0$, $A_0 = \frac{1}{3}mg^2T^3$. Notice that $A_{op} = A_0 - A_d$. A_d is given by

$$A_d = \frac{mg^2}{\zeta^2} \left(\frac{1}{4\zeta} e^{-2\zeta T} - \frac{2}{\zeta} e^{-\zeta T} + \frac{7}{4\zeta} - \frac{3}{2}T + \frac{1}{2}\zeta T^2 \right) \quad (4.20)$$

which becomes $A_d \approx \frac{1}{12}mg^2\zeta T^4$ for small ζ and tends to zero for $\zeta \rightarrow 0$. For large ζ (10^4 s^{-1} for example as the particle is in glycerin at ambient conditions) and moderate T (larger than, say, 1 s), the actions become $A_0 \approx \frac{mg^2}{\zeta^2}(-\frac{1}{2}T + \frac{1}{2}\zeta T^2)$, $A_d \approx \frac{mg^2}{\zeta^2}(-\frac{3}{2}T + \frac{1}{2}\zeta T^2)$ and $A_{op} \approx \frac{mg^2}{\zeta^2}T$, which all decrease with increasing ζ and increase with increasing duration of motion T . In order to see the ζ and T dependence of A_{op} , A_0 and A_d , these actions are calculated numerically for discrete motion along the optimal path. The particle moves from the initial point to the final point during the time interval $T = n_s \delta t = 1 \text{ s}$ where $n_s = 1000$ is the number of steps and $\delta t = 10^{-3} \text{ s}$ is the time increment of each step. The results are shown in Figs. 4.2 and 4.3. The sharp drop in A_{op} and A_0 is due to the increase of A_d (before its maximum) around $\zeta = 1 \text{ s}^{-1}$ and to the decrease of the velocity $\dot{x}(t) = \frac{g}{\zeta}(e^{-\zeta t} - 1)$ with increasing ζ for given t . The drop point ζ_c can be roughly estimated by $\zeta_c T = 1$, as expected from the exponential factors in Eqs. (4.18-4.20). The reader will find later that this point is also a critical point in the change of nature of the extrema of action.

4.5 Transition of extrema of action

At this stage, it is not yet clear whether the vanishing first variation $\delta A = 0$ yields a minimum, maximum or an saddle point action A_{op} . We know that when $A_{op} \approx A_0$ or $A_d \rightarrow 0$, the optimal action A_{op} is a least one in this case of linear potential. The question is whether this minimum holds for any ζ and T and how eventually it changes with these parameters. We propose in this work to investigate this matter by comparing the actions calculated along a large number of paths created by arbitrary variation of the optimal one. In our calculation algorithm, the arbitrary variation of position is made at each step of the motion by using a Gaussian distributed random displacements superposed on the optimal path $x(t)$ according to $x'_i = x'_{i-1} + \chi_i + x(t_i) - x(t_{i-1})$ where χ_i is the Gaussian random displacement at the step i and $i = 1, 2, \dots, n_s$. A deformed path is then a sequence of variation of positions $\{x'_0, x'_1, x'_2, \dots, x'_{n_s}\}$. The magnitude of the deformation of position at each step can be characterized by the standard deviation σ of the Gaussian distribution. Vanishing deformation of the optimal path can be obtained with vanishing σ . Examples of these deformed paths can be seen in Fig. 4.4.

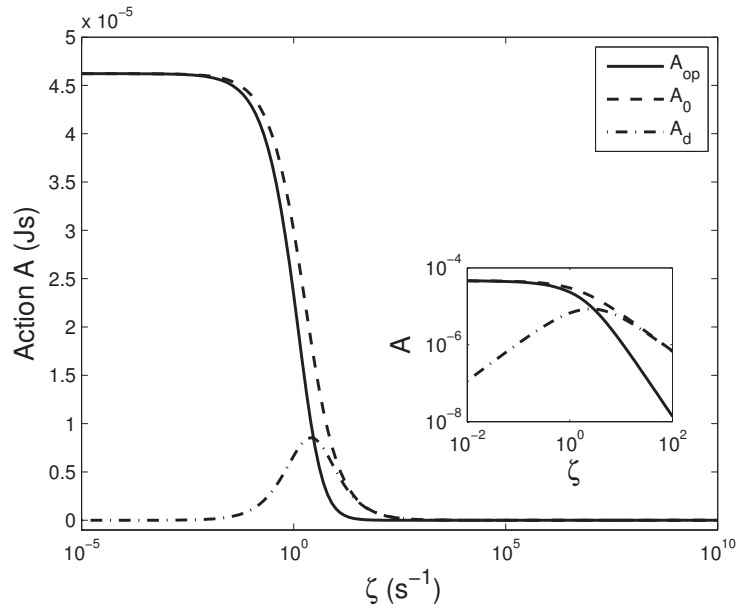


Fig. 4.2: ζ dependence of the actions for the optimal path with $T = 1$ s (for $n_s = 1000$ steps with 10^{-3} s each step). $A_{op} = A_0 - A_d$ is the optimal action (solid line), A_0 is the usual action (dashed line), A_d is the dissipative part of the action (dot dashed line). The drop point ζ_c can be roughly estimated by $\zeta_c T = 1$. The inset is a zoom of the zone around ζ_c in double logarithm plot.

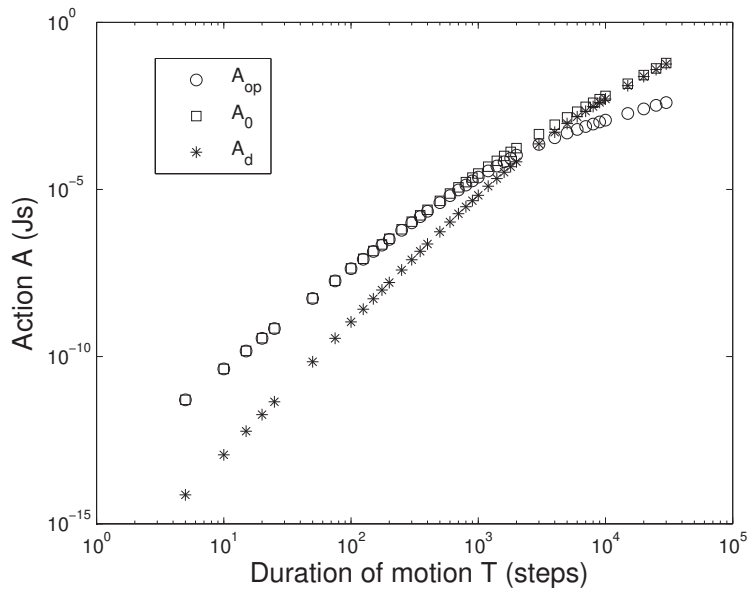


Fig. 4.3: T dependence of the actions for the optimal path with $\zeta = 1$ s $^{-1}$, where $A_{op} = A_0 - A_d$ is the optimal action (circles), A_0 is the usual action (squares), A_d is the dissipative part of the action (stars).

These paths are sufficiently smooth and their number of steps n_s is sufficiently large in order to calculate reliable velocity, energy, action and dissipative energy etc. The actions are calculated with different damping coefficient and duration of motion to see the evolution of the stationarity of action with these parameters.

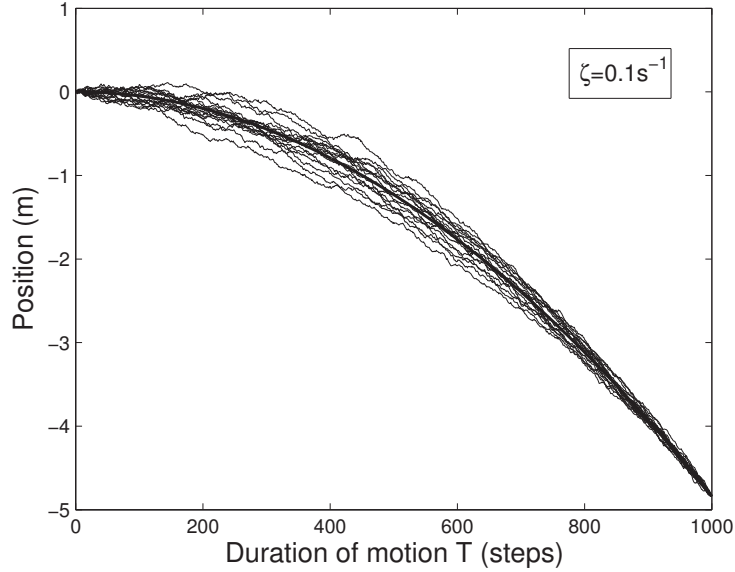


Fig. 4.4: Samples of the different paths $x'(t)$ created randomly around the optimal path $x(t)$ (thick line) given by the solution of Eq. (4.19) for a small particle moving between two fixed points in linear potential (constant force) and a medium of small viscous damping coefficient $\zeta = 0.1 \text{ s}^{-1}$ of Stokes' drag. The duration of motion is $T = 1 \text{ s}$ with $n_s = 1000$ steps and $\delta t = 10^{-3} \text{ s}$ each step.

A comparison of the actions calculated along about 100 paths is shown in Fig. 4.5 (a), (b) and (c) for three values of the drag constant $\zeta = 0.1$, $\zeta = 1$ and $\zeta = 10$, respectively. The duration of motion is $n_s = 1000$ steps with $\delta t = 10^{-3} \text{ s}$ each step ($T = 1 \text{ s}$). In (a), the optimal path (dot) has the smallest action A_{op} with respect to other paths (circles). In (b) A_{op} is neither the smallest nor the largest action. In (c) A_{op} becomes the largest action. The first observation is that, when ζ increases, there is an obvious transition of the stationary $\delta A = 0$ from a minimum regime (a) to a maximum regime (c) in passing by a saddle point regime (b).

We characterize these three regimes by the quantity $\Delta A = \frac{\bar{A} - A_{op}}{|\bar{A}| + |A_{op}|}$ where \bar{A} is the average action over all the paths. This quantity is positive when A_{op} is a minimum, negative when A_{op} is a maximum, and close to zero when A_{op} has a saddle point. Fig.

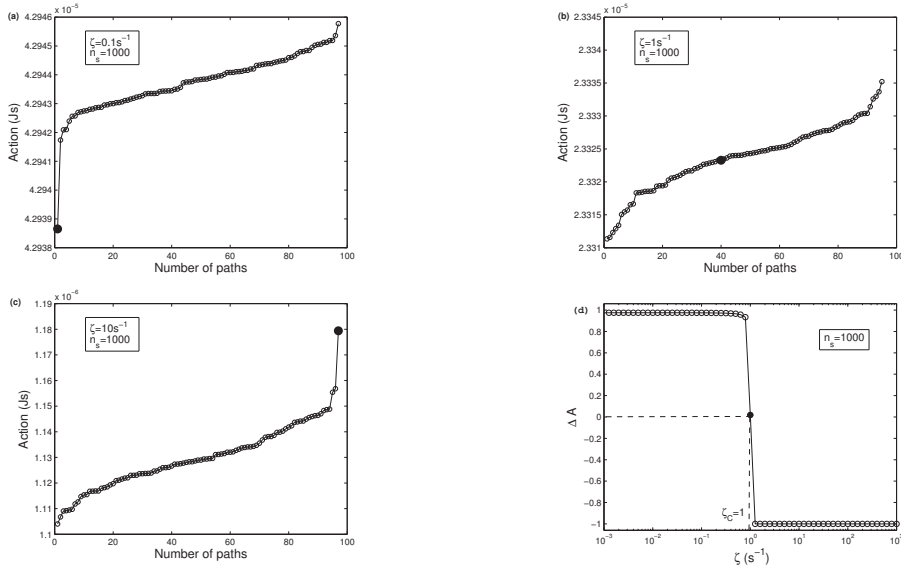


Fig. 4.5: Illustration of the transition of extrema by comparison of the action of the optimal path (dots) with the actions of other paths (circles) created by random deformation of the optimal one with $n_s = 1000$ steps and $\delta t = 10^{-3}$ s each step ($T = 1$ s). (a) For $\zeta = 0.1$ s $^{-1}$, A_{op} is in the bundle of smallest actions. (b) for $\zeta = 1$ s $^{-1}$, A_{op} is in the middle rank. (c) for $\zeta = 10$ s $^{-1}$, A_{op} is in the bundle of largest actions. All calculations were made with an amplitude of variation $\sigma = 0.1$ mm for a total displacement of about 5 m during T . (d) ζ dependence of the quantity $\Delta A = \frac{\bar{A} - A_{op}}{|\bar{A}| + |A_{op}|}$ where \bar{A} is the average action over all the paths. ΔA can be used to characterize the evolution of extrema of A in three regimes: the minimum regime ($\Delta A > 0$), the maximum regime ($\Delta A < 0$) and the saddle point regime around $\Delta A = 0$ corresponding to a critical $\zeta_c = 1$. The step increases at the two extremities of the ranking are due to the insufficient number of paths around the smallest and largest actions.

4.5 (d) shows the ζ dependence of ΔA which can be characterized with the critical point ζ_c determined by $\bar{A} = A_{op}$. The T -dependence of ζ_c is depicted in Fig. 4.6. It can be approximated by $\zeta_c T = 1$. Hence A_{op} corresponding to $\delta A = 0$ is in the minimum (maximum) regime for ζ much smaller (larger) than ζ_c , and in the saddle point regime for $\zeta \approx \zeta_c = 1$.

For given ζ , the evolution of extrema $\delta A = 0$ is a function of the duration of motion T . The critical point T_c for $\Delta A = 0$ can be approximately determined with $\zeta T_c = 1$, as shown in Fig. 4.7 which reveals that the three regimes of the evolution of extrema can be characterized by $\zeta T \ll 1$ (minimum regime), $\zeta T \gg 1$ (maximum regime),

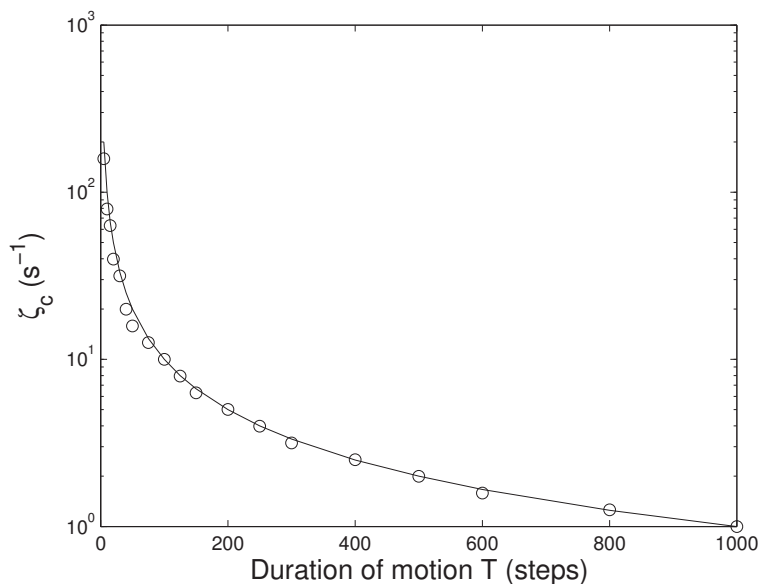


Fig. 4.6: T dependence of the critical value ζ_c which decreases with increasing T . It can be approximated by $\zeta_c T = 1$.

and $\zeta T \approx 1$ (saddle point regime).

Further study for different ζ and σ revealed that this evolution of extrema begins by the lose of the least action whenever ζ is different from zero. This means that, for arbitrarily small ζ , we could always find a σ sufficiently small to create paths having smaller actions than A_{op} of the optimal path. For example, Fig. 4.5 (a) was created with $\zeta = 0.1 \text{ s}^{-1}$ and $\sigma = 0.1 \text{ mm}$. If we use $\sigma = 1 \text{ nm}$, other circles below the dot will appear. In other words, the least action $\delta A_0 = 0$ is definitely lost whenever A_d is nonzero with nonzero variation $\delta A_d \neq 0$. Hence from mathematical point of view, $\delta A = \delta A_0 - \delta A_d = 0$ can be only a saddle point. However, very small σ produces so small deformations of the optimal path and the deformed paths are all so close to the optimal one that they can be considered as a part of the bundle of optimal paths. Therefore, from practical point of view, for very small ζ or negligible dissipation, $\delta A \approx \delta A_0 = 0$ is a minimum. We can say that, the bundle of paths determined by $\delta A = 0$ or equivalently by Newtonian equation, are the set of paths having smallest actions (A in plural) among all other possible paths, much more numerous, with arbitrary deformations.

Similar discussion can be made for the maximum regime illustrated in Fig. 4.5 (c). For arbitrarily large ζ (10^{10} s^{-1} for instance), we could always find sufficiently small σ (10^{-10} m for instance) to create paths having larger action than A_{op} (circles above the

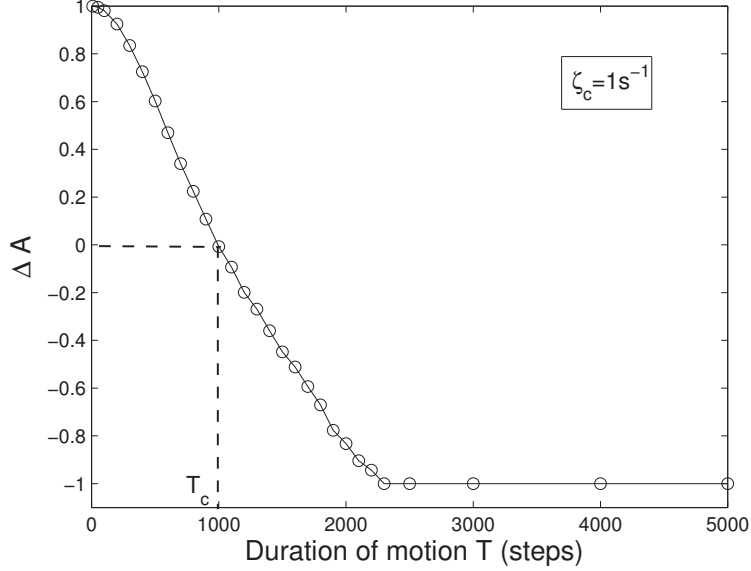


Fig. 4.7: T dependence of the quantity ΔA for $\zeta = 1 \text{ s}^{-1}$. A study shown that the critical point T_c of the evolution can be approximated by $T_c = 1/\zeta$.

dot). But these paths are so close to the optimal one and their number is so less than all the other arbitrarily deformed paths (all the circles below the dot), that they can be considered as the set (bundle) of paths having the largest actions. In this sense, we can say that $\delta A = 0$ is a maximum for large ζ or overdamped motion.

4.6 Other forces

From the above results, it is clear that the transition of extrema of action from minimum to maximum is caused by the increasing dissipative energy E_d or its time integral A_d . In principle, whenever A_d is no more negligible with respect to A_0 , the minimum action is lost, and when A_d approaches A_0 , the maximum action occurs as can be seen from Fig. 4.2, Fig. 4.3 and Fig. 4.5. From this point of view, similar transition of extrema of action can be expected for other friction and conservative forces. We have made same simulations as above with constant friction $f_d = m\zeta$ and the quadratic friction $f_d = m\zeta\dot{x}^2$, as well as harmonic oscillator damped by Stokes' drag. All these cases have similar evolution of extrema from minimum to maximum in three regimes. The maximum regime is shown for the three cases in Fig. 4.8.

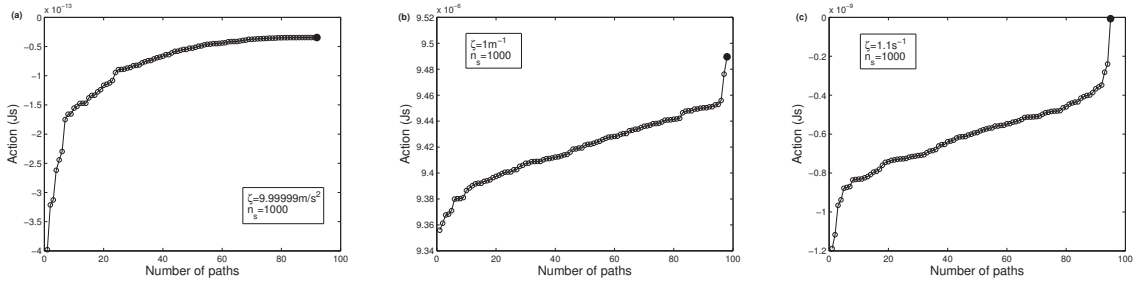


Fig. 4.8: Illustration of the maximum regime by comparison of the action of the optimal path (dots) with the actions of other paths (circles) created by random deformation of optimal one. The number of steps is $n_s = 1000$ with $\delta t = 10^{-3}$ s each step ($T = 1$ s). (a) for constant conservative force damped by constant friction $f_d = m\zeta$, where $\zeta = 9.99999$ $m s^{-2}$ is close to $g = 10$ $m s^{-2}$ and $\sigma = 0.1$ nm , (b) for constant conservative force damped by the quadratic drag $f_d = m\zeta\dot{x}^2$, where $\zeta = 1$ m^{-1} and $\sigma = 0.1$ mm , and (c) for harmonic oscillator damped by Stokes' drag, where $\zeta = 1.1$ s^{-1} and $\sigma = 0.1$ mm .

4.7 Concluding remarks

By numerical calculation of action A_{op} along the optimal path given by Newtonian equation Eq. (4.8) and a large number of paths arbitrarily deformed around the optimal one, we studied the nature of the stationarity of action for dissipative systems, where A is the time integral of the Lagrangian $L = K - V - E_d$ and $-E_d$ is the work of the friction force. Three frictions have been considered: the constant friction independent of position and velocity, the Stokes' drag, and the quadratic friction.

The result is that the extrema of A_{op} in the underdamped and overdamped cases are confirmed by the calculation results without ambiguity. $\delta A = 0$ does exist in these case. More precisely, when the dissipative energy is negligible (underdamping), A_{op} is a least action in the strict sense as can be inferred from the case of zero friction. When the dissipative energy is strong (overdamping), A_{op} is a largest action. In the intermediate case, the stationarity of A_{op} undergoes evolution from minimum regime to maximum regime in passing by a saddle point regime as the motion duration T and the drag coefficient ζ increase. For example, in the case of Stokes' drag, the vanishing first variation $\delta A = 0$ is a minimum, saddle point or maximum for $\zeta T \ll 1$, $\zeta T \approx 1$ or $\zeta T \gg 1$, respectively. This evolution of dynamics can also be seen in the form of the optimal path $x(t) = \frac{g}{\zeta^2}(1 - e^{-\zeta t}) - \frac{g}{\zeta}t$ which becomes gradually, during the saddle point regime, a straight line $x(t) = -\frac{g}{\zeta}t$ with the constant velocity $-\frac{g}{\zeta}$. For example, when

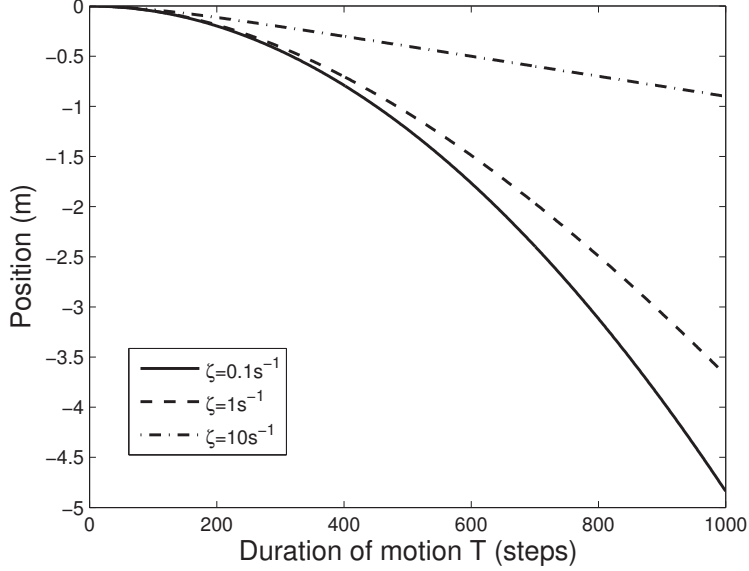


Fig. 4.9: Optimal paths for three values of ζ and $T = 1$ s with constant conservative force. For $\zeta = 0.1$ s $^{-1}$ or $\zeta T \ll 1$, the path seems identical to the path of zero friction. The paths begin to be different from the zero friction one for $\zeta T \approx 1$ and become straight line for $\zeta = 10$ s $^{-1}$ or $\zeta T \gg 1$.

$T = 1$ s, the optimal path is close to the path of zero friction for $\zeta T \ll 1$, begins to be less curved for $\zeta T \approx 1$ and becomes a straight line for $\zeta T = 10$ s $^{-1}$, as shown in Fig. 4.9 for Stokes' drag.

We would like to mention a hint of this maximum optimal action to the optimization of energy dissipation. In general, LAP and the variational principles of energy dissipation are two independent families of axioms, each being valid for its own systems. Many variational principles of dissipation have been formulated in relation with thermodynamic phenomena and entropy production [43, 110, 111]. There are even assumptions combining LAP and a dissipation principle which hold simultaneously for a dissipative fluid system [112]. However, in view of the relation $A = A_0 - A_d$, the maximum of A implies the minimum of A_d along the optimal path. Let us make a variation of the optimal path by a tiny but very intensive zigzag motion close to the optimal path. In the expression $A = \int_0^T (K - V - E_d) dt$ almost does not change because the variational path is very close to the optimal one, but the integral $A_K = \int_0^T K dt$ and $A_d = \int_0^T E_d dt$ will increase enormously due to the larger variational velocity caused by the violent zigzag motion. Hence the maximum action implies A over the variational path must

be smaller than A_{op} . In other words, A_d must increase, and more quickly than A_K . This is a minimum energy dissipation over the optimal path of overdamped motion. Therefore, the path given by the “least action principle” (a maximum now) is just the path of least dissipation. To our knowledge, this was the first relation established between a basic principle of Hamiltonian/Lagrangian mechanics and the optimization of energy dissipation.

Few attention has been paid to extremum principles of dissipation in mechanical motion. An example of this is the path of least dissipation which, rather by intuition, states that a mechanical system should follow the path of least energy dissipation in the case of damped motion. But in view of the present LAP, this principle is not that evident. From the vanishing variation $\delta \int_0^T (K - V - E_d) dt = 0$ it is obvious that $\delta A_d \neq 0$. Hence in general there is no extremum or stationary of A_d on the path of least action if we do not change the conditions of the vanishing variation $\delta A = 0$, i.e., fixed time duration T and fixed initial and final points a and b . These conditions can be of course modified for different variational problems. It is instructive to see the case of Maupertuis’ action. It is easy to verify that, in the case of Stokes friction, the Maupertuis’ action can be written as $A_m = \frac{1}{\zeta} \int_{x_a}^{x_b} m \zeta \dot{x} dx = \frac{E_d^b}{\zeta}$, where $E_d^b = \int_{x_a}^{x_b} \zeta \dot{x} dx$ is the negative work of the friction force over the entire trajectory from a to b . Hence Maupertuis’ principle implies $\delta E_d^b = 0$. In other words, the path of least action is just the path of least resistance in the case of Stokes friction.

In summary, we formulated a possible answer to a longstanding question of classical mechanics about the least action principle for damped motion, in keeping all the four conventional formulations of mechanics, i.e., Newtonian, Lagrangian, Hamiltonian and Hamilton-Jacobi equations. This work based on the model of a conservative system composed of the moving body and its environment coupled by friction. It was shown that this system with “internal dissipation” satisfies both Lagrangian and Hamiltonian mechanics, leading to correct equation of damped motion in a general way. It was also shown that, within this formulation, the Maupertuis’ principle is equivalent to a least dissipation principle in the case of Stokes damping. A more general least dissipation principle is also discussed for the overdamped motion. We hope that these results are helpful for further study of the relations between the variational principles of energy dissipation and the fundamental principles of Lagrangian and Hamiltonian mechanics (see the efforts for stochastic dissipative systems in, for example [115, 116, 117]). It is also hoped that the present result is useful for the study of quantum dissipation in

view of the role of action in the quantum wave propagator $\psi = e^{iA/\hbar}$ [12] and the close relationship between the Schrodinger equation and the Hamilton-Jacobi equation [1].

Chapter 5

The path probability of stochastic motion of dissipative systems

5.1 Introduction

The numerical experiments [118] showed that, for the stochastic motion of non dissipative systems or weakly dissipative systems, the path probability decreases exponentially with increasing action (Lagrangian one) of the paths, and that the most probable path is just the least action path of Hamiltonian/Lagrangian mechanics. This is a reasonable result of the model since, with diminishing noise, more and more paths shrink onto the bundle of least action paths. In the limiting case of vanishing noise, all paths will collapse on the least action path and the motion will recover the Hamiltonian/Lagrangian dynamics. But this result does not apply to Brownian motion [16] studied with Langevin, Fokker-Planck, Kolmogorov equations [97]-[101] which include important dissipation due to friction. The present work is to study the path probability for stochastic motion of dissipative systems. We considered a whole isolated conservative system containing a damped moving body and its environment, coupled to each other by friction. The Lagrangian is $L = K - V - E_d$ [56, 119] with an effective conservative Hamiltonian $H = K + V + E_d$ where K is the kinetic energy of the damped body, V its potential energy and E_d is the negative work of the friction force \vec{f}_d from point a to a position $x(t)$ along a given path $s = s(t)$ ($0 \leq t \leq T$) where T is a fixed time period. The friction is given by the Stokes' drag, i.e., $\vec{f}_d = -m\zeta\vec{\dot{x}}$, where $\zeta = \gamma/m$, γ is the viscous drag coefficient. The three associated actions of the whole system on

a given path between point a and point b is then given by $A_L = \int_0^T (K - V - E_d) dt$ (called Lagrangian action), the time integral of Hamiltonian $A_H = \int_0^T (K + V + E_d) dt$ (called Hamiltonian action) and the time integral of kinetic energy $A_K = \int_0^T K dt$ (called kinetic action).

To our knowledge, less experimental work or numerical experiment has been made to measure the path probability. This is certainly related to, among many reasons, the difficulty of experimental observation of a large number of stochastic motions. This large number is necessary to determine correctly the path probability. The purpose of the chapter is to overcome this difficulty by making numerical experiments of stochastic motion with dissipation in order to measure the path probability and to study its dependence on the conventional mechanics quantities such as position, velocity, energy and action. It is worth mentioning the instantaneous velocity has been experimentally measured with sufficiently small measuring time scale [120, 121, 122]. The measured result should be more and more precise with smaller and smaller scale. This is certainly an experimental argument for the use of velocity in the Langevin equation [123] and the Ornstein-Uhlenbeck model [124, 125].

5.2 Numerical simulation

We use a large number ($\sim 10^9$) of silica (SiO_2) particles of mass $m = 1.39 \times 10^{-15}$ kg undertaking one-dimensional stochastic motion in conservative force field. The spherical particles with 1- μm -diameter, moving in air or liquid water under the noise, move from the initial point a to the destination point b in the interval $z_b - \delta/2 \leq x_b \leq z_b + \delta/2$ (see below), over a given n steps, through different paths. A path is a sequence of random positions $\{x_a, x_1, x_2 \cdots x_{n-1}, x_b\}$, where x_i is the position at time t_i with $x_a = x_0$ and $x_b = x_n$. We chose $n=10$ (due to the limited computation time) with equal time increments $dt = t_i - t_{i-1}$.

The random motion can be described by the Langevin equation

$$m \frac{d^2 x}{dt^2} = -\frac{dV(x)}{dx} - m\zeta \frac{dx}{dt} + R, \quad (5.1)$$

where x is the position, t is the time, $V(x)$ is the potential energy and R is the Gaussian distributed random force. The Gaussian noise or random displacement at t_i is given

by the following

$$p(\chi_i, t_i - t_{i-1}) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{\chi_i^2}{2\sigma^2}}, \quad (5.2)$$

where χ_i is the Gaussian displacement at the step i , $\sigma = \sqrt{2D(t_i - t_{i-1})} = \sqrt{2Ddt}$ the standard deviation, $D = \frac{k_B T}{6\pi r \eta}$ the diffusion constant, k_B the Boltzmann constant, T the absolute temperature, $r = 0.5 \mu\text{m}$ the radius of the particle and $\eta = 8.5 \times 10^{-4} \text{Pas}$ (for $T = 293 \text{K}$) the viscosity of water. For example, when $T = 293 \text{K}$ and $dt = 10^{-5} \text{s}$, one obtain $D \approx 4.3 \times 10^{-13} \text{m}^2/\text{s}$ and $\sigma \approx 3 \times 10^{-9} \text{m}$, with a relaxation time close to 10^{-7}s . With this reference, the simulations were made with different time increments dt ranging from 10^{-7} to 10^{-3}s .

The motion of the particle is generated by the following equation combining two parts by superposition: a random Gaussian displacement from Eq. (5.2) and a part described by the solution $y_i = f(t_i) - f(t_{i-1})$ of the Newtonian equation of damped motion $m\ddot{x} = -\frac{\partial V}{\partial x} - m\zeta\dot{x}$ [56] for conservative and friction forces. The total displacement of each step is then given by

$$x_i = x_{i-1} + \sigma\chi_i + f(t_i) - f(t_{i-1}). \quad (5.3)$$

It is obvious that, in the case of vanishing noise, the motion of effective Hamiltonian/Lagrangian mechanics is recovered [56]. The damping effect related to ζ is considered in the Newtonian equation of damped motion.

The left panels of Figs. 5.1-5.4 illustrate some sample paths generated by Eq. (5.3) for friction force and two kinds of conservative forces. The samples are around the least action path with sufficiently different actions from the least one. In the simulation, each sample path is in fact a bundle or a tube of a small thickness δ whose axial line is a sequence of positions $\{z_0, z_1, z_2 \cdots z_{n-1}, z_n\}$. The larger δ is, the more particles will go through each path from a to b . The δ used in this work is chosen to be $1/2$ of the standard deviation σ of the distribution of random displacements.

For each sample path, the instantaneous velocity at time step i is calculated by $v_i = \frac{z_i - z_{i-1}}{t_i - t_{i-1}}$ along the axial line of its tube. This velocity can be approximately considered as the average velocity of all the trajectories passing through the tube of the sample path, i.e., the trajectories satisfying $z_i - \delta/2 \leq x_i \leq z_i + \delta/2$ for every step i . The kinetic energy is given by $K_i = \frac{1}{2}mv_i^2$, the dissipative energy is $E_d = m\zeta \int_0^{x(t)} \dot{x}_i(\tau) dx_i(\tau)$, the actions are $A_K = \sum_{i=1}^{10} \frac{1}{2}mv_i^2 dt$, $A_L = \sum_{i=1}^{10} [\frac{1}{2}mv_i^2 - V(x_i) - m\zeta \text{cumsum}(x_i v_i)] \cdot dt$, and $A_H = \sum_{i=1}^{10} [\frac{1}{2}mv_i^2 + V(x_i) + m\zeta \text{cumsum}(x_i v_i)] \cdot dt$, where ‘‘cumsum’’ is the cumulative

sum from $i=1$ to $i = f \leq 10$ in the matlab program.

The numerical experiment consists in observing the total number of particles N moving from point a to point b through all the sample paths and the number of particles N_k moving along a given sample path k from a to b . The probability that the path k is taken is determined by $P_k = N_k/N$ (with large N). Simulations are performed with two potential energies: constant force with potential $V(x) = mgx$ and harmonic force with potential $V(x) = \frac{1}{2}kx^2$. The results presented below for each potential were obtained with $dt = 10^{-5}$ s.

5.3 Path probability distributions

5.3.1 Particles with constant force and Stokes' drag

We considered the particles subject to Stokes' drag force and the constant force with potential $V(x) = mgx$. The Newtonian equation of damped motion is given by [56]:

$$m\ddot{x} = mg - m\zeta\dot{x}, \quad (5.4)$$

where $g = 10 \text{ ms}^{-2}$. The solution is

$$x(t) = \frac{g}{\zeta^2}(1 - e^{-\zeta t}) - \frac{g}{\zeta}t. \quad (5.5)$$

For a small ζ or the underdamped motion, the dissipative energy is negligible, the result of the right panel of Fig. 5.1 shows a path probability of the form

$$P_k(A) = \frac{1}{Z}e^{-\gamma A_k}, \quad (5.6)$$

where A_k is the Lagrangian action of the path k , the slope is $\gamma \approx 6.3 \times 10^{26} \text{ J}^{-1}\text{s}^{-1}$ and the normalization function Z can be analytically determined by the path integral technique [12]

$$\prod_{i=1}^{n-1} \int_{-\infty}^{\infty} \frac{dx_i}{\delta} P_k(A) = 1 \quad (5.7)$$

with fixed x_a and x_b , or numerically by the value of $\ln P(A=0)$ which can be found with the distribution curves in the figures. It recovers the result of particles subject to constant force in non dissipative systems.

For a large ζ or the overdamped motion, the dissipative energy is strong, the middle panel of Fig. 5.2 shows the Newtonian path has the most probable and the maximum

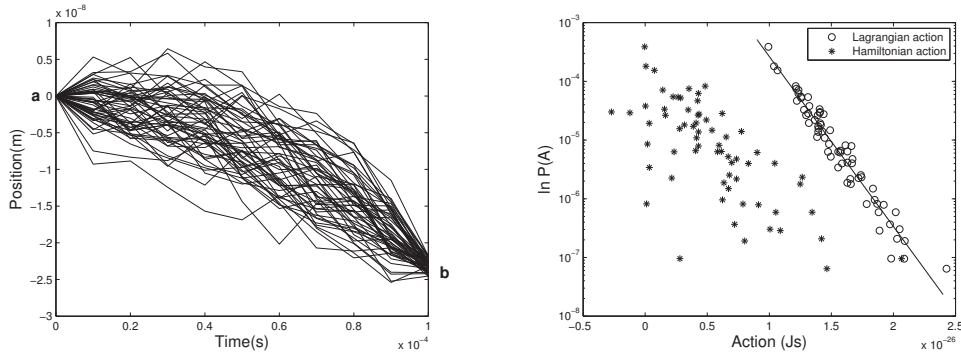


Fig. 5.1: The result of numerical simulation of the underdamped motion with 10^9 particles subject to the friction force $f_d = m\zeta\dot{x}$ where $\zeta = 1 \text{ s}^{-1}$ and the constant force with potential $V(x) = mgx$. The left panel shows the axial lines of sample paths. The right panel shows the path probability distribution against the Lagrangian (circles) and Hamiltonian (stars) actions. The straight line is a best fit of the points. It implies an exponential dependence on the Lagrangian action with negative slope $\gamma \approx 6.3 \times 10^{26} \text{ J}^{-1}\text{s}^{-1}$ in Eq. (5.6). There seems no correlation between the path probability and the Hamiltonian action.

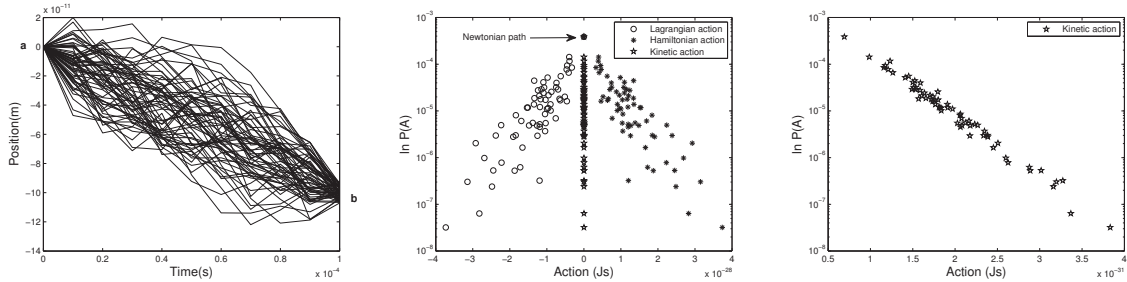


Fig. 5.2: The result of numerical simulation of the overdamped motion with 10^9 particles subject to the friction force $f_d = m\zeta\dot{x}$ where $\zeta = 10^7 \text{ s}^{-1}$ and the constant force with potential $V(x) = mgx$. The left panel shows the different sampled paths between the given points *a* and *b*. The middle panel shows the path probability distribution against the Lagrangian (circles), Hamiltonian (stars) and Kinetic (pentagrams) actions. The right panel is a zoom of the middle panel in kinetic action. The right panel shows the path probability distribution against the kinetic (pentagrams) action. It implies the path probability plays an exponential dependence on the kinetic action with $\gamma \approx 2.8 \times 10^{31} \text{ J}^{-1}\text{s}^{-1}$.

Lagrangian action, i.e., the most probable path is the maximum action path. The right panel of Fig. 5.2 shows the path probability distribution increases exponentially with increasing kinetic action with a slope $\gamma \approx 2.7 \times 10^{31} J^{-1}s^{-1}$. It is novel to find that the path probability does not play exponentially with Lagrangian action again for the overdamped motion.

5.3.2 Particles with harmonic force and Stokes' drag

We considered particles subject to Stokes' drag force and the harmonic force with potential $V(x) = \frac{1}{2}kx^2$, where k is the spring constant. The Newtonian equation of damped motion is given by [56]:

$$m\ddot{x} = -kx - m\zeta\dot{x}, \quad (5.8)$$

Thus, the solution to the damped harmonic oscillator equation is written

$$x(t) = Ae^{-\frac{\zeta}{2}t} \sin(\omega_1 t), \quad (5.9)$$

where $A = 1.5 \times 10^{-8} m$ is the amplitude, $\omega_1 = \sqrt{\omega_0^2 - \zeta^2/4}$ is the angular frequency and $\omega_0 = \sqrt{k/m} = 4.7 \times 10^4 s^{-1}$ is the underdamped oscillation frequency. Incidentally, if the damping is sufficiently large that $\zeta \geq 2\omega_0$, which we shall assume is not the case, then the system does not oscillate at all, and any motion simply decays away exponentially in time.

As for the constant force, the path probability distribution decreases exponentially with increasing Lagrangian action with a negative slope $\gamma \approx 6.8 \times 10^{26} J^{-1}s^{-1}$ of the straight line for the underdamped motion in the right panel of Fig. 5.3. From the middle and right panels of Fig. 5.4, the most probable path is the maximum Lagrangian action path and the path probability distribution decreases exponentially with increasing kinetic action with a slope $\gamma \approx 3.1 \times 10^{29} J^{-1}s^{-1}$.

5.4 Discussion

From the above figures, the exponential dependence of the path probability on the Lagrangian action is obvious. This correlation can be characterized by a correlation function between A (A_L or A_H) and $-\ln P(A)$ given by

$$c(A) = \frac{\sum_{i=1}^n (A_i - \langle A_i \rangle) [-\ln P(A_i) + \langle \ln P(A_i) \rangle]}{\sqrt{[\sum_{i=1}^n (A_i - \langle A_i \rangle)^2][\sum_{i=1}^n (-\ln P(A_i) + \langle \ln P(A_i) \rangle)^2]}}, \quad (5.10)$$

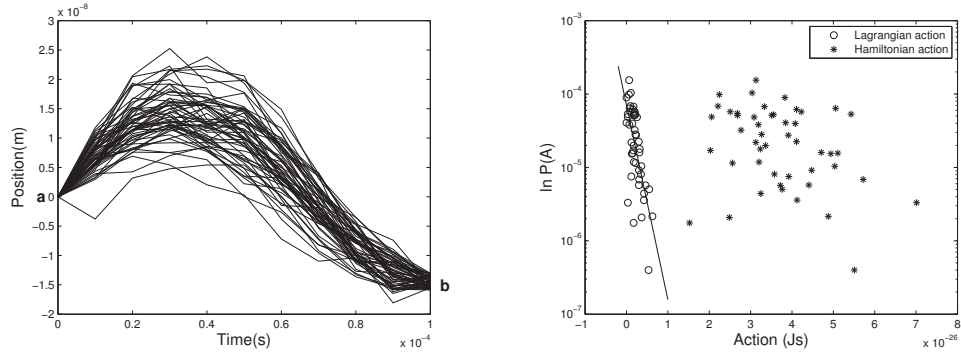


Fig. 5.3: The result of numerical simulation of the underdamped motion with 10^9 particles subject to the friction force $f_d = m\zeta\dot{x}$ where $\zeta = 1 \text{ s}^{-1}$ is close to $2\omega_0$ and harmonic force with potential $V(x) = \frac{1}{2}kx^2$. The left panel shows the different sampled paths between the given points a and b . The right panel shows the path probability distribution against Lagrangian (circles) and Hamiltonian (stars) actions. The straight line is a best fit of the points whose slope gives $\gamma \approx 6.8 \times 10^{26} \text{ J}^{-1}\text{s}^{-1}$ in Eq. (5.6). There is no correlation between the path probability and the Hamiltonian action.

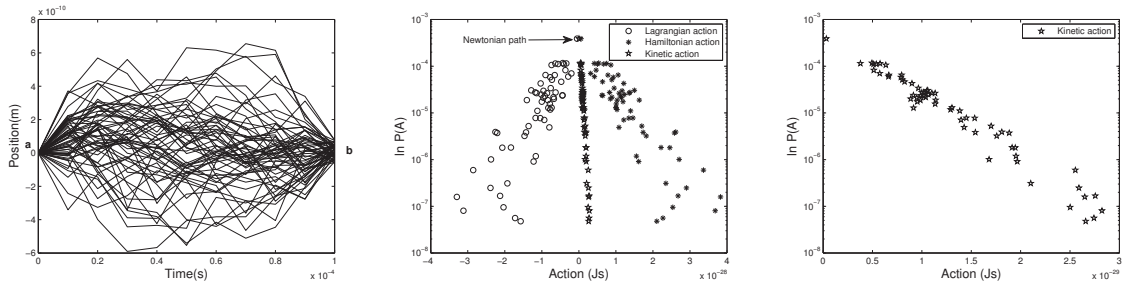


Fig. 5.4: The result of numerical simulation of the overdamped motion with 10^9 particles subject to the friction force $f_d = m\zeta\dot{x}$ where $\zeta = 9.39 \times 10^4 \text{ s}^{-1}$ and harmonic force with $V(x) = \frac{1}{2}kx^2$. The left panel shows the different sampled paths between the given points a and b . The middle panel shows the path probability distribution against the Lagrangian (circles), Hamiltonian (stars) and Kinetic (pentagrams) actions. The right panel is a zoom of the middle panel in kinetic action. The right panel shows the path probability distribution against the kinetic (pentagrams) action. It implies the path probability plays an exponential dependence on the kinetic action with $\gamma \approx 3.1 \times 10^{29} \text{ J}^{-1}\text{s}^{-1}$.

Table 5.1: Values of the correlation function $c(A)$ between the logarithm of the path probability $-\ln P(A)$ and actions (the Lagrangian action A_L , the Hamiltonian action A_H , the kinetic action A_K) for the two potentials $V(x)$ and two kinds of motion used in the numerical experiments. For the underdamped motion, $-\ln P(A)$ and A_L are linear correlation; For the overdamped motion, $-\ln P(A)$ and A_K are linear correlation.

$V(x)$	$c(A_L)$	$c(A_H)$	$c(A_K)$
mgx (underdamped)	0.9734	0.4945	
mgx (overdamped)	-0.8495	0.8499	0.9906
$\frac{1}{2}kx^2$ (underdamped)	0.9114	0.3298	
$\frac{1}{2}kx^2$ (overdamped)	-0.831	0.8593	0.9781

where $\langle A_i \rangle$ and $\langle \ln P(A_i) \rangle$ are the means of action A and $-\ln P(A)$ respectively. $|c(A, -\ln P(A))| \approx 1$ would indicate that A and $-\ln P(A)$ would indicate that A and $-\ln P(A)$ are linearly correlated. The results obtained from the numerical experiments are shown in Table 5.1.

It can be concluded from the Table 5.1 that $-\ln P(A)$ has a linear correlation with the Lagrangian action for the underdamped motion, but a linear correlation with the kinetic action for the overdamped motion. It should be indicated that all the numerical simulations have been done with different time scale of each step. No dependence of $c(A)$ on time scale was observed.

5.5 Conclusions

Based on the extension of least action principle to random motion, we studied the path probability of Gaussian stochastic motion of dissipative systems. The model of the simulation is small silica particles subject to conservative forces, friction force and Gaussian noise. It is found that the path probability still depends exponentially on Lagrangian action for the underdamped motion, but plays exponentially with kinetic action for the overdamped motion. The difference from the non dissipative motion is that, for the underdamped motion, the most probable path is the least Lagrangian action path; for the overdamped motion, the most probable path is the maximum La-

grangian action path. This is a reasonable results of the model. For the underdamped motion, the dissipative energy is negligible, with diminishing noise, more and more paths shrink onto the bundle of least action paths. In the limiting case of vanishing noise, all paths will collapse on the least action path and the motion will recover the Hamiltonian/Lagrangian dynamics. For the overdamped motion, the dissipative energy is strong, the path given by the “least action principle” (the maximum) is just the path of least dissipation.

We would like to stress that the result of present work is a preliminary development of the exponential of action of path probability in dissipative systems, but not the final result. It is unimaginable that the Lagrangian action is no more a characteristic variable of the paths in the overdamped motion. We hope that this result can be improved by more precise computation. The path probability depends on which actions for stochastic motion of dissipative systems is still in the process of exploration.

Chapter 6

Conclusions

In this thesis, we have done the numerical investigation on path probability of stochastic motion from non dissipative systems to dissipative systems. An extension of least action principle to dissipative mechanical systems has been described. The extremum of action undergoes evolution from a minimum to a maximum has been confirmed. We will here shortly review the essential of our work.

Based on the theoretical extension of Hamiltonian and Lagrangian mechanics to a stochastic formalism which predicts that path probability depending exponentially on action is possible in the non dissipative systems, we have made the numerical experiments of stochastic motion to verify its validity. The numerical experiments show that, for non dissipative systems or weakly dissipative systems undergoing Gaussian stochastic motion, the path probability decreases exponentially with increasing action (Lagrangian one) of the paths, and that the most probable path is just the least action path of Hamiltonian/Lagrangian mechanics. It can be predicted that, for such kind of ideal motion, the probability of occurrence of a path from a given point to any arbitrarily chosen point, within a given duration of motion, must decrease exponentially with increasing action. Hence the application of this result does not need the condition of a motion between two fixed points. The decay rate increases with decreasing Gaussian randomness. The decay rate increases with decreasing Gaussian randomness. This result is a confirmation of the existence of a classical analogue of the Feynman factor $e^{iA/\hbar}$ for the path integral formalism of quantum mechanics of Hamiltonian systems.

The least action principle has been generalized to dissipative systems with a unique well defined Lagrangian function $L = K - V - E_d$, where E_d is the dissipated energy

by friction force. We formulated for dissipative system a least action principle that can keep all the main features of the conventional Hamiltonian/Lagrangian mechanics such as the Hamiltonian, Lagrangian and Hamilton-Jacobi equations, three formulations of the classical mechanics. This least action principle can also be derived from the virtual work principle. It was also shown that, within this formulation, the Maupertuis' principle is equivalent to a least dissipation principle in the case of Stokes damping. By variational calculus and numerical simulation, we made a comparison of the action of the optimal Newtonian path (A_{op}) to those of a large number of deformed paths. This comparison revealed that the least action only persist in the case of weak dissipation, and is replaced by maximum action in the case of strong dissipation. Hence the extrema of A_{op} in the underdamped and overdamped cases seem to have been confirmed by the simulation results. More precisely, when the dissipative energy is negligible (underdamping), A_{op} is in the bundle of the least actions as expected. When the dissipative energy is strong (overdamping), A_{op} is in the bundle of the largest actions. On this basis, we studied the path probability of Gaussian stochastic motion of dissipative systems. It is found that the path probability still depends exponentially on Lagrangian action $A = \int_0^T L dt$ for the underdamped motion, but depends exponentially on kinetic action $A = \int_0^T K dt$ for the overdamped motion. The difference from the non dissipative motion is that, for the underdamped motion, the most probable path is the least Lagrangian action path; for the overdamped motion, the most probable path is the maximum Lagrangian action path.

We formulated a possible answer to a longstanding question of classical mechanics about the least action principle for damped motion. We hope that these results are helpful for further study of the relations between the variational principles of energy dissipation and the fundamental principles of Lagrangian and Hamiltonian mechanics. It is also hoped that the present result is useful for the study of quantum dissipation in view of the role of action in the quantum wave propagator and the close relationship between the Schrodinger equation and the Hamilton-Jacobi equation. Unlike the Feynman factor which is just a mathematical object, $e^{-\gamma A}$ is a real function characterizing the path probability. This probabilistic view of mechanical motion can possibly open a way to review some aspects of the relationship between mechanics and thermodynamics.

We would like to mention that, this exponential path probability is one of the possible path probability distributions underlying a stochastic formalism of Hamilto-

nian/Lagrangian mechanics. It is unimaginable that the Lagrangian action is no more a characteristic variable of the paths in the overdamped motion. The path probability depends on which actions for stochastic motion of dissipative systems is still a open question. It has been an unremitting ambition of physicists to date.

Appendix A

Calculation of the path probability distribution from the motion equation

$$x_i = x_{i-1} + \chi_i + f(t_i) - f(t_{i-1}),$$

where $f(t_i) = -\frac{1}{2}gt_i^2$, $t_i = idt$, $i = 1, 2, \dots, n$. The Wiener path measure probability P_k can be expressed as follows:

$$\begin{aligned} P_k &= \frac{1}{\sqrt{2\pi\sigma}} \prod_{i=1}^n \int_{z_i-\delta/2}^{z_i+\delta/2} \exp\left\{-\frac{[x_i - x_{i-1} - f(t_i) + f(t_{i-1})]^2}{2\sigma^2}\right\} dx_i \\ &= \frac{1}{\sqrt{2\pi\sigma}} \prod_{i=1}^n \int_{z_i-\delta/2}^{z_i+\delta/2} \exp\left\{-\frac{(x_i - x_{i-1})^2}{2\sigma^2} + \frac{2(x_i - x_{i-1})[f(t_i) - f(t_{i-1})]}{2\sigma^2}\right. \\ &\quad \left. - \frac{[f(t_i) - f(t_{i-1})]^2}{2\sigma^2}\right\} dx_i \\ &= \frac{1}{\sqrt{2\pi\sigma}} \int_{z_i-\delta/2}^{z_i+\delta/2} \exp\left\{-\sum_{i=1}^n \frac{(x_i - x_{i-1})^2}{2\sigma^2} + \sum_{i=1}^n \frac{(x_i - x_{i-1})[f(t_i) - f(t_{i-1})]}{\sigma^2}\right. \\ &\quad \left. - \sum_{i=1}^n \frac{[f(t_i) - f(t_{i-1})]^2}{2\sigma^2}\right\} dx_i \end{aligned}$$

The last term in the exponent is constant for given starting and final points and duration of motion. The second term in the exponent can be expressed as follows:

$$\begin{aligned} &\exp\left\{\sum_{i=1}^n \frac{(x_i - x_{i-1})[f(t_i) - f(t_{i-1})]}{\sigma^2}\right\} \\ &= \exp\left\{-\sum_{i=1}^n \frac{(x_i - x_{i-1})(i - \frac{1}{2})gdt^2}{\sigma^2}\right\} \\ &= \exp\left\{-\frac{gdt^2}{\sigma^2} \left[\sum_{i=1}^n (x_i - x_{i-1})(i - \frac{1}{2})\right]\right\} \\ &= \exp\left\{-\frac{gdt^2}{\sigma^2} [(x_1 - x_0) + 2(x_2 - x_1) + 3(x_3 - x_2) + \dots + n(x_n - x_{n-1})]\right. \\ &\quad \left.- \frac{1}{2}[(x_1 - x_0) + (x_2 - x_1) + (x_3 - x_2) + \dots + (x_n - x_{n-1})]\right\} \\ &= \exp\left\{-\frac{gdt^2}{\sigma^2} [-x_1 - x_2 - x_3 - \dots - x_n + (n+1)x_n - x_0 - \frac{1}{2}(x_n - x_0)]\right\} \\ &= \exp\left\{\frac{gdt^2}{\sigma^2} \left[\sum_{i=1}^n x_i - (n + \frac{1}{2})x_n + \frac{1}{2}x_0\right]\right\} \\ &= \exp\left[\frac{1}{2mD} \sum_{i=1}^n V(x_i)dt\right] \exp\left\{-\frac{gdt}{2D} \left[(n + \frac{1}{2})x_n - \frac{1}{2}x_0\right]\right\} \end{aligned}$$

where $\sigma = \sqrt{2Ddt}$, $V(x_i) = mgx_i$, and $\exp\{-\frac{gdt}{2D}[(n + \frac{1}{2})x_n - \frac{1}{2}x_0]\}$ is constant since g, D, n, dt, x_0 and x_n are all constant. Let $\gamma = \frac{1}{2mD}$,

$$\begin{aligned}
P_k &= \frac{1}{\sqrt{2\pi\sigma}} N_1 \int_{z_i-\delta/2}^{z_i+\delta/2} \exp\left[-\frac{1}{2}m\gamma \sum_{i=1}^n \frac{(x_i - x_{i-1})^2}{dt} + \gamma \sum_{i=1}^n V(x_i)dt\right] dx_i \\
&= \frac{1}{\sqrt{2\pi\sigma}} N_1 \int_{z_i-\delta/2}^{z_i+\delta/2} \exp(-\gamma A_k) dx_i \\
&\approx \frac{1}{\sqrt{2\pi\sigma}} N_1 \delta \exp(-\gamma A_k[z_0, z_1, z_2, \dots, z_n])
\end{aligned}$$

where $\frac{1}{\sqrt{2\pi\sigma}} N_1 = \frac{1}{\sqrt{2\pi\sigma}} \exp\{-\frac{gdt}{2D}[(n + \frac{1}{2})x_n - \frac{1}{2}x_0]\} - \sum_{i=1}^n \frac{[f(t_i) - f(t_{i-1})]^2}{4Ddt}$ is a constant which can be determined by the normalization of P_k , and the action is $A_k = \sum_{i=1}^n [\frac{1}{2}m \frac{(x_i - x_{i-1})^2}{dt^2} - V(x_i)]dt$.

This can be done inversely from the exponential probability distribution of action to the Wiener path measure probability if $V(x_i)$ is linear or approximately linear when developed up to the first order (linear term in δx_i) on each step $\delta x_i = x_i - x_{i-1}$ which should be small with respect to the total distance of the motions.

Appendix B

The dissipative action being defined by $A = \int_0^T (K - V - E_d)dt$ with $E_d = \int_0^t f(\tau)d\tau$ and $f = f_d(\tau)\dot{x}(\tau)$. The ‘‘global’’ variational calculus, which consists in considering both the variation $\delta x(t)$ and the antecedent $\delta x(\tau)$, is given by

$$\delta A = \int_0^T \delta(K - V - E_d)dt,$$

where the variation of the first part $A_0 = \int_0^T \delta(K - V)dt$ is:

$$\delta A_0 = \int_0^T \left[\frac{\partial(K - V)}{\partial x(t)} \delta x(t) + \frac{\partial(K - V)}{\partial \dot{x}(t)} \delta \dot{x}(t) \right] dt.$$

Integrating the second term by parts and using the boundary conditions $\delta x(0) = \delta x(T) = 0$, we get

$$\begin{aligned} \delta A_0 &= \frac{\partial(K - V)}{\partial \dot{x}(t)} \delta x(t) \Big|_0^T + \int_0^T \left[\frac{\partial(K - V)}{\partial x(t)} - \frac{d}{dt} \left(\frac{\partial(K - V)}{\partial \dot{x}(t)} \right) \right] \delta x(t) dt \\ &= \int_0^T \left[\frac{\partial(K - V)}{\partial x(t)} - \frac{d}{dt} \left(\frac{\partial(K - V)}{\partial \dot{x}(t)} \right) \right] \delta x(t) dt. \end{aligned}$$

The variation of the second part $A_d = \int_0^T \delta E_d dt$ is:

$$\delta A_d = \int_0^T \int_0^t \left[\frac{\partial f}{\partial x(\tau)} \delta x(\tau) + \frac{\partial f}{\partial \dot{x}(\tau)} \delta \dot{x}(\tau) \right] d\tau dt.$$

Making the same trick of integration by parts, we get

$$\begin{aligned} \delta A_d &= \int_0^T \left[\int_0^t \frac{\partial f}{\partial x(\tau)} \delta x(\tau) d\tau + \frac{\partial f}{\partial \dot{x}(\tau)} \delta x(\tau) \Big|_0^t - \int_0^t \frac{d}{d\tau} \left(\frac{\partial f}{\partial \dot{x}(\tau)} \right) \delta x(\tau) d\tau \right] dt \\ &= \int_0^T \frac{\partial f}{\partial \dot{x}(\tau)} \delta x(\tau) \Big|_0^t dt + \int_0^T \int_0^t \left[\frac{\partial f}{\partial x(\tau)} - \frac{d}{d\tau} \left(\frac{\partial f}{\partial \dot{x}(\tau)} \right) \right] \delta x(\tau) d\tau dt. \end{aligned}$$

Due to the boundary condition $\delta x(0) = 0$ causes the first term is equal to $\int_0^T \frac{\partial f}{\partial \dot{x}(t)} \delta x(t) dt$.

Making an integration by parts of $\int_0^t \left[\frac{\partial f}{\partial x(\tau)} - \frac{d}{d\tau} \left(\frac{\partial f}{\partial \dot{x}(\tau)} \right) \right] \delta x(\tau) d\tau$ with respect to t , δA_d turns out to be

$$\begin{aligned} \delta A_d &= \int_0^T \frac{\partial f}{\partial \dot{x}(t)} \delta x(t) dt + \left\{ t \int_0^t \left[\frac{\partial f}{\partial x(\tau)} - \frac{d}{d\tau} \left(\frac{\partial f}{\partial \dot{x}(\tau)} \right) \right] \delta x(\tau) d\tau \right\} \Big|_0^T \\ &\quad - \int_0^T t \frac{d}{dt} \left\{ \int_0^t \left[\frac{\partial f}{\partial x(\tau)} - \frac{d}{d\tau} \left(\frac{\partial f}{\partial \dot{x}(\tau)} \right) \right] \delta x(\tau) d\tau \right\} dt \end{aligned}$$

$$\begin{aligned}
&= \int_0^T \frac{\partial f}{\partial \dot{x}(t)} \delta x(t) dt + T \int_0^T \left[\frac{\partial f}{\partial x(\tau)} - \frac{d}{d\tau} \left(\frac{\partial f}{\partial \dot{x}(\tau)} \right) \right] \delta x(\tau) d\tau \\
&\quad - \int_0^T t \left[\frac{\partial f}{\partial x(t)} - \frac{d}{dt} \left(\frac{\partial f}{\partial \dot{x}(t)} \right) \right] \delta x(t) dt.
\end{aligned}$$

Since τ is an arbitrary time variable, we can write:

$$\delta A_d = \int_0^T \left\{ \frac{\partial f}{\partial \dot{x}(t)} + (T-t) \left[\frac{\partial f}{\partial x(t)} - \frac{d}{dt} \left(\frac{\partial f}{\partial \dot{x}(t)} \right) \right] \right\} \delta x(t) dt.$$

Finally, δA is:

$$\delta A = \int_0^T \left\{ \frac{\partial(K-V)}{\partial x(t)} - \frac{d}{dt} \left(\frac{\partial(K-V)}{\partial \dot{x}(t)} \right) - \frac{\partial f}{\partial \dot{x}(t)} - (T-t) \left[\frac{\partial f}{\partial x(t)} - \frac{d}{dt} \left(\frac{\partial f}{\partial \dot{x}(t)} \right) \right] \right\} \delta x(t) dt.$$

According to the least action principle $\delta A = 0$, Eq. (4.17) can be obtained:

$$\frac{\partial(K-V)}{\partial x} - \frac{d}{dt} \left(\frac{\partial(K-V)}{\partial \dot{x}} \right) - \frac{\partial f}{\partial \dot{x}} - (T-t) \left(\frac{\partial f}{\partial x} - \frac{d}{dt} \left(\frac{\partial f}{\partial \dot{x}} \right) \right) = 0.$$

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Publications

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