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► **To cite this version:**

| Qiuping Wang. Seeing maximum entropy from the principle of virtual work. 2007. hal-00140657v3

HAL Id: hal-00140657

<https://hal.science/hal-00140657v3>

Preprint submitted on 17 Oct 2007 (v3), last revised 28 Jan 2008 (v5)

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Why entropy tends to maximum?

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Abstract

We propose an extension of the principle of virtual work of classical mechanics to mechanical systems in random motion, i.e., the total virtual work of all the forces including random ones on all the elements (particles) of a mechanical system in stochastic motion should vanish when the system is in thermodynamic equilibrium. This extension allows us to establish a relation between the fundamental principle of mechanics and the maximum entropy principle for thermodynamics. This is an attempt to give the maximum entropy principle, considered by many as only an inference principle based on the subjectivity of probability and entropy, the status of a fundamental physics law.

PACS numbers : 02.30.Xx, 05.40.-a, 05.20.-y, 02.50.-r

1) Introduction

The principle of maximum entropy (maxent) is widely used in statistical science and engineering as a very useful fundamental rule. The maxent approach in statistical mechanics can be traced back to the works of Boltzmann and Gibbs[4] and finally be given the status of principle thanks to the work of Jaynes[5][6]. However, due to its mysterious nature, maxent has always been at the center of scientific and philosophical discussions and has raised many questions and controversies in the past[1][5][6][7]. One of the central questions is why entropy always gets to maximum for equilibrium state and why the optimal entropy takes the form of Boltzmann-Gibbs-Shannon one (see below).

In the present work, instead of answering these questions directly, we will establish a connection between maxent and a mechanical variational principle, the virtual work principle[2][3] (**viwop**) which is a widely used fundamental law of mechanics and capable of yielding all the basic laws of regular motion. It is in addition a simple, clearly defined, easily understandable and palpable law of physics. We think that this connection will be scientifically and pedagogically beneficial for the understanding of maxent and other controversial topics around it. In what follows, we use the term entropy, denoted by S , in the general sense as a measure of uncertainty or randomness of stochastic motion (also called information). In the case of equilibrium thermodynamics, S is the entropy of the second law of thermodynamics.

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 discuss maxent for the thermodynamic entropy of equilibrium state. Then we show that this entropy to be maximized should take the form of Boltzmann-Gibbs-Shannon one for the ordinary thermodynamic systems that can be studied with the ideal gas model having exponential probability distribution. For other systems with different distribution, the entropy form for maxent may be different.

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

the principle of virtual work (or virtual displacement¹) which is given unified and concise mathematical forms by Lagrange[2] and D’Alembert[3]. 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 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 ($i=1,2,\dots,n$), we have $\sum_{i=1}^n \bar{F}_i = 0$, and imagine a small displacement $\delta\bar{r}$ of the particle, the principle stipulates

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

This principle for statics was extended to dynamics by D’Alembert[3] in the Lagrange-d’Alembert principle given by

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

where m is the mass and \bar{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 with \bar{v}_i the velocity of the particle i . Without any loss of generality, let us suppose an equilibrium system without macroscopic motion, i.e., $\sum_{i=1}^N \bar{v}_i = 0$.

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

¹ 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.

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

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., $\vec{f}_i = -\nabla_i e_i$, such that

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

where δe_i is an infinitesimal variation of the energy e_i of the particle i . 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 δQ 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 β is the inverse absolute temperature according to the second law of thermodynamics. From the Lagrange-D'Alembert principle in Eq.(2), we straightforwardly change 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 α , 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., maxent applied to thermodynamic entropy for canonical ensemble. Note that we can write entropy as $S(p_j)$ as a function of the probability distribution, but we do not know yet its functional form which will be discussed below.

For microcanonical ensemble, the internal energy is constant, i.e., $\overline{\delta E} = 0$, 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 maxent under appropriate constraints is a consequence of the equilibrium condition of mechanical systems subject to the random motion. 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

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

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 $p_j = \frac{1}{w}$. This means that this entropy form must be used in maxent for the systems with exponential distributions.

5) Are other entropies possible?

The above calculation in section 4 is trivial and can be found in textbooks. It shows that the importance of Eq.(14) as optimal entropy measure is restricted to the cases where probability is exponential and energy is additive. For different probabilities and conditions, different optimal entropy forms are possible. For example, it was proved[9] that, for a distribution

such as $p_j = \frac{1}{Z_a} [1 - a\beta E_j]^{\frac{1}{a}}$ for finite system in equilibrium with finite heatbath[8], the

entropy defined by Eq.(12) is the Tsallis one $S = -\frac{\sum_j p_j^{1+a} - 1}{a} = -\sum_j \frac{p_j - p_j^q}{1-q}$ where $q=1+a$ and

$\sum_j p_j = 1$, and for $p_j = \frac{1}{Z} x_j^{-a}$ (Zipf law or large x_j Lévy flight), it is $S = \frac{\sum_j p_j^{1-1/a} - 1}{1-1/a}$. These

two entropies can be maximized to give the corresponding probability distributions, respectively.

6) Concluding remarks

It is argued that the maximum entropy principle has a close connection with a fundamental principle of classical mechanics, i.e., the principle of virtual work. In other words, for a mechanical system in thermodynamics equilibrium, the thermodynamic entropy gets to maximum when the total virtual work of all random forces on all the elements (particles) of the system vanishes. This means that the optimization of thermodynamic entropy can be considered as a consequence of another basic law of physics. Indeed, if one

admits that thermodynamic entropy is a measure of dynamical disorder and randomness (uncertainty), it is natural to state that this disorder must get to maximum in order that all the random forces act on each degree of freedom of the motion such that over any possible (virtual) displacement in any degree of freedom the possible work done by all the forces (not only the random forces) is zero. In other words, this vanishing work can 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.

To our opinion, the present result is useful especially for pedagogical purpose to introduce maxent from a more basic and well understood mechanical principle instead of postulating it as a first principle. In this way, we also show that entropy in general 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.

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