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Non quantum uncertainty relations of stochastic dynamics

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Abstract

After a recapitulation of an information-action method for the study of stochastic dynamics of hamiltonian systems perturbed by thermal noise and chaotic instability, we show that, for the ensemble of all the possible paths between two state points, the action principle acquires a statistical form $\langle \delta A \rangle = 0$. The main objective of this paper is to prove that, via this information-action description, some uncertainty relations such as $\langle \Delta A \rangle \geq \frac{1}{2\eta}$ for action, $\langle \Delta x \rangle \langle \Delta P \rangle \geq \frac{1}{\eta}$ for position and momentum, and $\langle \Delta H \rangle \langle \Delta t \rangle \geq \frac{1}{2\eta}$ for hamiltonian and time, exist for stochastic dynamics of hamiltonian systems. These relations describe, through action or its conjugate variables, the fluctuation of stochastic dynamics due to random perturbation characterized by the parameter η .

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1 Introduction

The discussion of this work is limited to mechanical systems without considering the quantum effect. We use the term *regular dynamics* to mean the mechanical processes with *time reversible* trajectories (geodesics) uniquely determined for each system by the Hamiltonian equations, or equivalently, by least action principle. Compared to this deterministic character of regular dynamics, one of the strong difference of irregular (random, stochastic, or

statistical) dynamics is the uncertainty (unpredictability) of the trajectories of the system. This uncertainty can be illustrated in Figure 1 showing the diffusion of perfume molecules in the air. Clearly, from the point of view of classical mechanics, if there is no random perturbation of the molecules of air, an isolated perfume molecule leaving the hole a of the bottle at time t_a has only one possible path or a fine bundle of paths having least action and arrives at a sole point b at time t_b . With the random perturbation of thermal noise of air molecules, however, the perfume molecules can arrive at many very different points b at a time t_b . This is the first dynamical uncertainty due to the random noise. In the theories of chaos, this uncertainty is usually measured by Kolmogorov-Sinai entropy or by Lyapunov exponent[1]. Another uncertainty is that, at time t_b , the perfume molecules can arrive at a point b through different paths. This uncertainty in path space has been considered, e.g., in the path integral approach to quantum[2] and non quantum[3] dynamics and in the large deviation theory[4]. In general, these two uncertainty are not independent from each other. It is obvious that, without the first uncertainty, the second one cannot take place.

While the mathematics of regular dynamics can be perfectly formulated on the basis of the least action principle in classical mechanics, irregular or random dynamics, found in diffusion, chaotic and other nonequilibrium phenomena, is much more complicated to be described due to its stochastic and random feature. Nowadays, statistical and thermodynamic theories of irregular dynamics are still in development, among which we can cited nonequilibrium statistical mechanics[5, 6], chaotic dynamics theory[1], anomalous transport theory[7], large deviation theory[4], small random perturbation theory[8] and path integral method starting from Brownian motion[3]. Many questions and topics concerning, e.g., time irreversibility[9], variational approaches[3, 10, 11, 12], chaotic nature of dynamic process[14, 15], connection with quantum physics[16, 17, 18] are still open to investigation. Much efforts have been made to clarify the origin of diffusion laws[19] such as the Fokker-Planck equation, the Fick's laws, the Fourier law, the Ohm's law and the anomalous diffusion laws (fractional or nonlinear)[7].

As a starting point of what we will describe in this paper, we would like to mention some characteristics shared by large deviation theory, perturbation theory, and path integral approach. In these theories, variational method is use to find the most probable (or optimal) paths (histories, trajectories) with the help of rate functional[4], action functional[5, 8, 12, 13], or path integral[3, 18]. All these functionals can be called *effective action* S whose

optimization, through a postulated exponential transition probability with a factor $\exp(-\alpha S)$, allows one to find the most probable paths. Note that S are not necessarily the mechanistic action defined in classical mechanics with the Lagrangian $L = E - U$ [3], where E and U are respectively kinetic and potential energy. Here L is defined for hamiltonian systems satisfying (in one dimensional space)

$$\dot{x} = \frac{\partial H}{\partial P} \text{ and } \dot{P} = -\frac{\partial H}{\partial x} \quad (1)$$

where x is the coordinates, $P = m\dot{x}_i$ the momenta, and $H = E + U$ is the hamiltonian of the system. The mechanistic action is defined by $A = \int_a^b L(x, P, t)dt$. Its stationary $\delta A = 0$ according to least action principle leads to the Euler-Lagrange equations[20]

$$\frac{\partial}{\partial t} \frac{\partial L}{\partial \dot{x}} - \frac{\partial L}{\partial x} = 0. \quad (2)$$

If we consider the Legendre transformation $H = P\dot{x} - L$, Eqs.(1) can be easily derived from Eq.(2). It is worth noticing that, when the effective actions mentioned above are calculated by time integral of an effective Lagrangian, Eq.(2) is always satisfied by the optimal paths[3, 5, 8, 13, 18].

A point to be noticed is that, in the above theories and their applications, one is most interested by the most probable paths whose neighborhood provides the basic contribution to the transition probability[3, 8, 12, 18]. The other less probable paths of larger actions are often neglected or only taken into account (or buried) in the path integrals[2, 3]. As a matter of fact, the extension of classical action principle only to the optimal paths is, to our opinion, incomplete. The physics represented by the larger action paths is an inseparable part of the dynamics and may be essential for the fundamental understanding of irregular dynamics. Recently, an informational method was proposed[21, 22] to treat all the possible paths as an ensemble. The method considers *hamiltonian systems* under random perturbation of thermal noise and chaotic instability leading to the uncertainties shown in Fig. 1. These uncertainties are measured by a path information associated with different paths between two points in phase space. This path information is optimized in connection with the average action of the hamiltonian system calculated over all the possible paths. We have here an exponential probability of action. In principle, this action can be any effective action mentioned above. But in our previous work, the classical mechanistic action is used. It is worth

noticing that this variational method is proven to be equivalent to an “extended least action principle”, i.e., instead of $\delta A = 0$, we have $\langle \delta A \rangle = 0$ where the average $\langle \cdot \rangle$ is taken over all the paths. Using classical action turns out to be an useful choice since we have been able to derive the diffusion laws mentioned above for all the possible paths not only for the optimal paths. In this paper we will describe some mathematical consequences of this approach. Our main objective here is to derive non quantum uncertainty relations. The results can be extended to other type of actions.

2 Optimizing information-action

First let us recapitulate briefly the method. Let $p_k(b|a)$ be the transition probability along a path k ($k = 1, 2, \dots, w$) from a phase points a and to another point b . The dynamic uncertainty associated with $p_k(b|a)$ is measured with the following Shannon information

$$I_{ab} = - \sum_{k=1}^w p_k(b|a) \ln p_k(b|a). \quad (3)$$

We have the following normalization $\sum_{k=1}^w p_k(b|a) = 1$. If w is very large in an ergodic phase volume and if the paths are sufficiently smooth, the sum \sum_k should be replaced by a path integral in the Feynman sense[2], e.g., $I_{ab} = - \int \mathcal{D}(x) p_k(b|a) \ln p_k(b|a)$ in keeping a and b fixed. The average action between a and b is given by

$$\langle A_{ab} \rangle = \sum_{k=1}^w p_k(b|a) A_{ab}(k). \quad (4)$$

where $A_{ab}(k)$ is the classical action along a path k . Our optimal information-action method consists in the following operation:

$$\delta [I_{ab} + \alpha \sum_{k=1}^w p_k(b|a) - \eta \sum_{k=1}^w p_k(b|a) A_{ab}(k)] = 0 \quad (5)$$

leading to

$$p_k(b|a) = \frac{1}{Z} \exp[-\eta A_{ab}(k)], \quad (6)$$

where the partition function $Z = \sum_k \exp[-\eta A_{ab}(k)] = \int \mathcal{D}(x) \exp[-\eta A_{ab}(k)]$. It is straightforward to see the following relationships :

$$I_{ab} = \ln Z + \eta \langle A_{ab} \rangle \quad (7)$$

and

$$\langle A_{ab} \rangle = -\frac{\partial}{\partial \eta} \ln Z, \quad (8)$$

It is proved that[21] the distribution Eq.(6) is stable with respect to the fluctuation of action. It is also shown in [21] that if one uses the action of a free particle, $p_k(b|a)$ is just the transition probability of Brownian particles[2, 3, 6]. In this case, we have a precise physical meaning of the multiplier η , i.e., $\eta = \frac{1}{2mD}$ where m is the mass and D the diffusion constant of the Brownian particle. The signification of η will be discussed later in a general way for particles moving in a potential field $U(x)$.

3 Extended action principle for irregular dynamics

As expected, Eq.(6) is a least action distribution, i.e., the most probable paths are just the paths of least action $\delta A_{ab}(k) = 0$ satisfying Euler-Lagrange equation and Hamiltonian equations. The other paths do not satisfy Eqs.(1) and (2). In general, the paths have neither $\delta A_{ab}(k) = 0$ nor $\delta \langle A_{ab} \rangle = 0$. Eq.(5) implies following relationship

$$-\eta \delta A_{ab} + \delta I_{ab} = 0. \quad (9)$$

By using Eqs.(3), (4) and the distribution (6), it is easy to calculate that Eq.(9) is equivalent to

$$\langle \delta A_{ab}(k) \rangle = \sum_k p_k(b|a) \delta A_{ab}(k) = 0. \quad (10)$$

This extension of action principle can also be derived from normalization of probability implying $\delta \sum_k p_k(b|a) = 0$ and, from Eq.(6),

$$\delta \sum_k p_k(b|a) \propto \sum_k p_k(b|a) \delta A_{ab}(k) = \langle \delta A_{ab}(k) \rangle = 0. \quad (11)$$

On the other hand, in mimicking equilibrium thermodynamics, we can define a dynamic potential

$$\Psi = \frac{1}{\eta} \ln Z$$

as an analog of the free energy of Helmholtz. From Eqs.(7) and (9), it is straightforward to see that the extended action principle Eq.(11) is equivalent to the following variational principle

$$\delta\Psi = 0. \tag{12}$$

A remarkable application of this above variational approach to computation of thermodynamic properties of hamiltonian systems was (independently) carried out recently[10]. The authors derived thermodynamic equations of motions for equilibrium systems with different Hamiltonians, already known in the literature and used in simulations of molecular dynamics, by considering the particle histories in phase space on constant energy surface.

The extension of action principle has some consequences on the equations of motion as discussed in [23]. For example, for the paths whose action is not at stationary, we get $\frac{\partial}{\partial t} \frac{\partial L_k(t)}{\partial \dot{x}} - \frac{\partial L_k(t)}{\partial x} \neq 0$ and $\dot{P} \neq -\frac{\partial H}{\partial x}$ which implies a stochastic equation like

$$\dot{P}_k = -\frac{\partial H}{\partial x} + R \tag{13}$$

where R is a random force representing the random perturbation of thermal noise and chaotic instability. On the other hand, using the action principle Eq.(10), we recover Eqs.(1) and (2) for the ensemble of paths:

$$\left\langle \frac{\partial}{\partial t} \frac{\partial L_k(t)}{\partial \dot{x}} \right\rangle - \left\langle \frac{\partial L_k(t)}{\partial x} \right\rangle = 0 \tag{14}$$

and

$$\langle \dot{x} \rangle = \left\langle \frac{\partial H}{\partial P} \right\rangle \quad \text{and} \quad \langle \dot{P} \rangle = -\left\langle \frac{\partial H}{\partial x} \right\rangle. \tag{15}$$

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

In what follows, we are concerned with the spreads of the distribution of the stochastic dynamics, in other words, the deviation of the irregular

dynamics from the regular one due to random perturbation. This uncertainty is a priori measured by the path information we introduced. But here it will be analyzed at the level of mechanical quantity like position, momentum, action and energy.

4 Uncertainty relations

For the sake of simplicity, we suppose the point a at x is very close to the point b at x_0 and the transition takes place in the infinitesimal time interval $\delta t = t - t_0$. This segment can be considered as a factor (a small element of a long path) in path integral technique[2]. Let $\delta x = x(t) - x_0(t_0)$, the action is given by

$$A_{ab}(x) = \frac{m(\delta x)^2}{2\delta t} + F\frac{\delta x}{2}\delta t - U(x_0)\delta t, \quad (16)$$

where $F = -\left(\frac{\partial U}{\partial x}\right)_{(x+x_0)/2}$ is the force on the path and m the mass of the studied system. The transition probability is

$$p_k(b|a) = \frac{1}{Z} \exp\left(-\eta \left[\frac{m}{2\delta t}\delta x^2 + F\frac{\delta t}{2}\delta x\right]\right) \quad (17)$$

with

$$\begin{aligned} Z &= \int_{-\infty}^{\infty} dx \exp\left(-\eta \left[\frac{m}{2\delta t}\delta x^2 + F\frac{\delta t}{2}\delta x\right]\right) \\ &= \exp\left[F^2\frac{\eta\delta t^3}{8m}\right] \sqrt{\frac{2\pi\delta t}{m\eta}}. \end{aligned} \quad (18)$$

The potential energy of the point x_0 disappears after normalization because it does not depend on x . F is considered constant on small δx . It is easy to show[22] that the probability of Eq.(17) satisfies the Fokker-Planck equation and that other diffusion laws can be trivially derived from it.

How far are the randomly perturbed paths deviated from the optimal paths? How different are Eqs.(15) from Eqs.(1)? This question can be answered, under different angles, by the standard deviation of action $\langle\Delta A\rangle^2 = \langle A^2\rangle - \langle A\rangle^2 = \langle A^2\rangle - \langle A_{ab}\rangle^2 = -\frac{\partial\langle A_{ab}\rangle}{\partial\eta}$, of position $\langle\Delta x\rangle^2 = \langle x^2\rangle - \langle x\rangle^2$, of

momentum $\langle \Delta P \rangle^2 = \langle P^2 \rangle - \langle P \rangle^2$ and of Hamiltonian $\langle \Delta H \rangle^2 = \langle H^2 \rangle - \langle H \rangle^2$. Using the formula below¹, we obtain

$$\langle x \rangle = -\frac{F\delta t^2}{2m}, \quad (19)$$

$$\langle P \rangle = -\frac{F\delta t}{2}, \quad (20)$$

$$\langle x^2 \rangle = \frac{\delta t}{m\eta} + \frac{F^2\delta t^4}{4m^2}, \quad (21)$$

and

$$\langle P^2 \rangle = \frac{m}{\delta t\eta} + \frac{F^2\delta t^2}{4}. \quad (22)$$

This means

$$\langle \Delta x^2 \rangle = \frac{\delta t}{m\eta} \quad (23)$$

and

$$\langle \Delta P^2 \rangle = \frac{m}{\delta t\eta}. \quad (24)$$

Cancelling the time δt and m in the above two equations, we get a “classical uncertainty relation” for irregular dynamics

$$\langle \Delta x^2 \rangle \langle \Delta P^2 \rangle = \frac{1}{\eta^2}. \quad (25)$$

Notice that this is only a asymptotic relation for $\delta t \rightarrow 0$. For a measurable (longer) length of time and path, we divide them into small segments of the order of δt and δx . Eq.(25) should be valid for each segment. Thus it can be trivially proven that the total deviation $\langle \Delta \rangle^2$ of whatever quantity on a path

¹ $\int_{-\infty}^{\infty} dx \exp(-\alpha x^2 + 2\gamma x) = \exp(\gamma^2/\alpha) \sqrt{\frac{\pi}{\alpha}}$ and $\int_{-\infty}^{\infty} x^n dx \exp(-\alpha x^2 + 2\gamma x) = \frac{1}{2^{n-1}\alpha} \sqrt{\frac{\pi}{\alpha}} \frac{d^{n-1}}{d\gamma^{n-1}} [\gamma \exp(\gamma^2/\alpha)]$.

is a sum of all the deviations on its small segments (Gaussian law of errors, see for example [6]). So in general, we must write

$$\langle \Delta x \rangle^2 \langle \Delta P \rangle^2 \geq \frac{1}{\eta^2} \quad (26)$$

which is valid for any period of time and path length. If the system is in rotation with $\delta x/R = \delta\theta$ where θ is the rotation angle and $1/R$ the curvature of δx , then we get

$$\langle \Delta\theta \rangle^2 \langle \Delta J \rangle^2 \geq \frac{1}{\eta^2}, \quad (27)$$

where J is the angular momentum.

The action uncertainty can be calculated from Eqs.(8) and (18) :

$$\langle A_{ab} \rangle = \frac{1}{2\eta} - \frac{F^2 \delta t^3}{8m} \quad (28)$$

so that

$$\begin{aligned} \langle \Delta A \rangle^2 &= -\frac{\partial \langle A_{ab} \rangle}{\partial \eta} \\ &= \frac{1}{2\eta^2}. \end{aligned} \quad (29)$$

This relation can be written as $\langle \Delta L \rangle^2 \langle \delta t \rangle^2 = \frac{1}{2\eta^2}$ where $\langle \Delta L \rangle^2 = \langle L^2 \rangle - \langle L \rangle^2$ is the standard deviation of Lagrangian. For arbitrary time and path length, we must write

$$\langle \Delta A \rangle^2 \geq \frac{1}{2\eta^2}. \quad (30)$$

and

$$\langle \Delta L \rangle^2 \langle \Delta t \rangle^2 \geq \frac{1}{2\eta^2} \quad (31)$$

where $\langle \Delta t \rangle^2 = \langle t^2 \rangle - \langle t \rangle^2$ is the standard deviation of time measure. Eq.(31) can be verified in the same way as for position and momentum, through the calculation of $\langle t \rangle$ and $\langle t^2 \rangle$ with the distribution Eq.(17) in relaxing δt and fixing δx .

Now let $H(t)$ be the Hamiltonian on the considered path segment at moment t , we have the Legendre transformation $H(t) = P\dot{x} - L(t)$. Considering $L = E - U$ and $E = P\dot{x}/2$, we get

$$\langle \Delta H \rangle^2 = \langle \Delta L \rangle^2 + 4(\langle EU \rangle - \langle E \rangle \langle U \rangle). \quad (32)$$

E and U are two independent variable, so $\langle EU \rangle = \langle E \rangle \langle U \rangle$, we obtain

$$\langle \Delta H \rangle^2 = \langle \Delta L \rangle^2 \quad (33)$$

and

$$\langle \Delta H \rangle^2 \langle \Delta t \rangle^2 \geq \frac{1}{2\eta^2}. \quad (34)$$

Before giving an interpretation of these non quantum uncertainty relations of irregular dynamics, i.e., Eq.(26), Eq.(27), Eq.(30), Eq.(31) and Eq.(34), we would like to indicate two points. First, it seems that Eq.(30), the action uncertainty relation, is the most essential one because it tell us the spread of the action distribution and the deviation of the extended action principle $\langle \delta A \rangle = 0$ from the conventional one $\delta A = 0$. The other relations concerns the conjugate variables of action and can be a priori derived from action uncertainty. Second, the coefficient η plays a central role in this description of the dynamics. Roughly speaking, $\eta \rightarrow 0$ represents large deviation of the perturbed dynamics from the regular one (large uncertainty), large η represents small random perturbation and deviation (small uncertainty), and $\eta \rightarrow \infty$ implies vanishing perturbation and convergence of irregular dynamics to regular one (zero uncertainty).

A quantitative relationship between the uncertainty and thermal noise can be shown with a special example, Brownian motion ($F = 0$) with diffusion constant $D = \mu k_B T$ [6], where μ is the mobility of the particles, k_B is the Boltzmann constant and T the temperature. Here we see a relationship between η and temperature characterizing the thermal noise: $\eta = \frac{1}{2m\mu k_B T} = \frac{\gamma}{2k_B T}$ where $m\gamma$ is the friction coefficient. In this case, we can write, for example,

$$\langle \Delta x \rangle \langle \Delta P \rangle \geq 2k_B T / \gamma, \quad (35)$$

which implies that the paths may be distributed very widely in phase space around the optimal (least action) paths at high temperature.

5 Concluding remarks

We have briefly presented an information-action method for stochastic dynamics of hamiltonian systems. We see that in this approach the Euler-Lagrange equations, the Hamiltonian equations and the action principle only hold in averaged form over the ensemble of all the possible paths between two state points. The main result of this paper is to show that some uncertainty relations, very similar to those in quantum mechanics, exist for stochastic dynamics of hamiltonian systems.

We are in the realm of classical physics, no quantum effect is considered. There is normally the consensus that exact value of position and speed can be a priori assigned to a particle (consensus contested by an interpretation of quantum mechanics). Then how to understand the uncertainty relations in classical dynamics? A plausible understanding is that $\langle \Delta A \rangle \geq \frac{1}{\sqrt{2}\eta}$ implies the distribution of action cannot be arbitrarily narrow, or the fluctuation of action has a minimum depending on the random perturbation. $\langle \Delta x \rangle \langle \Delta P \rangle \geq \frac{1}{\eta}$ means that the fluctuations or the distributions of position and momentum cannot be arbitrarily narrow simultaneously. It has no meaning about the precision of the measure, because we know that a classical body does have exact position and speed and that the means $\langle x \rangle$ and $\langle P \rangle$ can be made arbitrarily close to the real values of the body whatever the fluctuation $\langle \Delta x \rangle$ and $\langle \Delta P \rangle$ of the separately measured values.

We would like to indicate that the above results have been obtained by using the mechanical Lagrangian and action. Nevertheless, as mentioned above, the same conclusions can be reached with other action functionals and Lagrangians. It can be trivially shown that similar uncertainty relations can be derived with, e.g., Onsager-Machlup Lagrangian $L_{OM} = (\dot{x} - \mu F)^2$ [3, 5] and Freidlin-Wentzell Lagrangian $L_{OM} = [\dot{\varphi} - b(\varphi)]^2$ where $\dot{\varphi} = b(\varphi)$ is the differential equation of some continuous function φ of paths when the perturbation vanishes[8]. If the Lagrangians do not have mechanistic interpretation, the uncertainty relations should be understood differently depending on the physical content of the variables.

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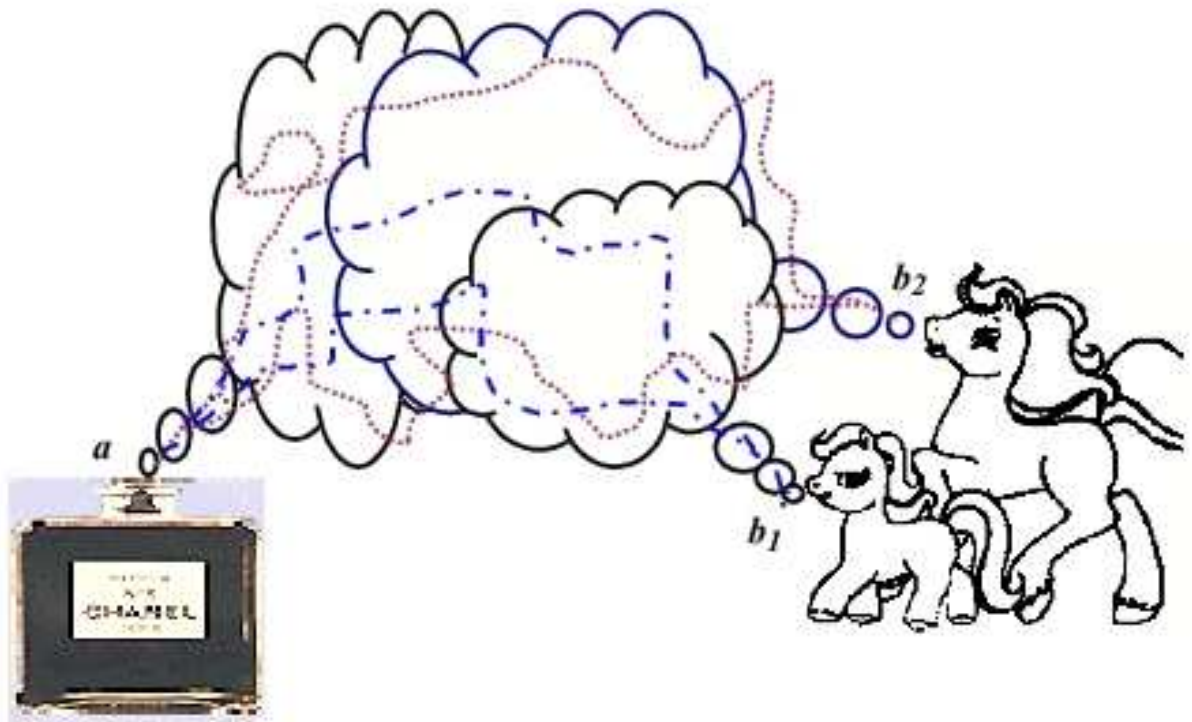


Figure 1: An example of random dynamics: the diffusion of scent. At time t_a , the molecules of the perfume get out of the bottle at point a . At time t_b , the molecules arrive at different points b_i ($i = 1, 2, \dots$) (first dynamical uncertainty) so the two ponies smell the scent at the moment. For a pony putting his nose at a given point b , all the molecules it receives at time t_b may arrive there via different paths (second dynamical uncertainty). Obviously, as shown by the dotted lines in the figure, the second uncertainty cannot take place without the first one.