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Abstract

After the work showing that the maximum entropy principle for equilibrium mechanical system is a consequence of the principle of virtual work, i.e., the virtual work of random forces on a mechanical system should vanish in thermodynamic equilibrium, we present in this paper an extension of that principle to dynamical systems out of equilibrium. The objective of the present work is to justify a least action principle and the concurrent maximum path entropy principle for mechanical systems in random motion.

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1) Introduction

The least action principle[1] first developed by Maupertuis[1][2] is originally formulated for regular dynamics of mechanical system. What is the fate of the principle when the system is perturbed by noise such that the dynamics becomes irregular and stochastic? There have been many efforts to answer this question. One can count Onsager[3] and De Broglie[4] among the first scientists who were interested in developing least action principle or its analog for random dynamics. Other efforts have also been made in the fields such as random dynamics[5][6], stochastic mechanics[7][8], quantum theory[9] and quantum gravity theory[10]. Recently, a new extension of the Maupertuis principle using the Lagrange action (see definition below) was suggested fort describing stochastic motion in a mean way[11]. The new ingredient in this approach is the introduction of informational entropy or probabilistic uncertainty in the variational calculus. This leads to a so called stochastic least action principle given by

$$\overline{\delta A} = 0 \qquad (1)$$

where A is the Lagrange action and the $\overline{\delta A}$ its variation averaged over all the possible paths between two points a and b in configuration space. When there is vanishing perturbation, this variation becomes the usual principle $\delta A = 0$. Eq.(1) is equivalent to a maximization of path entropy S_{ab} defined by $\delta S_{ab} = \eta \left(\delta \overline{A} - \overline{\delta A} \right)$.

This formalism seems not so strange and quite encouraging in many points. It has a diffusion probability in exponential of action. For free diffusing particles, this is the transition probability of Brown motion. For particles in a potential energy, the diffusion probability satisfies the Fokker-Planck equation of diffusion[11]. Questions have been asked about Eq.(1). For instance, why one use $\overline{\delta A} = 0$ instead of $\delta \overline{A} = 0$? Why the path entropy S_{ab} is defined as mentioned above? What is the physics making it maximal for the correct path probability distribution of action? In this work, we try to answer these questions on the basis of a fundamental principle of mechanics, the principle of virtual work [12][13].

We look at mechanical systems out of equilibrium. So the term “entropy” is used as a measure of uncertainty or randomness of stochastic motion. The first law and the second law of thermodynamics will be used formally to define a generalized “heat” as a measure of

[1] We continue to use the term "least action principle" here considering its popularity in the scientific community. We know nowadays that the term "optimal action" is more suitable because the action of a mechanical system can have a maximum, or a minimum, or a stationary for real paths[14].

uncertainty. It will be indicated if we use entropy in the sense of equilibrium thermodynamics. In what follows, we first recall the least action principle of Maupertuis and the principle of virtual work. Then we present a derivation of Eq.(1) from these principles.

2) Principle of least action

The least action principle is well formulated for non-dissipative Hamiltonian system satisfying following equations [2]:

$$\dot{x}_k = \frac{\partial H}{\partial P_k} \text{ and } \dot{P}_k = -\frac{\partial H}{\partial x_k} \text{ with } k=1,2, \ldots g \tag{2}$$

where x_k is the coordinates, P_k the momentum, H the Hamiltonian given by $H = T + V$, T the kinetic energy, V the potential energy, and g the number of degrees of freedom of the system.

The least action principle stipulates that the action of a motion between two point a and b in the configuration space defined by the time integral $A = \int_a^b L dt$ on a given path from a to b must be a stationary on the unique true path for given period of time τ of the motion between the two points, i.e.,

$$\delta A\big|_\tau = 0 \tag{3}$$

where the Lagrangian is defined by the $L = T - V$. In what follows, we will drop the index τ of the variation and the action variation is always calculated for fixed period of time τ. This principle yield the famous Lagrange-Euler equation given by

$$\frac{\partial}{\partial t}\frac{\partial L}{\partial \dot{x}_k} - \frac{\partial L}{\partial x_k} = 0 \tag{4}$$

and underlies a completely deterministic character of dynamic process ($\dot{x}_k = \frac{\partial x_k}{\partial t}$). Eq.(3) says that if the time period of the motion is given, there is only one path between two given points with all states of the systems completely determined by Eq.(4) for any moment of the motion. This uniqueness does not exist any more when the motion becomes random and stochastic[11]. This is the physical situation we encounter in the case of thermodynamic systems either in equilibrium or out of equilibrium.

3) Principle of virtual work

In mechanics, a virtual displacement of a system is a kind of hypothetical infinitesimal displacement with no time passage and no influence on the forces. It should be perpendicular to the constraint forces. The principle of virtual work says that the total work done by all forces acting on a system in static equilibrium is zero for any possible virtual displacement. Let us suppose the simple case of a particle in equilibrium under n forces F_i (i=1,2,…n) and a virtual displacement $\delta\vec{r}$, the principle stipulates

$$\delta W = \sum_{i=1}^{n} \vec{F}_i \cdot \delta\vec{r} = 0 \tag{5}$$

This principle for statics has been extended to dynamics by D'Alembert in the Lagrange-d'Alembert principle given by

$$\delta W = \sum_{i=1}^{n} (\vec{F}_i - m\vec{a}_i) \cdot \delta\vec{r} = 0 \tag{6}$$

where m is the mass and $\vec{a}_i$ the acceleration of the particle due to $\vec{F}_i$. Eqs.(5) et (6) are two of the most basic principles of classical mechanics.

For the stochastic dynamics mechanical systems in thermodynamic equilibrium, with the help of the first law and the second law, we have shown that[15]

$$\delta W = \delta\left(S + \alpha \sum_{j=0}^{w} p_j - \beta \sum_{j=0}^{w} p_j E_j\right) \tag{7}$$

where S is the entropy of the second law, p_j the probability that the system is found at the state j and E_j the energy of the state j. Eq.(7) implies that the virtual work of random forces corresponds to a variation of thermodynamic entropy under two constraints associated with the normalization and the mean energy, respectively. α and β are two Lagrange multipliers. If we apply the principle of virtual work Eq.(5), it follows that

$$\delta\left(S + \alpha \sum_{j=0}^{w} p_j - \beta \sum_{j=0}^{w} p_j E_j\right) = 0 \tag{8}$$

which is nothing but the Jaynes principle of maximum entropy[15].

4) Stochastic least action principle

Now let us consider a nonequilibrium mechanical system composed of an ensemble of particles moving in the configuration space starting from a point *a*. If the motion was regular, all the particles would follow a same trajectory from *a* to a given point *b* according to the least action principle. But if there are random forces perturbing the motion, the particles will take different paths to go to all the possible final positions allowed by the constraints. Suppose there are *N* particles arriving at point *b* by different paths linking *a* and *b*. At each moment of time, there are two kind of forces acting on a given particle of number *i*. One is the total conservative force $\vec{F}_i=-\nabla V$, another is the random force $\vec{R}_i$. In the sense of the D'Alembert extension, the total virtual work at any moment of time on a virtual displacement $\delta\vec{r}_i$ of the particle *i* should be

$$\delta W_i=(\vec{F}_i-m\vec{a}_i+\vec{R}_i)\cdot\delta\vec{r}_i \tag{9}$$

where $\vec{a}_i=(\vec{F}_i+\vec{R}_i)/m$ is the total acceleration of the particle. Remember that we are looking at an ensemble of nonequilibrium systems on their way from *a* to *b*, and some of them are not on the least action path. So the Lagrange-D'Alembert principle does not apply to all the particles, i.e., Eq.(9) does not vanish in general.

In order to overcome this difficulty, the following reasoning of virtual work will be based on the ensemble of the trajectories instead of a configuration point, i.e., the virtual displacement $\delta\vec{r}_i$ on a point will be replaced by an ensemble of point displacements forming a virtual deformation of the trajectory on a small time interval *dt*. $\delta W_i=(\vec{F}_i-m\vec{a}_i+\vec{R}_i)\cdot\delta\vec{r}_i$ is interpreted now as the virtual work on the particle *i* during *dt*. So the mean virtual work on the particle *i* from *a* to *b* can be written as

$$W_i=\frac{1}{\tau}\int_a^b dW_i dt=\frac{1}{\tau}\int_a^b(\vec{F}_i-m\vec{a}_i+\vec{R}_i)\cdot\delta\vec{r}_i\, dt\,. \tag{10}$$

Finally, the total virtual work on all the *N* particles

$$W=\sum_{i=1}^{N}W_i=\frac{1}{\tau}\sum_{i=1}^{N}\int_a^b(\vec{F}_i-m\vec{a}_i+\vec{R}_i)\cdot\delta\vec{r}_i\, dt\,. \tag{11}$$

which will be written below in terms of paths. Without loss of generality, the following discussion will be made with discrete paths denoted by *j*=1,2 … *w* (if the variation of path is continuous, the sum over j should be replaced by the path integral[9]). By using p_j as the probability that the path j is taken by the particles from a to b, Eq.(11) can be given by

$$W = \frac{1}{\tau}\sum_{j=1}^{w} p_j \int_a^b (\vec{F}_j - m\vec{a}_j + \vec{R}_j)\cdot \delta\vec{r}_j \, dt \,. \tag{12}$$

In what follows, for the sake of simplicity, we consider only one degree of freedom in Eq.(12), say x. The total virtual work is

$$W = \sum_{j=1}^{w} p_j \int_a^b (F_{xj} - m\ddot{x}_j + R_{xj})\,\delta x_j \, dt = \sum_{j=1}^{w} p_j \int_a^b (-\frac{\partial H}{\partial x_j} - \dot{P}_{xj})\,\delta x_j \, dt \tag{13}$$

$$= \sum_{j=1}^{w} p_j \int_a^b \left[\frac{\partial L}{\partial x_j} - \frac{\partial}{\partial t}\left(\frac{\partial L}{\partial \dot{x}}\right)\right]\delta x_j \, dt = \sum_{j=1}^{w} p_j \int_a^b (\frac{\partial L}{\partial x_j}\delta x_j + \left(\frac{\partial L}{\partial \dot{x}}\right)\delta\dot{x}_j) dt = \sum_{j=1}^{w} p_j \,\delta \int_a^b L_j \, dt = \overline{\delta}$$

.

where we used $F_{xj} + R_{xj} = -\frac{\partial H}{\partial x_j} = \frac{\partial L}{\partial x_j}$, $m\ddot{x}_j = \dot{P}_{xj} = \frac{\partial}{\partial t}\left(\frac{\partial L}{\partial \dot{x}}\right)$ and the integral $\int_a^b \frac{\partial}{\partial t}\left(\delta x_j \frac{\partial L}{\partial \dot{x}}\right) = \left(\delta x_j \frac{\partial L}{\partial \dot{x}}\right)_a^b = 0$ due to the zero variation at a and b.

Now we will make an extension of the Lagrange-D'Alembert principle, which is no more valid for single path, to the total virtual work W on the ensemble of particles moving between a and b, i.e., $W = 0$. This is equivalent to say that there is no work on the ensemble of particles. In other words, a Hamiltonian system will statistically remains Hamiltonian. This condition is crucial for the present work, because the least action principle, originally formulated for conservative system, can be used here in a mean way over an ensemble of systems. If the mean Hamiltonian is given by $H = \overline{T} + \overline{V}$ and the mean Lagrangian by $L = \overline{T} - \overline{V}$ where $\overline{T}$ is the means kinetic energy and $\overline{V}$ the potential one, the Lagrangian action on a given path is given by $A = \int_a^b L dt$ as defined in the Lagrangian mechanics.

Considering Eq.**(13)**, this generalization of Lagrange-D'Alembert principle implies

$$\overline{\delta A} = 0 \,. \tag{14}$$

This is the stochastic least action principle.

5) Maximum path entropy principle

Eq.(14) underlies an entropy variational approach. To see this, we calculate

$$\begin{aligned}\overline{\delta A} &= \sum_{j=1}^{w} p_j \delta A_j \\ &= \delta \sum_{j=1}^{w} p_j A_j - \sum_{j=1}^{w} \delta p_j A_j \\ &= \delta \overline{A} - \delta Q_{ab}\end{aligned} \tag{15}$$

where $\overline{A} = \sum_{j=1}^{w} p_j \delta A_j$ is the ensemble mean of action A_j, and δQ_{ab} is defined by

$$\delta Q_{ab} = \delta \overline{A} - \overline{\delta A}. \tag{16}$$

Eq. (16) is a definition of entropy as a measure of uncertainty of random variable (action in the present case). It mimics the first law of thermodynamics $dQ = d\overline{E} - \overline{dE}$ where $\overline{E} = \sum_i p_i E_i$ is the average energy, E_i the energy of the state i with probability p_i, and $\overline{dE} = \sum_i p_i dE_i = -\sum_k \left(\sum_i p_i \frac{\partial E_i}{\partial x_k} \right) dx_k = -dW$ with dW the work of the forces $F_k = -(\sum_i p_i \frac{\partial E_i}{\partial x_k})$ on a displacement dx_k of the extensive variables x_k such as volume, surface, magnetic moment etc. Eq. (16**)** defines a generalized "heat" Q as a measure the randomness of action. If we introduce an 'inverse temperature' η such that

$$\delta Q_{ab} = \frac{\delta S_{ab}}{\eta}, \tag{17}$$

the stochastic action principle Eq.(14) and Eq.(15) give us

$$\delta(S_{ab} - \eta \overline{A}) = 0\,. \tag{18}$$

This is a variational calculus with the constraint related to average action $\overline{A}$. One can add the normalization condition as another constraint, Eq.(18) then becomes:

$$\delta[S_{ab} - \eta \sum_j p_j A_j + \alpha \sum_j p_j] = 0 \tag{19}$$

which is nothing but the usual Jaynes principle of maximum entropy applied to path entropy defined in Eqs.**(16)** and (17) with two Lagrange multipliers α and β. S_{ab} is a measure of the uncertainty of the probability distribution of action and has been investigated in a detailed way in reference [16].

6) Concluding remarks

Recently, it was shown that the maximum entropy principle for equilibrium mechanical system is a consequence of the principle of virtual work. This work is an extension of that result to dynamical systems out of equilibrium. For this purpose, we have generalized the Lagrange-D'Alembert principle of virtual work with point virtual displacement to the case of virtual deformation of trajectories. The objective is to justify a stochastic least action principle $\overline{\delta A}=0$ postulated previously for mechanical systems in random motion. The conclusion of the present work is that this stochastic action principle and the concurrent maximum path entropy principle are prescribed by the statistically vanishing virtual work of random forces on the ensemble of conservative dynamical systems in motion. The approach can be applied to many stationary diffusion processes in which the diffusing particles have statistically the same velocity in time even there is dissipation (in stationary Brownian motion or stationary electrical currant for instance). However, whether and when it is necessary to include dissipative effects and how to do it in the present variational approach to random dynamics are still matter of investigation.

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