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# A mathematical method for irregular hamiltonian systems

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## Abstract

We present certain mathematical aspects of an information method which was formulated in an attempt to investigate diffusion phenomena. We imagine a regular dynamical hamiltonian systems under the random perturbation of thermal (molecular) noise and chaotic motion. The random effect is taken into account via the uncertainty of irregular dynamic process produced in this way. This uncertainty due to different paths between two phase points is measured by a path information which is maximized in connection with the action defined originally for the unperturbed regular hamiltonian systems. The obtained transition probability depends exponentially on this action. The usefulness of this information method has been demonstrated by the derivation of diffusion laws without the usual assumptions. In this work, some essential mathematical aspects of this irregular dynamics is reviewed. It is emphasized that the classical action principle for single least action path is no more valid and the formalism of classical mechanics for regular hamiltonian systems is no more exact for irregular hamiltonian dynamics. There is violation of the fundamental laws of mechanics by randomly perturbed hamiltonian systems. However, the action principle is always present for the ensemble of paths through the average action. This average action principle leads to a formalism of stochastic mechanics in which, in spite of the violation of fundamental laws, the mathematical form of classical mechanics can be recovered by a consideration of the statistical averaging of the dynamics.

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# 1 Introduction

The dynamics of a Hamiltonian system can be roughly classified into two categories: regular and irregular. The mathematics of the regular dynamics can be perfectly formulated on the basis of the least action principle in classical mechanics. But the stochastic character of irregular dynamics makes it much more complicated to be formulated. Description of random dynamic process with Newtonian type equations is possible if one introduces random forces like in Langevin equation[1]. Other statistical method by informational consideration without introducing the details of the dynamic randomness are proved to be very useful. The description of the stochastic behavior of chaotic systems using Kolmogorov-Sinai entropy is an example[2].

The method we address in this paper is originally intended to study diffusion process by a informational consideration. Diffusion is an irregular dynamic process in which components of a mixture are transported around the mixture by means of random molecular motion. Over 200 years ago, Berthelot postulated[3] that the flow of mass by diffusion across a plane, was proportional to the concentration gradient of the diffusant across that plane. About 50 years later, Fick introduced[4] two differential equations that quantified the above statement for the case of transport through thin membranes. Fick's First Law states that the flux  $J$  of a component of concentration  $n$  across a membrane is proportional to the concentration gradient in the membrane:

$$J(x) = -D \frac{\partial n(x)}{\partial x} \quad (1)$$

where  $x$  is the position variable for one dimensional systems. Fick's Second Law states that the rate of time change of concentration of diffusant at a point is proportional to the rate of spacial change of concentration gradient at that point within the mixture

$$\frac{\partial n}{\partial t} = \frac{\partial}{\partial x} \left[ D \frac{\partial n(x)}{\partial x} \right]. \quad (2)$$

If  $D$  is constant everywhere in the mixture, the above equation becomes  $\frac{\partial n}{\partial t} = D \frac{\partial^2 n(x)}{\partial x^2}$ .

Above normal diffusion laws are very precisely tested in experiments in most of solids, liquids and gases and are widely studied in nonequilibrium

thermostatistics together with the Fokker-Planck equation of diffusion probability, the Fourier law of heat conduction and the Ohm's law of electrical charge conduction. Many efforts to derive theoretically the above diffusion laws were concentrated on special models of solids in which particles are transported. Other phenomenological derivations are also possible if one supposes Brownian motion and Markovian process[1], or Kolmogorov conditions[5]. Recently, an attempt is made to derive these laws with a different method based on information theory. The method consists in considering hamiltonian systems under the perturbation of thermal noise and chaotic instability. The dynamic uncertainty of this perturbed dynamic process is measured by a path information connected with different paths. In order to derive the transition probability distribution of the irregular process, the path information is maximized in connection with, *faute de mieux*, the action defined with the unperturbed Hamiltonian. The diffusion laws is simply the differential equation of the transition probability distribution in exponential of action. Although we can hardly talk about the exact action of a system subject to random forces and that the action here is only the *unperturbed* action of the system, the least action principle is still present in this approach through the average action. This description of irregular dynamics underlies a probabilistic formalism of mechanics which is logically different from the conventional one based on the action principle for single path of the unperturbed hamiltonian systems. In what follows, we discuss some mathematical aspects of this stochastic mechanics.

## 2 Regular dynamics of hamiltonian systems

A hamiltonian system is a mechanical system which satisfies the following Hamiltonian equations[2] :

$$\dot{x}_i = \frac{\partial H}{\partial p_i} \text{ and } \dot{p}_i = -\frac{\partial H}{\partial x_i}, \text{ with } i = 1, 2, \dots, n \quad (3)$$

where  $n$  is the number of degrees of freedom,  $x_i$  is the coordinates,  $P_i = m\dot{x}_i$  the momenta and  $H$  is the hamiltonian of the system. The solutions of these equations are geodesics in phase space  $\Gamma$  of  $2n$  dimension, i.e., the paths between a initial point  $a$  and a final point  $b$  whose action  $A_k = \int_a^b L_k(t)dt$  has a stationary (least action principle). From this action principle, we can

derive Euler-Lagrange equations[6]

$$\frac{\partial}{\partial t} \frac{\partial L_k(t)}{\partial \dot{x}} - \frac{\partial L_k(t)}{\partial x} = 0 \quad (4)$$

where  $L_k = T - V$  (we suppose  $n = 1$  from now on) is the Lagrangian of the system along a path  $k$ . If we consider the Legendre transformation  $H = P\dot{x} - L_k$ , Eqs.(3) can be easily derived from Eq.(4)[6]. This formalism of mechanics underlies a completely deterministic character of dynamic process: if the initial conditions are given, there is no uncertainty, no information, no probability distribution associated with the future evolution of the systems. The geodesics are determined for any time by the above equations plus initial conditions.

### 3 A path information

Now we imagine a hamiltonian system under the perturbation of thermal noise and chaotic instability. This perturbation can be either internal or external to the system. A hamiltonian system containing a large number of particles in random motion is an example of internal perturbation. The dynamic instability of chaotic systems is another example of internal perturbation leading to stochastic deviation from regular behavior. The motion of a Brownian particle is an example of external perturbation due to the random molecular motion around the particle. Under these perturbations, the geodesics of regular dynamics will be deformed and fluctuate in such a stochastic way that following exactly the evolution of each mechanical quantity (e.g., action) is inconceivable. We call this dynamic process irregular since there is uncertainty about the future evolution even if the initial condition is given. We will consider two dynamic uncertainties:

1. Between any two phase space points  $a$  and  $b$ , there may be different possible paths (labelled by  $k=1,2,...w$ ) each having a probability  $p_k(b|a)$  to be followed by the system. This is the uncertainty considered by Feynman in his formulation of quantum mechanics[7]. Here we introduce it within randomly perturbed classical mechanics.
2. There are different possible paths leaving the point  $a$  and leading to different final points  $b$ , each having a probability  $p_k(x|a)$  to be followed

by the system, where  $x$  is the position of arbitrary  $b$ . This uncertainty is the basic consideration for the definition of Kolmogorov-Sinai entropy[2] in the description of chaotic systems.

In what follows, we first discuss the transition probability  $p_k(b|a)$  between two fixed phase points (or cells of a given partition of the phase space): the cell  $a$  in the initial phase volume  $A$  and a cell  $b$  in the final phase volume  $B$  via a path  $k$  ( $k = 1, 2, \dots, w$ ). We suppose that the uncertainty concerning the choice of paths by the systems between two points is measured with the following path information

$$I_{ab} = - \sum_{k=1}^w p_k(b|a) \ln p_k(b|a). \quad (5)$$

We have the following normalization

$$\sum_{k=1}^w p_k(b|a) = 1. \quad (6)$$

## 4 Maximum path information

An essential assumption of our informational method is that each path is characterized by its action  $A_{ab}(k)$  defined as if there was no random perturbation. This action is given by

$$A_{ab}(k) = \int_{t_{ab}(k)} L_k(t) dt \quad (7)$$

where  $L_k(t) = E - U$  is the Lagrangian of the system at time  $t$  along the path  $k$ . The average action is given by

$$A_{ab} = \sum_{k=1}^w p_k(b|a) A_{ab}(k). \quad (8)$$

For irregular dynamic process, the least action principle does not apply since, firstly, there is no exact calculation of real action due to dynamic randomness, and secondly, the action we defined here has no stationary  $\delta A_{ab}(k) = 0$  for all the possible paths. We use the information method which consists in saying that the stable probability distribution of paths must correspond

to a stationary uncertainty or path information  $I_{ab}$  under the constraint associated with the average action  $A_{ab}$ . This means the following operation:

$$\delta[I_{ab} + \alpha \sum_{k=1}^w p_k(b|a) - \eta \sum_{k=1}^w p_k(b|a) A_{ab}(k)] = 0 \quad (9)$$

leading to

$$p_k(b|a) = \frac{1}{Z} \exp[-\eta A_{ab}(k)], \quad (10)$$

where the partition function

$$Z = \sum_k \exp[-\eta A_{ab}(k)]. \quad (11)$$

The physical meaning of the multiplier  $\eta$  will be discussed below.

It is proved that[8] the distribution Eq.(10) is stable with respect to the fluctuation of action. It is also proved that Eq.(10) is a least (stationary) action distribution, i.e., the most probable paths are just the paths of least action. Indeed, we have  $\delta p_k(b|a) = -\eta p_k(b|a) \delta A_{ab}(k) = 0$  which means  $\delta A_{ab}(k) = 0$  and yields Euler-Lagrange equation and Hamiltonian equations given in Eqs.(3) and (4). Consequently, the most probable paths are just the geodesics of the unperturbed hamiltonian dynamics. The other paths do not satisfy Eqs.(3) and (4). In general, the paths have neither  $\delta A_{ab}(k) = 0$  nor  $\delta A_{ab} = 0$ . Nevertheless, the average action  $A_{ab}$  defined over all these paths does have a stationary associated with the stationary of the uncertainty  $I_{ab}$  in Eq.(9), i.e.,

$$-\eta \delta A_{ab} + \delta I_{ab} = 0. \quad (12)$$

Here we considered  $\sum_{k=1}^w \delta p_k(b|a) = 0$ . Eq.(12) implies that, although the least action principle of classical mechanics cannot apply when the dynamics is perturbed by random and instable noise, the maximum path information introduced above underlies in fact the same physics in which the action principle is present as a average effect in association with the stationary dynamic uncertainty. Eq.(12) implies a probabilistic version of classical mechanics and will be used below to derive the averaged Euler-lagrange equation for irregular dynamics.

## 5 A calculation of least action distribution

In what follows, the *unperturbed* action is analyzed for different paths with the Euler method. Let us look at a system of mass  $m$  moving along a given path  $k$  from a point  $a$  to a point  $b$ . The path is cut into  $N$  infinitesimally small segments each having a spatial length  $\Delta x_i = x_i - x_{i-1}$  with  $i = 1 \dots N$  ( $x_0 = x_a$  and  $x_N = x_b$ ).  $t = t_i - t_{i-1}$  is the time interval spent by the system on every segment. The Lagrangian on the segment  $i$  is given by

$$L(x_i, \dot{x}_i, t) = \frac{m(x_i - x_{i-1})^2}{2(t_i - t_{i-1})^2} - \left( \frac{\partial U}{\partial x} \right)_i \frac{(x_i - x_{i-1})}{2} - U(x_{i-1}) \quad (13)$$

where the first term on the right hand side is the kinetic energy of the particle, the second and the third terms are the average potential energy on the segment  $i$ . The action of segment  $i$  is given by

$$A_i = \frac{m(\Delta x_i)^2}{2t} + F_i \frac{\Delta x_i}{2} t - U(x_{i-1})t, \quad (14)$$

where  $F_i = - \left( \frac{\partial U}{\partial x} \right)_i$  is the force on the segment  $i$ . According to Eq.(10), the transition probability  $p_{k,i}$  from  $x_{i-1}$  to  $x_i$  on the path  $k$  is given by

$$p_{k,i} = \frac{1}{Z_i} \exp \left( -\eta \left[ \frac{m}{2t} \Delta x_i^2 + F_i \frac{t}{2} \Delta x_i \right]_k \right) \quad (15)$$

where  $Z_i$  is calculated as follows

$$\begin{aligned} Z_i &= \int_{-\infty}^{\infty} dx_i \exp \left( -\eta \left[ \frac{m}{2t} \Delta x_i^2 + F_i \frac{t}{2} \Delta x_i \right]_k \right) \\ &= \exp \left[ F_i^2 \frac{\eta t^3}{8m} \right] \sqrt{\frac{2\pi t}{m\eta}}. \end{aligned} \quad (16)$$

The potential energy of the point  $x_{i-1}$  disappears in the expression of  $p_{k,i}$  because it does not depend on  $x_i$ .

The total action is given by

$$A_{ab}(k) = \sum_{i=1}^N A_i = \sum_{i=1}^N \left[ \frac{m(\Delta x_i)^2}{2t} + F_i \frac{t}{2} \Delta x_i - U(x_{i-1})t \right]_k. \quad (17)$$

According to Eq.(10), the transition probability from  $a$  to  $b$  via the path  $k$  is the following:

$$\begin{aligned} p_k(b|a) &= \frac{1}{Z} \exp \left( -\eta \sum_{i=1}^N \left[ \frac{m(\Delta x_i)^2}{2t} + F_i \frac{t}{2} \Delta x_i \right]_k \right) \\ &= p(b|a)^{-1} \prod_{i=1}^N p_{k,i} \end{aligned} \quad (18)$$

where

$$\begin{aligned} Z &= \sum_{k=1}^w \exp \left( -\eta \sum_{i=1}^N \left[ \frac{m(\Delta x_i)^2}{2t} + F_i \frac{t}{2} \Delta x_i \right]_k \right) \\ &= \int_{-\infty}^{\infty} dx_1 dx_2 \dots dx_{N-1} \exp \left( -\eta \sum_{i=1}^N \left[ \frac{m(x_i - x_{i-1})^2}{2t} + F_i \frac{t}{2} (x_i - x_{i-1}) \right]_k \right) \\ &= \left( \exp \left[ F_i^2 \frac{\eta t^3}{8m} \right] \sqrt{\frac{2\pi t}{m\eta}} \right)^N p(b|a) = Z_i^N p(b|a) \end{aligned} \quad (19)$$

and

$$\begin{aligned} p(b|a) &= \exp \left[ F_i^2 \frac{\eta(t_b - t_a)^3}{8m} \right] \sqrt{\frac{m\eta}{2\pi(t_b - t_a)}} \\ &\times \exp \left( -\eta \left[ \frac{m(x_b - x_a)^2}{2(t_b - t_a)} + F_i \frac{t_b - t_a}{2} \Delta x_i \right] \right). \end{aligned} \quad (20)$$

Remember that in the above calculation, the point  $x_0 = x_a$  and the final point  $x_N = x_b$  are fixed.

Now in order to see the behavior of transition probability with respect to final point, we have to relax  $x_b = x$  and let it vary arbitrarily as other intermediate points. This implies we take into account the second uncertainty due to chaos mentioned in the introduction. The corresponding transition probability  $p_k(x|a)$  from  $a$  to arbitrary  $x$  via the path  $k$  has been derived with the maximum path information combined with action[9]. Here we only introduce it in the following way:

$$\begin{aligned} p_k(x|a) &= p(b|a)p_k(b|a) \\ &= \prod_{i=1}^N p_{k,i/i-1}, \end{aligned} \quad (21)$$

normalized by

$$\sum_b \sum_{k=1}^w p_k(x_b|a) = \int dx_1 dx_2 \dots dx_{N-1} dx p_k(x|a) = 1. \quad (22)$$

The uncertainty or path information associated with this transition probability between  $a$  and arbitrary  $b$  is given by

$$\begin{aligned} I_a &= - \sum_b \sum_{k=1}^w p_k(x|a) \ln p_k(x|a) \\ &= - \sum_b p(b|a) \ln p(b|a) - \sum_b p(b|a) \sum_{k=1}^w p_k(b|a) \ln p_k(b|a) \\ &= h_{ab} + \langle I_{ab} \rangle \end{aligned} \quad (23)$$

where  $h_{ab} = - \sum_b p(b|a) \ln p(b|a)$  is the uncertainty of the transition from  $a$  to an arbitrary  $b$  via whichever path, and  $\langle I_{ab} \rangle$  is the average of  $I_{ab}$  over all the possible point  $b$  in the final phase volume  $B$ .

The average action defined with  $p_k(x|a)$  over all the possible paths and final points is given by

$$\begin{aligned} \langle A_{ab} \rangle &= - \sum_b \sum_{k=1}^w p_k(x|a) A_{ab}(k) \\ &= \sum_b p(b|a) \sum_{k=1}^w p_k(b|a) A_{ab}(k) \\ &= \sum_b p(b|a) A_{ab}. \end{aligned} \quad (24)$$

Remember that  $p(b|a)$  does not depend on the paths. So if  $A_{ab}$  has a stationary,  $\langle A_{ab} \rangle$  must have a stationary as well.

## 6 Fokker-Planck equation

A derivation of the diffusion laws from Eq.(15) and Eq.(21) is given in [10]. In what follows, we only illustrate this straightforward method with Fokker-Planck equation which describes the time evolution of transition probability. This equation can be derived if we suppose that the diffusion particles follow Brownian motion and Markovian process[1], or Kolmogorov conditions[5].

From Eq.(15), a simple calculation of the derivatives  $\frac{\partial p_i}{\partial t}$ ,  $\frac{\partial(F_i p_i)}{\partial x_i}$  and  $\frac{\partial^2 p_i}{\partial x_i^2}$  yields

$$\frac{\partial p_i}{\partial t} = -\frac{\tau}{m} \frac{\partial(F_i p_i)}{\partial x_i} + \frac{1}{2m\eta} \frac{\partial^2 p_i}{\partial x_i^2}. \quad (25)$$

This is the Fokker-Planck equation, where  $\tau$  is the mean free time supposed to be the time interval  $t$  of the particle on each segment of its path. In view of the Eq.(21), it is easy to show that this equation is also satisfied by  $p_k(x|a)$  if  $x_i$  is replaced by  $x$ , the final position. Other diffusion laws can be easily obtained from the above equation. We think that this derivation is a proof of the usefulness of the present informational approach to irregular dynamics.

As discussed in [10], Eq.(25) yields in general:

$$\frac{\partial n}{\partial t} = -\frac{\tau}{m} \frac{\partial(nF)}{\partial x} + \frac{1}{2m\eta} \frac{\partial^2 n}{\partial x^2}. \quad (26)$$

where  $n$  is the particle density at point  $x$  and time  $t$ . In order to clarify the physical meaning of  $\eta$ , we consider here a gas in equilibrium (hence  $\frac{\partial n}{\partial t} = 0$ ) in a constant force  $F$  with the distribution  $n(x) = n(x_0) \exp[F(x - x_0)/k_B T]$  where  $k_B$  is the Boltzmann constant. From Eq.(26), we straightforwardly get

$$\eta = \frac{1}{2\tau k_B T} \quad (27)$$

Now let us focus on the modification imposed upon the formalism of classical mechanics by the above probabilistic description of stochastic mechanics.

## 7 Euler-Lagrange equations

Let us look at, not the most probable paths (geodesics) of the dynamics from  $A$  to  $B$  which satisfy Eqs.(3) and (4), but all the other paths whose *unperturbed* action is not a stationary. When a system travels along these paths,  $\delta A_{ab}(k) \neq 0$ . It is either positive or negative. On the other hand, we have[6]

$$\delta A_{ab}(k) = \int_a^b \left[ \frac{\partial}{\partial t} \frac{\partial L_k(t)}{\partial \dot{x}} - \frac{\partial L_k(t)}{\partial x} \right] \varepsilon dt \quad (28)$$

where  $\varepsilon$  is an arbitrary variation of  $x$  ( $\varepsilon$  is zero at  $a$  and  $b$ ). If  $\delta A_{ab}(k) > 0$  (or  $< 0$ ), we get

$$\frac{\partial}{\partial t} \frac{\partial L_k(t)}{\partial \dot{x}} - \frac{\partial L_k(t)}{\partial x} > 0 \text{ (or } < 0 \text{)}. \quad (29)$$

which can be proved as follows. Suppose  $\int_a^b f(t)\varepsilon dt > 0$  and  $f(t) < c < 0$  during a small period of time  $\Delta t$  somewhere between  $a$  and  $b$ . Since  $\varepsilon$  is arbitrary, let it be zero outside  $\Delta t$  and a positive constant within  $\Delta t$ . We clearly have  $\int_a^b f(t)\varepsilon dt < c\varepsilon < 0$  which contradicts our starting assumption. This proves Eq.(29).

Legendre transformation  $H = P\dot{x} - L_k$  implies[6]

$$P = \frac{\partial L_{k_{ab}}}{\partial \dot{x}}. \quad (30)$$

Put this relationship back into Eq.(29), we get

$$\dot{P} > \text{ (or } < \text{)} \frac{\partial L_k}{\partial x} \quad (31)$$

for  $dA_{ab}(k) > 0$  (or  $< 0$ ). In view of the fact that the deviation of  $\dot{P}$  from the regular force  $\frac{\partial L_k}{\partial x}$  is due to the dynamic irregularity, by introducing a “force”  $R$  of the random perturbation, Eq.(31) can be recast into

$$\dot{P} = \frac{\partial L_k}{\partial x} + R. \quad (32)$$

According to Eq.(31),  $R$  is positive if  $dA_{ab}(k) > 0$  and negative if  $dA_{ab}(k) < 0$ .

## 8 Hamiltonian equations

The total differential of  $H$  is

$$dH = \frac{\partial H}{\partial P}dP + \frac{\partial H}{\partial x}dx + \frac{\partial H}{\partial t}dt. \quad (33)$$

From Legendre transformation, we can also write[6]

$$dH = \dot{x}dP - \frac{\partial L_k}{\partial x}dx - \frac{\partial L_k}{\partial t}dt. \quad (34)$$

Comparing Eq.(33) to Eq.(34), we get

$$\dot{x} = \frac{\partial H}{\partial P} \text{ and } \dot{P} > (\text{or } <) - \frac{\partial H}{\partial x}, \quad (35)$$

which are the Hamiltonian equations for irregular dynamic process following the paths whose action is not at stationary. The second equation above violates the Newton's second law. Remember that  $>$  (or  $<$ ) is for the case where  $dA_{ab}(k) = \frac{\partial A_{ab}(k)}{\partial x} dx - \frac{\partial A_{ab}(k)}{\partial \dot{x}} d\dot{x} > (\text{or } <) 0$ .

Considering the random force  $R$ , Eq.(35) can be written as

$$\dot{P}_k = -\frac{\partial H}{\partial x} + R. \quad (36)$$

This is a Langevin equation.

## 9 Energy conservation

From Eq.(33), we see that if the Hamiltonian of the system is not an explicit function of time ( $\frac{\partial H}{\partial t} = 0$ ), we get

$$\frac{dH}{dt} = \frac{\partial H}{\partial P} \dot{P} + \frac{\partial H}{\partial x} \dot{x}. \quad (37)$$

For the geodesics, using Eq.(3), we get  $\frac{dH}{dt} = 0$ . So the energy is conserved during the time evolution of the system. But if the system travels along other paths than the unperturbed geodesics, Eq.(35) occurs, we should write  $\frac{dH}{dt} > (\text{or } <) 0$  for the paths having  $dA_{ab}(k) > 0$  (or  $< 0$ ). The energy is no more conserved.

The fluctuation of energy is defined by  $\sigma_H^2 = \langle (H_k - \langle H_k \rangle)^2 \rangle = \langle H_k^2 \rangle - \langle H_k \rangle^2$  which we will calculate for a segment  $i$  of the paths in the time interval  $\tau = t_i - t_{i-1}$  (see section 5). The action on this segment of the path  $k$  can be written as

$$A_i = (P_i \dot{x}_i - H_i)_k \tau \quad (38)$$

So the transition probability is given by

$$p_{k,i} = \frac{1}{Z_i} \exp [-\eta \tau (P_i \dot{x}_i - H_i)_k] \quad (39)$$

where  $Z_i = \sum_k \exp [-\eta\tau(P_i\dot{x}_i - H_i)_k]$ . After some mathematics, we get

$$\begin{aligned}\sigma_H^2 &= \frac{1}{Z_i} \sum_k (H_i - \langle H_i \rangle)^2 \exp [-\eta\tau(P_i\dot{x}_i - H_i)_k] \\ &= \frac{1}{\tau} \frac{\partial \langle H_i \rangle}{\partial \eta} + \langle P\dot{x}H_i \rangle - \langle P\dot{x} \rangle \langle H_i \rangle.\end{aligned}\quad (40)$$

Let's see an example with *free particle*. We have in this case  $\langle P\dot{x}H_i \rangle = 2\langle H_i^2 \rangle$  and  $\langle P\dot{x} \rangle \langle H_i \rangle = 2\langle H_i \rangle^2$ , leading to

$$\sigma_H^2 = -\frac{1}{\tau} \frac{\partial \langle H_i \rangle}{\partial \eta}.\quad (41)$$

For this kind of systems,  $\langle H_i \rangle$  can be calculated by using Eq.(15) with  $F_i = 0$ . We have  $\langle \Delta x_i^2 \rangle = \frac{\tau}{m\eta}$  and  $\langle H_i \rangle = \frac{m\langle \Delta x_i^2 \rangle}{2\tau^2} = \frac{1}{2\tau\eta} = k_B T$ . Finally, we get

$$\sigma_H^2 = \frac{1}{2\tau^2\eta^2} = 2k_B^2 T^2.\quad (42)$$

Don't forget that we are addressing one dimensional system which can have only one particle under thermal noise. For  $N$ -particle systems, the result is different. From Eqs.(27) and (41), one can write

$$\sigma_H^2 = -2C_i k_B T^2\quad (43)$$

where  $C_i = \frac{\partial \langle H_i \rangle}{\partial T}$  is the heat capacity of the system on the segment  $i$  of the paths.

## 10 Liouville theorem

Now we look at the time change of state density  $\rho(\Gamma)$  in phase space. The time evolution neither creates nor destroys state points, so the number of the phase points is conserved. The conservation law in a 2-dimensional phase space is

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\dot{x}\rho)}{\partial x} + \frac{\partial(\dot{P}\rho)}{\partial P} = 0\quad (44)$$

which means

$$\frac{d\rho}{dt} = \frac{\partial\rho}{\partial t} + \frac{\partial\rho}{\partial x}\dot{x} + \frac{\partial\rho}{\partial P}\dot{P} = -\left(\frac{\partial\dot{x}}{\partial x} + \frac{\partial\dot{P}}{\partial P}\right)\rho. \quad (45)$$

For the least action paths which satisfy Eqs.(3), the right hand side of the above equation is zero, leading to the *Liouville theorem*

$$\frac{d\rho(\Gamma, t)}{dt} = 0, \quad (46)$$

i.e., the state density in phase space is a constant of motion.

For a system travelling along a perturbed paths having  $dA_{ab}(k) \neq 0$ , Eqs.(3) vanishes and so does Eq.(46). Considering Eqs.(36) and (45), we find

$$\frac{d\rho(\Gamma, t)}{dt} = -\frac{\partial R}{\partial P}\rho. \quad (47)$$

Nevertheless, the determination of the sign of  $\frac{\partial R}{\partial P}$  is not evident in general. In any case, this result means that, in general, if a system does not travel along the paths of stationary *unperturbed* action due to random or molecular noise, then its state density may change with time.

The first consequence of Eq.(47) is that, in general, the phase volume  $\Omega$  is no more conserved for irregular dynamic systems since

$$\frac{d\Omega}{dt} = \frac{d}{dt} \int \rho(\Gamma, t) d\Gamma = \int \frac{d\rho(\Gamma, t)}{dt} d\Gamma = -\overline{\frac{\partial R}{\partial P}} \neq 0, \quad (48)$$

where the average  $\overline{\frac{\partial R}{\partial P}}$  is over all the phase volume occupied by the system at time  $t$ .

## 11 Averaged formalism of stochastic mechanics

### 11.1 Euler-Lagrange equations

It is mentioned above that the dynamics described by the distribution Eq.(10) has a *stationary average action* in association with the stationary path information. In what follows, we use this fact to derive the averaged version of the equations of motion of classical mechanics.

$\delta A_{ab}$  can be calculated as follows:

$$\delta A_{ab} = \sum p_k(b|a) \delta A_{ab}(k) + \sum \delta p_k(b|a) A_{ab}(k). \quad (49)$$

The first term on the right hand side of this equation is

$$\begin{aligned} \sum p_k(b|a) \delta A_{ab}(k) &= \sum p_k(b|a) \int_a^b \left[ \frac{\partial}{\partial t} \frac{\partial L_k(t)}{\partial \dot{x}} - \frac{\partial L_k(t)}{\partial x} \right] \varepsilon dt \\ &= \int_a^b \left[ \left\langle \frac{\partial}{\partial t} \frac{\partial L_k(t)}{\partial \dot{x}} \right\rangle - \left\langle \frac{\partial L_k(t)}{\partial x} \right\rangle \right] \varepsilon dt \end{aligned} \quad (50)$$

where  $\langle \cdot \rangle$  is the average over all the possible paths.

The second term on the right hand side of Eq.(49) is

$$\sum \delta p_k(b|a) A_{ab}(k) = -\frac{1}{\eta} \sum \delta p_k(b|a) \ln[Z p_k(b|a)] \quad (51)$$

$$= -\frac{1}{\eta} \delta \sum p_k(b|a) \ln p_k(b|a) = \frac{\delta I_{ab}}{\eta}. \quad (52)$$

where we have used  $\sum \delta p_k(b|a) = 0$ . Considering Eq.(12), we get

$$\int_a^b \left[ \left\langle \frac{\partial}{\partial t} \frac{\partial L_k(t)}{\partial \dot{x}} \right\rangle - \left\langle \frac{\partial L_k(t)}{\partial x} \right\rangle \right] \varepsilon dt = \delta A_{ab} - \frac{\delta I_{ab}}{\eta} = 0. \quad (53)$$

Now considering that  $\varepsilon$  is arbitrarily chosen, we obtain

$$\left\langle \frac{\partial}{\partial t} \frac{\partial L_k(t)}{\partial \dot{x}} \right\rangle - \left\langle \frac{\partial L_k(t)}{\partial x} \right\rangle = 0. \quad (54)$$

This is the *averaged Euler-Lagrange equation*.

From Eq.(30), we can write

$$\langle \dot{P} \rangle = \left\langle \frac{\partial L_k(t)}{\partial x} \right\rangle \quad (55)$$

where  $\left\langle \frac{\partial L_k(t)}{\partial x} \right\rangle$  is an averaged force.

## 11.2 Averaged Hamiltonian equations

By means of Eq.(35) and  $\frac{\partial H(t)}{\partial x} = -\frac{\partial L_{kab}(t)}{\partial x}$ , the following averaged equations exist

$$\langle \dot{x} \rangle = \left\langle \frac{\partial H}{\partial P} \right\rangle \quad \text{and} \quad \langle \dot{P} \rangle = - \left\langle \frac{\partial H}{\partial x} \right\rangle. \quad (56)$$

This implies that the mean of the “random force”  $R$  over all possible paths must vanish, i.e.,  $\langle R \rangle = 0$ .

## 11.3 Energy conservation law

From the energy conservation problem discussed above, we see that the only Hamiltonian which is physically significant for randomly perturbed hamiltonian systems is the average Hamiltonian  $\langle H \rangle$ . Its derivative with respect to time (change rate of average energy) is

$$\frac{d\langle H \rangle}{dt} = \left\langle \frac{dH}{dt} \right\rangle + \sum_k \frac{dp_{k,i}}{dt} H. \quad (57)$$

The first term of this equation is just

$$\left\langle \frac{dH}{dt} \right\rangle = \left\langle \frac{\partial H}{\partial P} \dot{P} \right\rangle + \left\langle \frac{\partial H}{\partial x} \dot{x} \right\rangle = \langle \dot{x} R \rangle = \left\langle \frac{dW_R}{dt} \right\rangle \quad (58)$$

where  $W_R$  is a random work done by the “random force”  $R$ .

With the help of the least action distribution  $p_{k,i}$  and the definition of path information, the second term of Eq.(57) can be given by

$$\sum_k \frac{dp_{k,i}}{dt} H = \sum_k \frac{dp_{k,i}}{dt} P \dot{x} - \frac{1}{\tau \eta} \frac{dI_i}{dt} \quad (59)$$

where  $I_i = -\sum_k p_{k,i} \ln p_{k,i}$  is the path information on the segment  $i$  and in the time interval  $\tau$ . Simple calculation leads to

$$\frac{dI_i}{dt} = \eta \left[ \frac{d\langle A_i \rangle}{dt} - \left\langle \frac{dA_i}{dt} \right\rangle \right] = \eta(\Delta_t A) \quad (60)$$

On the other hand,

$$\begin{aligned}
\sum_k \frac{dp_{k,i}}{dt} P\dot{x} &= \frac{d\langle P\dot{x} \rangle}{dt} - \sum_k p_{k,i} \frac{d(P\dot{x})}{dt} \\
&= \frac{d\langle P\dot{x} \rangle}{dt} - 2 \sum_k p_{k,i} \left[ -\frac{\partial H}{\partial x} + R \right] \dot{x} \\
&= \frac{d\langle P\dot{x} \rangle}{dt} + 2 \left\langle \frac{\partial H}{\partial x} \dot{x} \right\rangle - 2 \langle \dot{x} R \rangle.
\end{aligned} \tag{61}$$

Hence we get

$$\sum_k \frac{dp_{k,i}}{dt} H = \frac{d\langle P\dot{x} \rangle}{dt} + 2 \left\langle \frac{\partial H}{\partial x} \dot{x} \right\rangle - 2 \langle \dot{x} R \rangle - \frac{1}{\tau} (\Delta_t A). \tag{62}$$

This means

$$\begin{aligned}
\frac{d\langle H \rangle}{dt} &= \frac{d\langle P\dot{x} \rangle}{dt} + 2 \left\langle \frac{\partial H}{\partial x} \dot{x} \right\rangle - \langle \dot{x} R \rangle - \frac{1}{\tau} (\Delta_t A) \\
&= 2 \frac{d\langle T \rangle}{dt} - 2 \left\langle \frac{dW_H}{dt} \right\rangle - \langle \dot{x} R \rangle - \frac{1}{\tau} (\Delta_t A)
\end{aligned} \tag{63}$$

where  $T$  is the kinetic energy of the system,  $W_H$  is the work done by the conservative force. We suppose that our hamiltonian system neither gains nor loses energy through the irregular random process. So the average energy must be a constant of motion, i.e.,  $\frac{d\langle H \rangle}{dt} = 0$ . This means the random work must satisfy the following relation:

$$\langle \dot{x} R \rangle = 2 \left( \frac{d\langle T \rangle}{dt} - \left\langle \frac{dW_H}{dt} \right\rangle \right) - \frac{1}{\tau} (\Delta_t A). \tag{64}$$

This condition seems reasonable because a random force, though statistically vanishing, can made non vanishing average work which may change the average energy of a system. So if we require that the system statistically remain hamiltonian, this work or its power  $\langle \dot{x} R \rangle$  should satisfy some condition. If ever we have  $\langle \dot{x} R \rangle = 0$ , we can write  $\left\langle \frac{dH}{dt} \right\rangle = 0$ , meaning that the time variation of energy is statistically null. But the average energy may always change in time due to the deviation from the least action paths. We have the following condition for statistical energy conservation:

$$\left( \frac{d\langle T \rangle}{dt} - \left\langle \frac{dW_H}{dt} \right\rangle \right) = \frac{1}{2\tau} (\Delta_t A). \tag{65}$$

## 12 Passage from stochastic mechanics to regular one

Of course, when the randomness diminishes, this stochastic mechanics formalism should recover the regular classical one. In fact, the dispersion of action or the width of the least action distribution can be measured by the variance  $\sigma^2 = \overline{A^2} - \overline{A}^2 = \overline{A^2} - A_{ab}^2$ . From Eqs.(5), (8), (10) and (11), we get

$$\sigma^2 = -\frac{\partial A_{ab}}{\partial \eta}, \quad (66)$$

$$A_{ab} = -\frac{\partial}{\partial \eta} \ln Z, \quad (67)$$

and

$$I_{ab} = \ln Z + \eta A_{ab} = \ln Z - \eta \frac{\partial}{\partial \eta} \ln Z \quad (68)$$

When the system becomes less and less irregular,  $\sigma^2$  diminishes and the paths become closer and closer to the least action ones having stationary action  $A_{ab}^{stat}$ . When  $\sigma^2 \rightarrow 0$ , the significant contribution to the partition function  $Z$  comes from the geodesics having  $A_{ab}^{stat}$ , i.e.,  $Z \rightarrow \exp[-\eta A_{ab}^{stat}]$ . From Eq.(67),  $A_{ab} \rightarrow A_{ab}^{stat}$ . Then considering Eq.(68), it is clear that the path information  $I_{ab} \rightarrow 0$ . In this case, the stationary average action Eq.(12) becomes  $\delta A_{ab}^{stat} = 0$ , the usual action principle, and Eqs.(29) and (35) will recover Eqs.(3) and (4). At the same time, diffusion phenomena completely vanish and the diffusion laws are replaced by the laws of regular mechanics. The energy conservation law is also recovered because Eq.(65) becomes  $\left(\frac{dT}{dt} = \frac{dW_H}{dt}\right)$  due to  $\Delta_t A = \frac{d\langle A_i \rangle}{dt} - \left\langle \frac{dA_i}{dt} \right\rangle = 0$ .

## 13 Concluding remarks

The objective of this paper is to present certain mathematical aspects of an information method formulated in the attempt to describe diffusion phenomena within a formalism of stochastic mechanics. We address hamiltonian systems undergoing irregular dynamic process due to random perturbation

of thermal (molecular) noise and chaotic instability. The dynamic randomness or irregularity is taken into account via the uncertainty associated with different paths between two points in phase space and with the different final points from a given initial point. These uncertainties are measured by path informations maximized in connection with average action. It results that the probability of the irregular process depends exponentially on action (least action distribution). The usefulness of this information method is demonstrated by the derivation of diffusion laws such as the Fokker-Planck equation, Fick's laws, Ohm's law[10] and the Fourier's law[11].

This information approach with the least action distribution of paths implies a deviation from the classical regular dynamics and a formalism of stochastic mechanics. The instantaneous behaviors of irregular hamiltonian system may violate classical mechanics and its fundamental equations if only the unperturbed Hamiltonian is introduced. This is understandable because, due to the random noise and instability, exact mathematical treatment of the perturbed Hamiltonian is inconceivable even when the system remain statistically hamiltonian. In this case, only the average Hamiltonian is physically significant.

Another point is that this approach underlines a tight connection between the diffusion laws and the maximum dynamic uncertainty associated with the average action. Remember that the action here is that of the unperturbed regular system, not the real action (does it exist?) of the randomly perturbed system. This association of dynamic uncertainty with average action is in fact an application of the action principle to the whole dynamic situation, i.e., all the paths, not only the most probable paths or geodesics. As a consequence, it is the average action, instead of action, which has a stationary under the constraint of uncertainty.

This averaged action principle underlies a formalism of stochastic mechanics, which can be derived directly from the violated fundamental equations by probabilistic consideration. The mathematical form of classical mechanics can be recovered. The fundamental equations are statistically satisfied. It is shown that if the work of "random force" satisfy some condition like Eq.(49), the system remains Hamiltonian with a constant average energy. We would like to emphasize here that the Liouville theorem is also violated by the ensemble of paths or by the instantaneous behaviors of random hamiltonian system. But it seems not obvious to recover this theorem within the stochastic version of classical mechanics. This result may have impacts on some properties of mechanical systems, e.g., on the Poincaré recurrence theo-

rem and the mechanical interpretation of the second law of thermodynamics. Further work is in progress to tackle this topic.

## References

- [1] R. Kubo, M. Toda, N. Hashitsume, *Statistical physics II, Nonequilibrium statistical mechanics*, Springer, Berlin, 1995
- [2] J.R. Dorfmann, *An introduction to Chaos in nonequilibrium statistical mechanics*, Cambridge University Press, 1999
- [3] C.L. Berthelot, *Eassai de Statique Chimique*, Paris, France, 1803
- [4] A. Fick, *Ann. Physik, Leipzig*, **170**,59(1855)
- [5] G.M. Zaslavsky, Chaos, fractional kinetics and anomalous transport, *Physics Reports*, **371**,461(2002)
- [6] V.L. Arnold, *Mathematical methods of classical mechanics*, Springer-Verlag, New York, 1989
- [7] R.P. Feynman, *Quantum mechanics and path integrals*, McGraw-Hill Publishing Company, New York, 1965
- [8] Q.A. Wang, Maximum path information and the principle of least action for chaotic system, *Chaos, Solitons & Fractals*, **23**,1253(2004); cond-mat/0405373
- [9] Q.A. Wang, Maximum entropy change and least action principle for nonequilibrium systems, Invited talk at the Twelfth United Nations/European Space Agency Workshop on Basic Space Science, 24-28 May 2004, Beijing, P.R. China; cond-mat/0312329
- [10] Q.A. Wang, Diffusion laws, path information and action principle, cond-mat/0407570
- [11] Q.A. Wang, From maximum path information for irregular dynamics to Fourier's law, cond-mat/0407517