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# Why entropy tends to maximum?

Qiuping A. Wang

Institut Supérieur des Matériaux et Mécaniques Avancées du Mans,

44 Av. Bartholdi, 72000 Le Mans, France

## **Abstract**

It is argued that the maximum entropy is a requirement of the conventional mechanical equilibrium condition, i.e., the total virtual work of all the forces including random forces on all the elements (particles) of a mechanical system should vanish for the systems to stay in thermodynamic equilibrium. This is an attempt to give the maximum entropy principle, considered by many as only an inference principle based on a subjective quantity such as entropy, the status of a fundamental physics law.

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## 1) Introduction

Why does entropy always get its maximum for stable probability distributions?

The present work is an effort to answer this question in connection with a mechanical variational principle, the principle of virtual work[1][2]. Except the case of equilibrium thermodynamics where entropy is used in the sense of the second law of thermodynamics, we generally use the term entropy as a measure of uncertainty or randomness of stochastic motion.

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 the principle of virtual work (or virtual displacement<sup>1</sup>) which is given unified and concise mathematical forms by Lagrange[1] and D'Alambert[2]. This principle is considered as a most basic one of mechanics from which the fundamental laws of statics and dynamics can be understood thoroughly.

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 physical principle thanks to the work of Jaynes[4][5]. In contrary to the mechanical variational principles which are widely accepted and applied in physics with almost no opposition, the entropy variation approaches, often discussed in relation with the second law of thermodynamics, have raised many questions and controversies in the past[4][5]. Nowadays, although the scientists and engineers widely and successfully use the maxent principle in statistical sciences as a useful inference calculus, the underlying question why entropy and disorder always get their maximal value for stable probability distribution and correct inference results is still open.

It is helpful to recall certain famous arguments supporting maxent advanced by Jaynes, who thought that information and entropy were subjective quantity dependent on observers. So maxent is only a method of guess or inference but not deduction method of mechanics[4][5]. He argued that "if a system is in a state with lower entropy it would contain more information than previously specified", or that "higher entropy states are more probable" and "less predictable". Entropy and information are only anthropomorphic, but not objective quantities involved in fundamental laws of physics.

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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.

In the present work, we will try to eliminate plausible argument related to intuition and common sense and base our self on the physical laws of mechanical systems. Si this work is limited to mechanical systems and based on the first and second laws of thermodynamics. In what follows, we first recall the principle of virtual work before applying it to equilibrium thermodynamic system to discuss the maxent principle. We also try to extend some results of this work to non thermodynamic systems. In this case, the first law is used to define a generalized “heat” as a measure of uncertainty and disorder.

## 2) Principle of virtual work

The principle of virtual work 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 particle in equilibrium under  $n$  forces  $F_i$  ( $i=1,2,\dots,w$ ), we have  $\sum_{i=1}^n \vec{F}_i = 0$ , and imagine a small displacement  $\delta\vec{r}$  of the particle, the principle stipulates

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

This principle for statics was extended to dynamics by D’Alembert[2] in the Lagrange-d’Alembert principle given by

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

where  $m$  is the mass and  $\vec{a}$  the acceleration of the particle. This is the necessary and sufficient conditions for dynamical systems to move according to Newtonian equation.

## 3) Why maximum thermodynamic entropy?

Now let us consider a mechanical system composed of  $N$  particles in random motion. Without losing generality, suppose the system in equilibrium has no macroscopic motion, hence the total velocity is constant, i.e.,  $\sum_{i=1}^N \vec{v}_i = 0$ .

Let  $\vec{f}_i$  be the total force on each particle of the system. This is the sum of all forces including the external forces and the random internal forces. Imagine a virtual displacement  $\delta\vec{r}_i$  for each particle at a given time, the total dynamical virtual work is given by

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

However, due to the zero total velocity, the sum of the acceleration of all the particles vanishes. We finally get

$$\delta W = \sum_{i=1}^N \vec{f}_i \cdot \delta\vec{r}_i \quad (4)$$

At this stage, remember that the force  $\vec{f}_i$  is the total one on the particle  $i$  and can be given by the gradient of the energy of the particle, i.e.,  $\vec{f}_i = -\nabla_i e_i$ .

$$\delta W = -\sum_{i=1}^N \nabla_i e_i \cdot \delta\vec{r}_i = -\sum_{i=1}^N \delta e_i. \quad (5)$$

Now let us consider the microstates of the total system. Suppose  $p_j$  is the probability that the system is at the microstate  $j$  with total energy  $E_j$ , and there are  $w$  microstates, the above sum of energy variation of each particle can be written as an average (over different microstates) of the energy change of the total system at the time of the virtual displacements, i.e.

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

Considering the first law of thermodynamics in the virtual sense and imagine a virtual heat transfer  $\delta Q$  and a virtual variation  $\overline{\delta E}$  of internal energy  $\overline{E} = \sum_{j=1}^w p_j E_j$ , we can write

$$\overline{\delta E} = \delta Q + \delta W = \delta Q + \overline{\delta E}. \quad (7)$$

where  $\delta Q = \frac{\delta S}{\beta}$  and  $S$  is the equilibrium thermodynamic entropy and  $\beta$  is the inverse absolute temperature according to the second law of thermodynamics. From the Lagrange-D'Alembert principle in Eq.(2), we straightforwardly write Eq.(7) into

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

If we add the constraint due to the normalization  $\sum_{j=0}^w p_j = 1$  with a Langrange multiplier  $\alpha$ , we finally obtain

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

which is nothing but the variational calculus using entropy, i.e., the maxent principle of Jaynes applied to thermodynamic entropy for canonical ensemble.

For microcanonical, the internal energy is constant, i.e.,  $\delta \bar{E} = 0$ , hence we only have

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

The conclusion of this section is that, at thermodynamic equilibrium, the maximum entropy under appropriate constraints is a consequence of the equilibrium condition of mechanical systems subject to the random motion. This result is helpful to understand the maxent principle which is so important in statistical mechanics and other statistical sciences. From the above discussion, one notices that the maxent principle can be written in a concise form such as

$$\overline{\delta E} = 0. \quad (11)$$

#### 4) Why Boltzmann-Gibbs-Shannon entropy?

Let us write Eq.(7) as

$$\delta Q = \delta \bar{E} - \overline{\delta E}. \quad (12)$$

It is easy to calculate

$$\delta S = \beta \sum_{j=1}^w E_j \delta p_j \quad (13)$$

This equation makes it possible to calculate the entropy as a function of probability directly from known probability distribution. Take the example of ideal gas. It is a well known and experimentally observed fact that a particle in an ideal gas has exponential probability distribution of its energy  $p(e) \propto e^{-e/T}$ . If one assumes additive energy, the total energy of the gas will be the sum of the one particle energy. This means that the probability distribution of

state of the gas must be also exponential function of the total energy, i.e.,  $p_j \propto e^{-E_j/T}$  (let the Boltzmann constant  $k_B$  be unity). Normalize this probability and put it into Eq.(13), one obtain easily

$$S = -\sum_{j=1}^w p_j \ln p_j \quad (14)$$

which is Gibbs-Shannon entropy and becomes Boltzmann entropy  $S = \ln w$  for microcanonical ensemble for which all states  $j$  are equally probable with  $p_j = \frac{1}{w}$ .

### 5) Whether other entropy?

The above calculation is trivial and can be found in many textbooks. It shows obviously that the validity of the above derivation of Boltzmann-Gibbs-Shannon entropy is subject to many constraints (exponential probability and additivity of random variables for composite systems). With different conditions, the derivation may give different entropy forms. The question is what probability we have to choose for this derivation. First, it should not be forgotten that it concerns equilibrium systems. Second, we need probabilities which are scientifically sound, i.e., either experimentally observed or theoretically derived. Here is an example with small mechanical system.

We know that a small system without thermodynamic limit in volume or particle number is much more complex than large systems. Its energy may not be additive and extensive due to interaction and boundary effects. As a matter of fact, a large system can also show small system behavior (nonadditivity of energy for instance) if there are long range interaction or correlation in it. Even one assume additive energy for a small system as did Terletskii[7], one find

$$p_j = \frac{1}{Z_a} [1 - a\beta E_j]_a^{-1} \quad (15)$$

for the microstate  $j$  of the small system in equilibrium with a heat bath containing  $N$  particles, where  $a$  tends to zero if  $N$  is large, i.e.,  $p_j \xrightarrow{a \rightarrow 0} \frac{1}{Z_0} e^{-\beta E_j}$  with  $Z_a = \sum_j [1 - a\beta E_j]_a^{-1}$ . In a previous work [8], we have shown that the entropy defined by Eq.(12) could be given by Tsallis entropy

$$I = -\frac{\sum_j p_j^{1+a} - 1}{a} = -\sum_j \frac{p_j - p_j^q}{1-q} \quad (16)$$

where  $q=1+a$  and  $\sum_j p_j = 1$ .

As a matter of fact, small system effect (or small world effect) often occurs in non thermodynamic systems such as, among others, complex networks being often in equilibrium topological structures and showing power law degree distribution. Here the correlated elements may be separated far from each other in configuration space, much like the case of mechanical system with elements separated at large distance but in interaction (gravitation for instance). For this kind of systems, the entropy defined in Eq.(12) can take other functional forms such as

$S = \frac{\sum_j p_j^{1-1/a} - 1}{1-1/a}$  for Zipf distribution law  $p_j = \frac{1}{Z} x_j^{-a}$  of random variable  $x_j$  [8]. Obviously this

entropy does not have the same physical content as the thermodynamic entropy because the random variable is not energy. It is a measure of random uncertainty and disorder as defined by Eq.(12). The fact that this definition can lead to thermodynamic entropy means that this disorder measure coincides with the thermodynamic entropy when the random variable is energy. In reference [8], we gave a brief discussion about why the equality  $\delta S = \delta \bar{x} - \overline{\delta x}$  is a measure of uncertainty with the help of some graphics showing that  $\delta S = \delta \bar{x} - \overline{\delta x}$  defines a possible measure  $S$  of uncertainty of any probability distribution of  $p(x)$ . From this point of view,  $S$  is an uncertainty measure no more no less than, for example, the variance, the functional  $\ln p$ , or many other monotones function of  $p(x)$ . An advantage of  $\delta S = \delta \bar{x} - \overline{\delta x}$  with respect to all other possible measures seems to be that  $S$  always reaches maximum for corresponding probability distribution, which can be written as  $\overline{\delta x} = 0$ , as shown in [8].

## 6) Concluding remarks

It is argued that the maximum entropy is a requirement of the conventional mechanical equilibrium condition, i.e., the total virtual work of all random forces on all the elements (particles) of a mechanical system should vanish for the systems to be in thermodynamic equilibrium.

This is not a general derivation of the maxent principle for statistical and informational sciences. But through this work on maxent for mechanical system, we understand that the

optimization of thermodynamic entropy is simply the consequence of another much basic law of physics. There is no mystery in that. Indeed, if one admits that thermodynamic entropy is a measure of dynamical disorder and randomness (uncertainty), it is much natural to state that this disorder must get to maximum under some constraints of the equilibrium state, in order that all the random forces act on each degree of freedom of the motion in such a way that on any possible (virtual) displacement in any degree of freedom the possible work done by the forces (not only the random forces) should vanish. In other words, this vanishing work can only be obtained if and only if the randomness of the forces is at maximum in all degree of freedom allowed by the constraints. This is why if we take off the constraint associated with average energy for microcanonical ensemble, all microstates (combination of the possible characteristic values taken by all the degree of freedom) becomes equally probable. Equiprobability is a distribution of disorder in which no degree of freedom is privileged in the motion. Any privileged degree of freedom by the random forces may cause non vanishing virtual work.

Hence entropy is not necessarily a subjective quantity to be able to reach maximum for correct inference and probability deduction. Maximum entropy is not merely an inference principle. It is a law of physics at least for mechanical systems.

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