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# Seeing maximum entropy from the principle of virtual work

Qiuping A. Wang

Institut Supérieur des Matériaux et Mécaniques Avancées du Mans,

44 Av. Bartholdi, 72000 Le Mans, France

## **Abstract**

We propose an application of the principle of virtual work of mechanics to random dynamics of mechanical systems. The total virtual work of the interacting forces and inertial forces on every particle of the system is calculated by considering the motion of each particle. Then according to the principle of Lagrange-d'Alembert for dynamical equilibrium, the vanishing virtual work gives rise to the thermodynamic equilibrium state with maximization of thermodynamic entropy with suitable constraints. This approach establishes a close relationship between the maximum entropy approach for statistical mechanics and a fundamental principle of mechanics, and constitutes an attempt to give the maximum entropy approach, considered by many as only an inference principle based on the subjectivity of probability and entropy, the status of fundamental physics law.

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## 1) Introduction

The principle of maximum entropy (maxent) is widely used in the statistical sciences and engineering as a powerful tool and fundamental rule. The maxent approach in statistical mechanics can be traced back to the works of Boltzmann and Gibbs[3] and finally be given the status of principle thanks to the work of Jaynes[4] who used it with Boltzmann-Gibbs-Shannon (BGS) entropy (see below) to derive the canonical probability distribution for statistical mechanics in a simple manner. However, in spite of its success and popularity, maxent has always been at the center of scientific and philosophical discussions and has raised many questions and controversies[4][5][6]. A central question is why a thermodynamic system chooses the equilibrium microstates such that the BGS entropy gets to maximum. As a basic assumption of scientific theory, maxent is not directly or indirectly related to observation and undoubted facts. In the literature, maxent is postulated as such or justified either a priori by the second laws with additional hypothesis such as the entropy functional (Boltzmann or Shannon entropy)[6], or a posteriori by the correctness of the probability distributions derived from it[4]. In statistical inference theory, it was often justified by intuitive arguments based on the subjectivity of probability[4] or by relating it to other principles such as the consistency requirement and the principle of insufficient reason of Laplace, which have been the object of considerable criticisms[5].

Another important question about maxent is whether or not the BGS entropy is unique as the measure of uncertainty or disorder that can be maximized in order to determine probability distributions. This was already an question raised 40 years ago by the scientists who tried to generalize the Shannon entropy by mathematical considerations [9][10]. Nowadays, the answer to this question becomes much more urgent and waited due to the controversy and debate surrounding the development of the statistical theories using maxent with different entropy functionals [11].

In the present work, we try to contribute to the debate around maxent by an attempt to derive maxent from a well known fundamental principle of classical mechanics, the virtual work principle or Lagrange-d'Alembert principle (LAP) [1][2] without additional hypotheses to LAP and about entropy property. LAP is widely used in physical sciences as well as in mechanical engineering. It is a basic principle capable of yielding all the basic laws of statics and of dynamics of mechanical systems. It is in addition a simple, clearly defined, easily understandable and palpable law of physics. It is hoped that this derivation is scientifically

and pedagogically beneficial for the understanding of maxent and of the relevant questions and controversies around it. In this work, the term entropy, denoted by  $S$ , is used in the sense of the second law of thermodynamics for equilibrium system.

The paper is organized as follows. In the first section, we recall the principle of virtual work before applying it to equilibrium thermodynamic system to derive maxent for the thermodynamic entropy of equilibrium state. Then we will briefly mention a previous result in order to show that other maximizable entropy functionals different from the BGS forms are possible even for equilibrium system.

## 2) Principle of virtual work

The variational calculus in mechanics has a long history which may be traced back to Galilei and other physicists of his time who studied the equilibrium problem of statics with LAP (or virtual displacement<sup>1</sup>). LAP gets unified and concise mathematical forms thanks to Lagrange[1] and d'Alembert[2] and is considered as a most basic principle of mechanics from which all the fundamental laws of statics and dynamics can be understood thoroughly.

LAP says that the total work done by all forces acting on a system in static equilibrium is zero on all possible virtual displacements which are consistent with the constraints of the system. Let us suppose a simple case of a system of  $N$  points of mass in equilibrium under the action of  $N$  forces  $\mathbf{F}_i$  ( $i=1,2,\dots,N$ ) with  $\mathbf{F}_i$  on the point  $i$ , and imagine virtual displacement of each point  $\delta\vec{r}_i$  for the point  $i$ . According to viwop, the virtual work  $\delta W$  of all the forces  $\mathbf{F}_i$  on all  $\delta\vec{r}_i$  cancels itself for static equilibrium, i.e.

$$\delta W = \sum_{i=1}^N \vec{F}_i \cdot \delta\vec{r}_i = 0 \quad (1)$$

This principle for statics was extended to dynamical equilibrium by d'Alembert[2] in the LAP by adding the initial force  $-m_i\vec{a}_i$  on each point:

$$\delta W = \sum_{i=1}^N (\vec{F}_i - m_i\vec{a}_i) \cdot \delta\vec{r}_i = 0 \quad (2)$$

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<sup>1</sup> In mechanics, the virtual displacement of a system is a kind of imaginary infinitesimal displacement with no time passage and no influence on the forces. It should be perpendicular to the constraint forces.

where  $m_i$  is the mass of the point  $i$  and  $\vec{a}_i$  its acceleration. From this principle, we can not only derive Newtonian equation of dynamics, but also other fundamental principles such as least action principle.

### 3) Why maximum thermodynamic entropy ?

We suppose that the mechanics laws are usable not only for mechanical system containing small number of particles in regular motion, but also for large number of particles in random and stochastic motion for which one has to use statistical approach introducing probability distribution of mechanical states. Let us first consider a canonical ensemble with *equilibrium* systems, each composed of  $N$  particles in random motion with  $\vec{v}_i$  the velocity of the particle  $i$ . It will be shown that the result for canonical ensemble can be easily extended to microcanonical ensemble and grand-canonical ensemble. Without loss of generality, let us look at a system without macroscopic motion, i.e.,  $\sum_{i=1}^N \vec{v}_i = 0$ .

We imagine that the system in thermodynamic equilibrium leaves the equilibrium state by a reversible infinitesimal virtual process. Let  $\vec{F}_i$  be the force on a particle  $i$  of the system at that moment.  $\vec{F}_i$  includes all the interacting forces particles-particles and particles-walls of the container. During the virtual process, each particle with acceleration  $\ddot{\vec{r}}_i$  has a virtual displacement  $\delta \vec{r}_i$ . The total virtual work on this displacement is given by

$$\delta W = \sum_{i=1}^N (\vec{F}_i - m\ddot{\vec{r}}_i) \cdot \delta \vec{r}_i \quad (3)$$

Although the sum of the accelerations of all the particles vanishes, i.e.,  $\sum_{i=1}^N m\ddot{\vec{r}}_i = 0$ , the

acceleration  $\ddot{\vec{r}}_i$  on each particle can be nonzero. So in general  $\sum_{i=1}^N m\ddot{\vec{r}}_i \cdot \delta \vec{r}_i \neq 0$ . As a matter of

fact, we have  $m\ddot{\vec{r}}_i \cdot \delta \vec{r}_i = m\dot{\delta \vec{r}}_i \cdot \dot{\vec{r}}_i = \delta(\frac{1}{2}m\dot{\vec{r}}_i^2) = \delta e_{ki}$  where  $e_{ki}$  is the kinetic energy of the

particle. On the other hand, we suppose there are no dissipative forces in the system or on the particles. It means that the energy of the system will not change if the system is completely closed and isolated. Let  $e_{pi}$  be the potential energy of a particle  $i$  subject to the force  $\vec{F}_i$ , we should have  $\vec{F}_i = -\nabla e_{pi}$  and

$$\sum_{i=1}^N \vec{F}_i \cdot \delta \vec{r}_i = \sum_{i=1}^N -\nabla_i e_i \cdot \delta \vec{r}_i = -\sum_{i=1}^N \delta e_{pi} \quad (4)$$

So finally it follows that

$$\delta W = -\sum_{i=1}^N (\delta e_{pi} + \delta e_{ki}) = -\sum_{i=1}^N \delta e_i \quad (5)$$

where  $\delta e_i$  is a virtual variation of the total energy  $e_i = e_{pi} + e_{ki}$  of the particle  $i$ .

At this stage, no statistics has been done. The particles are treated as if they had a regular dynamics. As a matter of fact, for a canonical system, the random dynamics can leads the  $N$  particles to different microstates  $j$  with different energy  $E_j$  and probability  $p_j$  ( $j=1,2 \dots w$ ). A microstate  $j$  is a distribution of the  $N$  particles over the one particle states  $k$  with energy  $\varepsilon_k$  where  $k$  varies from, say, 1 to  $g$ . For classical discernable particles,  $g$  can be very large and  $k$  undergoes continuous variation from 1 to  $g$ . We can imagine  $N$  identical particles distributed over the  $g$  states. A microstate  $j$  is a combination of  $g$  numbers  $n_k$  of particles over the  $g$  states, i.e.,  $j = \{n_1, n_2, \dots, n_g\}$ . For a given  $j$  with probability  $p_j$ , the virtual energy variation  $\delta E_j$  due

to the virtual work  $\delta W$  can be given by  $\delta E_j = \sum_{k=1}^g n_k \delta \varepsilon_k$  since a work does not affect the

population. Finally, the sum  $\sum_{i=1}^N \delta e_i$  of the energy variation of each particle can be written as

the statistical average (over different microstates  $j$ ) of the energy change  $\delta E_j$  of the system due to the virtual displacements, i.e.

$$\delta W = -\sum_{i=1}^N \delta e_i = -\sum_{j=1}^w p_j \delta E_j = -\overline{\delta E} \quad (6)$$

This is a well known relationship in statistical mechanics. Here we have derived it from the microscopic consideration of virtual work on each particle of the system. A simple calculation

shows that  $\sum_{j=1}^w p_j \delta E_j = \delta \sum_{j=1}^w p_j E_j - \sum_{j=1}^w E_j \delta p_j$  which means

$$\overline{\delta E} = -\delta W = \delta \bar{E} - \delta Q \quad (7)$$

where  $\bar{E} = \sum_{j=1}^w p_j E_j$  is the total average energy with a virtual change  $\delta \bar{E}$  and  $\delta Q = \sum_{j=1}^w E_j \delta p_j$  is

a virtual heat transfer. This is an expression of the first law of thermodynamics in the virtual

sense for canonical ensemble. If we consider a *reversible virtual process*, we have  $\delta Q = \frac{\delta S}{\beta}$  where  $\delta S$  is the infinitesimal virtual change of the thermodynamic entropy and  $\beta$  the inverse absolute temperature according to the second law of thermodynamics.

Now let us use LAP in Eq.(2), it follows that

$$\delta W = \frac{\delta S}{\beta} - \delta \bar{E} = 0. \quad (8)$$

Then we should add the constraint due to the normalization  $\sum_{j=0}^w p_j = 1$  into the variational expression with a Lagrange multiplier  $\alpha$ , the viwop in Eq.(8) becomes

$$\delta(S + \alpha \sum_{j=0}^w p_j - \beta \sum_{j=0}^w p_j E_j) = 0 \quad (9)$$

which is the variational calculus of maxent applied to thermodynamic entropy for canonical ensemble. Note that at this stage the entropy functional  $S(p_j)$  is not yet determined. Note that in Eq.(9), the average energy as a constraint for the maximization of entropy  $S$  is a natural consequence of LAP, in contrast to the introduction of this constraint in the inference theory or inferential statistical mechanics[4] by the argument that an averaged value of an observable quantity represents a factual information to be put into the maximization of information in order to derive unbiased probability distribution[5].

For microcanonical ensemble, the system is completely closed and isolated with constant energy so that  $\delta \bar{E} = 0$ . When the virtual displacements occur, the total virtual work would be transformed into virtual heat such that Eq.(7) becomes  $\delta W - \delta Q = 0$ . According to LAP  $\delta W = 0$ , Eq.(9) reads

$$\delta(S + \alpha \sum_{j=0}^w p_j) = 0 \quad (10)$$

which necessarily leads to uniform probability distribution over the different microstates  $j$ , i.e.,  $p_j = 1/w$  whatever is the form of the entropy  $S$ . Note that here the uniform distribution over the microstates is not an a priori assumption, but a consequence of LAP.

For grand-canonical ensemble, according to the first law  $\delta \bar{E} = \delta Q - \delta W + \mu \delta N$ , Eq.(7) should be  $\delta \bar{E} = \delta \bar{E} - \delta Q - \mu \delta N$ , where  $\mu$  is the chemical potential and  $N$  the average particle

number of the system given by  $N = \sum_{j=1}^w p_j N_j$  with  $N_j$  the particle number of the microstate  $j$ .

According to LAP, we have

$$\delta(S + \alpha \sum_{j=0}^w p_j - \beta \sum_{j=0}^w p_j E_j + \beta \mu \sum_{j=0}^w p_j N_j) = 0 \quad (11)$$

which is the usual calculus of maxent for grand-canonical ensemble.

The conclusion of this section is that, at thermodynamic equilibrium, the maxent under suitable constraints is a consequence of the equilibrium condition LAP of mechanical systems subject to random motion. From the above discussion, one notices that maxent can be written in a concise form such as

$$\overline{\delta E} = 0. \quad (12)$$

We stress that in the above derivation, the only essential assumptions or fundamental physical hypotheses used before the LAP are the first and second laws of thermodynamics for equilibrium system and reversible process. Hence the three derived expressions of maxent from Eg.(9) to (11) for the three statistical ensembles are in principle valid for all systems for which the first and second laws are valid, whatsoever is the form of the entropy  $S$ . The maximizable entropy form is an issue we will briefly discuss below.

#### 4) Maximizable entropy functionals

In general, the entropy functionals are given either as a first hypothesis or from physical or mathematical considerations about the entropy property. The standard approach in statistical mechanics is to use maxent for given entropy in order to derive the probability distribution. As a matter of fact, in the standard textbook, the only entropy form widely used in BGS is the Shannon entropy. This is in addition a claim of uniqueness of the Shannon entropy as maximizable entropy to be used in maxent[4]. Of course this uniqueness claim becomes questionable when other entropy forms are used with maxent for systems in equilibrium or out of equilibrium.

In order to contribute to this discussion and to see the possible entropy forms, we will inverse the reasoning of maxent which is to yield probability distributions by maximizing entropy. Here we will derive the entropy forms from known probability distribution by a definition of entropy implying maxent. This is possible thanks to the Eq.(7) which is nothing but



$$\delta S = \beta(\delta \overline{E} - \overline{\delta E}). \quad (13)$$

This is just the definition of thermodynamic entropy for reversible process of canonical system. Obviously, this definition entails maxent if  $\overline{\delta E} = 0$ . But before application of LAP or  $\overline{\delta E} = 0$ , let us write Eq.(13) as follows

$$\delta S = \beta \sum_{j=1}^w E_j \delta p_j \quad (14)$$

which will enable us to derive the entropy form directly from probability distribution.

It is well known that  $p_j \propto e^{-\beta E_j}$  is a well known and confirmed distribution of thermostatics for canonical ensemble. This distribution can be directly derived from the Maxwell velocity distribution of dilute gas if we suppose additivity of energy for the particles in the gas. As shown in many textbook, if  $p_j \propto e^{-\beta E_j}$ , it is easy to derive the Gibbs-Shannon entropy using Eq.(14) (with Boltzmann constant  $k_B=1$ ):

$$S = -\sum_{j=1}^w p_j \ln p_j \quad (15)$$

whose optimization by  $\overline{\delta E} = 0$  obviously gives  $p_j \propto e^{-\beta E_j}$ .

Another possible probability distribution for canonical system in thermodynamic equilibrium is  $p_j = \frac{1}{Z_a} [1 - a\beta E_j]^{\frac{1}{a}}$  derived for finite system in equilibrium with finite heat

bath where  $a = \frac{2}{3N_2 - 2}$  and  $N_2$  is the particle number of the heat bath[7]. It was proved[8]

that the entropy defined by Eq.(13) is the Tsallis one  $S_q = -\frac{\sum_j p_j^{1+q} - 1}{q} = -\sum_j \frac{p_j - p_j^q}{1-q}$  where

$q=1+a$  and  $\sum_j p_j = 1$ . Obviously, when  $N_2$  is very large (a thermodynamic limit),  $a$  tends to 0

or  $q$  tends to 1. In this case,  $S_q$  becomes the Shannon one and the probability distribution

becomes exponential. The maxent applied to  $S_q$  naturally gives  $p_j = \frac{1}{Z_a} [1 - a\beta E_j]^{\frac{1}{a}}$ . This

means that the Shannon entropy form as maximizable one is non unique and subject to the condition such as additivity and thermodynamic limit in this investigation.

As a mathematical study, we have tried to see other maximizable entropy forms with other probability distributions[8]. In this case, the entropy, as a generic measure of probabilistic uncertainty (not only the thermodynamic entropy), is defined by  $\delta S = \beta(\delta \bar{x} - \bar{\delta x})$  where  $x$  is a random variable of a probability distribution  $p(x_j)$  and  $\beta$  is a generic parameter. We have

obtained the maximizable entropies  $S_\gamma = \frac{\sum_j p_j^{1-1/\gamma} - 1}{1-1/\gamma}$  for the distribution  $p_j = \frac{1}{Z} x_j^{-\gamma}$  (Zipf

law or large  $x_j$  Lévy flight), and  $S_\kappa = -\frac{1}{2\kappa} \sum_j \left( \frac{p_j^{1+\kappa}}{1+\kappa} - \frac{p_j^{1-\kappa}}{1-\kappa} \right)$  for  $p_j = \left( \sqrt{1+\kappa^2 x_j^2} + \kappa x_j \right)^{1/\kappa}$  for

the  $\kappa$ -statistics[12].

## 5) Concluding remarks

This work shows that the maximum entropy principle has a close connection with the fundamental principle of classical mechanics, the principle of virtual work, i.e., for a mechanical system to be in thermodynamics equilibrium with maximum entropy, the total virtual work of all the forces on all the elements (particles) of the system should vanish. Indeed, if one admits that thermodynamic entropy is a measure of dynamical disorder and randomness, it is natural to say that this disorder must get to maximum in order that all the random forces act on each degree of freedom of the motion in such a way that over any possible (virtual) displacement, the work of all the forces is zero. In other words, this vanishing work can be obtained if and only if the randomness of the forces is at maximum over all degree of freedom allowed by the constraints to get stable equilibrium state.

To our opinion, the present result is helpful not only for the understanding of maxent derived from a more basic and well understood mechanical principle, it also shows that entropy in physics is not necessarily a subjective quantity reaching maximum for correct inference, and that maximum entropy is a law of physics but not merely an inference principle.

After finishing this paper, the author became aware of the works of Plastino and Curado[13] on the equivalence between the particular thermodynamic relation  $\delta S = \beta \delta \bar{E}$  and maxent in the derivation of probability distribution. They consider the particular thermodynamic process affecting only the microstate population in order to find a different way from maxent to derive probability. The work part is not considered in their work. Their analysis is pertinent and consequential. The present work provides a substantial support of their reasoning from a basic principle of mechanics.

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