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On the robust thermodynamical structures against arbitrary entropy form and energy mean value

Takuya Yamano[a]

Faculty of Science, Tokyo Institute of Technology, Oh-okayama, Meguro-ku, Tokyo,152-8551, Japan

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Abstract. We discuss how the thermodynamical Legendre transform structure can be retained not only for the arbitrary entropic form but also for the arbitrary form of the energy constraints by following the discussion of Plastino and Plastino. The thermodynamic relation between the expectation values and the conjugate Lagrange multipliers are seen to be universal. Furthermore, Gibbs' fundamental equation is shown to be unaffected by the choice of the entropy and the definition of the mean values due to the robustness of the Legendre transform structure.

PACS. 05.70.-a Thermodynamics – 05.90.+m Other topics in statistical physics, thermodynamics, and nonlinear dynamical systems

1 Introduction

There exists subtleness in understanding the relation between thermodynamics and statistical mechanics. Nowadays, on the other hand, some alternative entropic functionals to the conventional Boltzmann-Gibbs-Shannon (BGS) entropy have been investigated, applied to a variety of physical situations. Among them, as one example, Tsallis' information measure $S_q = (1-\int \mathrm{d}x f^q)/(q-1)$ [1,2] where q is a real parameter characterizing S_q is attracting much attention. Thermostatistics based on this nonextensive measure has been shown to be useful for describing anomalous systems involving long-range interactions, long-term memory effect and (multi)fractal-like structure (see [3] for concrete applications). Another example is Fisher's information measure $I = \int \mathrm{d}x(f'^2/f)$ where f is a normalized probability distribution [4]. The connection between derivation of the variety of statistical laws of physics and the principle of minimum I has been shown [5]. In view of these examples, there is increasing interest in exploring the possibility of the associated thermodynamics with non-BGS entropies. In this sense, therefore, a certain mathematical relation among thermodynamical variables is considered to be in a crucial position in discussing the applicability of the alternative context.

The Legendre transform structure (LTS) [7–9] is considered to be a most fundamental relation which associates the phenomenologically based thermodynamics with the microscopically based statistical mechanics. Recently Plastino and Plastino [10,11] showed that the LTS is a universal property independent of the selection of the entropic functional if only we adopt the linear definition of an expectation value of observables. That is, weighting each quantity with the probability corresponding to the configurational states preserves the LTS for an arbitrary form of the entropy functional. At the present stage, it should be of interest to investigate the structure against a nonlinear definition of the mean value in a plurality of constraints.

In this paper, our discussion requires only the Jaynes maximum entropy principle [13–15]. Jaynes' information theoretical approach to statistical mechanics based on Shannon's extensive measure with a linear weighting of quantities as a mean value have been successfully extended to Fisher's information measure ([6] and references therein). Moreover it is well known that Tsallis' nonextensive measure with a nonlinear weighting has the LTS [2,16,17]. Therefore overall discussion based on the generic form of the entropy and a mean value with general weighting would illuminate the thermodynamical structures. It is the purpose of our present attempt to develop arguments along the line of the previous approach as mentioned above.

2 The thermodynamical relation in general context

We start with a consideration of what relation we have between an entropy and energies when we adopt the arbitrary form of entropy functional and the energy constraints with respect to a probability set. This problem was considered for the case of the canonical ensemble, that is, with one energy constraint to the entropy to be extremized [10]. We deal with the generalized entropy

[a] e-mail: tyamano@o.cc.titech.ac.jp

$S(\{p_i\})$ and the generalized expectation value of observables (generalized energy) $E^\sigma(\{p_i\}, \{M_i^\sigma\})$, where p_i denotes a probability of the microstate i of a quantity M_i^σ, $(i = 1, \cdots, W)$. The superscript σ labels a constraint number $(\sigma = 1, \cdots, N)$. We usually suppose $N < W$ since we treat a huge number of microstates W. The important thing is that the information we have at first is the N mean values E^σ and each p_i is not *a priori* known. The probability p_i should be given in terms of the Jaynes maximum entropy principle instead. Extremization of S with respect to p_i subject to N generalized energy and the normalization condition of the probability leads to

$$\frac{\delta}{\delta p_i}\left(S - \sum_{\sigma=0}^{N} \beta_\sigma E^\sigma\right) = 0 \tag{1}$$

where we have introduced the $N+1$ Lagrange multipliers β_σ ,$(\sigma = 0, \cdots, N)$ and set $E^0 = \sum_i^W p_i = 1$, *i.e.*

$$\frac{\partial S}{\partial p_i} - \sum_{\sigma=0}^{N} \beta_\sigma \frac{\partial E^\sigma}{\partial p_i} = 0. \tag{2}$$

Since the solution in equilibrium p_i^* should be of the form $p_i^* = p_i^*(\beta_0(\beta_1, \dots, \beta_N), \beta_1, \dots, \beta_N)$ with the normalization of p_i^*, we have the partial derivatives of S and E^σ with respect to the μ-th Lagrange parameter,

$$\frac{\partial S}{\partial \beta_\mu} = \sum_{i=1}^{W} \frac{\partial S}{\partial p_i^*}\left(\frac{\partial p_i^*}{\partial \beta_\mu} + \frac{\partial p_i^*}{\partial \beta_0}\frac{\partial \beta_0}{\partial \beta_\mu}\right), \tag{3}$$

and

$$\frac{\partial E^\sigma}{\partial \beta_\mu} = \sum_{i=1}^{W} \frac{\partial E^\sigma}{\partial p_i^*}\left(\frac{\partial p_i^*}{\partial \beta_\mu} + \frac{\partial p_i^*}{\partial \beta_0}\frac{\partial \beta_0}{\partial \beta_\mu}\right), \tag{4}$$

respectively. After multiplying equation (4) by β_σ and summing over σ, one finds

$$\begin{aligned}\sum_{\sigma=0}^{N} \beta_\sigma \frac{\partial E^\sigma}{\partial \beta_\mu} &= \sum_{i=1}^{W}\sum_{\sigma=0}^{N} \beta_\sigma \frac{\partial E^\sigma}{\partial p_i^*}\left(\frac{\partial p_i^*}{\partial \beta_\mu} + \frac{\partial p_i^*}{\partial \beta_0}\frac{\partial \beta_0}{\partial \beta_\mu}\right)\\ &= \sum_{i=1}^{W} \frac{\partial S}{\partial p_i^*}\left(\frac{\partial p_i^*}{\partial \beta_\mu} + \frac{\partial p_i^*}{\partial \beta_0}\frac{\partial \beta_0}{\partial \beta_\mu}\right)\\ &= \frac{\partial S}{\partial \beta_\mu},\end{aligned} \tag{5}$$

which gives the generalized thermodynamical relation that connects the arbitrary form of the entropy and the mean values, *i.e.*

$$\begin{aligned}\frac{\partial S}{\partial E^\sigma} &= \sum_{\nu=0}^{N} \frac{\partial S}{\partial \beta_\nu}\frac{\partial \beta_\nu}{\partial E^\sigma} = \sum_{\nu=0}^{N}\sum_{\mu=0}^{N} \beta_\mu \frac{\partial E^\mu}{\partial \beta_\nu}\frac{\partial \beta_\nu}{\partial E^\sigma}\\ &= \beta_\sigma \quad (\sigma \neq 0).\end{aligned} \tag{6}$$

$N = 1$ corresponds to the canonical ensemble theory and gives the fundamental thermodynamical relation [10],

$$\frac{\partial S}{\partial E} = \beta. \tag{7}$$

The above relation constitutes the basis of the justification that the Lagrange multiplier β appearing in the equilibrium statistical mechanics based on the BGS entropy is identified with the inverse temperature in thermodynamics. However, we stress that this thermodynamical relation is very robust in a general context if only there is one energy constraint. Although we give no explicit form of the entropy $S(\{p_i^*\})$ in the present consideration, the condition of extremization with respect to each Lagrange multipliers when fixing general energies is to be required, namely,

$$\left.\frac{\partial S\{p_i^*\}}{\partial \beta_\mu}\right|_{E^1, \cdots, E^N} = 0. \tag{8}$$

3 Legendre transform structure

Consider now the following general entropic form

$$S = \sum_{i=1}^{W} f(p_i), \tag{9}$$

where a measure $f(p_i)$ is an arbitrary function of the probability $\{p_i\}$ and we do not have to require the concavity property which is needed in physical stability in the following discussion. It should be noted that one form $f(p_i) = -p_i \ln p_i$ is the BGS measure when we choose Boltzmann's constant as the information unit and another form $f(p_i) = (p_i - p_i^q)/(q-1)$, $(q \in \mathbb{R})$ is the Tsallis one. Moreover let us define the mean value of quantities (eigenvalues)$\{M_i^\sigma\}$ in the following way,

$$\langle M^\sigma \rangle = \sum_{j=1}^{W} g_j(p_1, \dots, p_W) M_j^\sigma \quad (\sigma = 1, \cdots N), \tag{10}$$

where $g_j(p_1, \dots, p_W)$ determined by all probabilities is a weighting function for eigenvalues M_j^σ. In an ordinary case, we should constrain g_j as being $\sum_{j=1}^{W} g_j = 1$ from a physically acceptable definition of the mean value (the mean value of unity should be unity). As a specific form of g_j, an escort type of probability [8] satisfies this condition (hereafter referred to as a weighting condition) as a weighting function,

$$g_j(p_1, \dots, p_W) = \frac{\phi(p_j)}{\sum_{i=1}^{W} \phi(p_i)} \tag{11}$$

where $\phi(p_j)$ is a positive test function defined for all $p_j \in [0, 1]$. It is worth noting that the special test function of the form $\phi(p_j) = p_j^q$ constitutes the generalized expectation value in Tsallis statistical mechanics [2]. In the present consideration, however, we weigh the eigenvalues with an general g_j to proceed to a discussion. We will as a result see that our conclusion can be derived even without the weighting condition.

The variational approach applied to extremizing equation (9) in this context is quite similar to the one developed in Section 2

$$\frac{\delta}{\delta p_i}\left[S-\alpha\sum_{i=1}^{W}p_i-\sum_{\sigma=1}^{N}\beta_\sigma\sum_{j=1}^{W}M_j^\sigma g_j(p_1,\dots,p_W)\right]=0 \tag{12}$$

where α and β_σ ($\sigma=1,\cdots,N$) are Lagrange multipliers again yielding

$$f'(p_i)-\alpha-\sum_{\sigma=1}^{N}\beta_\sigma\sum_{j=1}^{W}\frac{\partial g_j(p_1,\dots,p_W)}{\partial p_i}M_j^\sigma=0. \tag{13}$$

The *prime* denotes the derivative with respect to p_i. For a given set of eigenvalues $\{M_j^\sigma\}$, we define Q as a function of the probability set $\{p_i\}$ and the Lagrange multipliers set $\{\beta_\sigma\}$ as follows,

$$Q(\{p_i\},\{\beta_\sigma\})=\sum_{j=1}^{W}\sum_{\sigma=1}^{N}\beta_\sigma M_j^\sigma g_j(p_1,\dots,p_W)\ . \tag{14}$$

Then the equation which determines the equilibrium probabilities $\{p_i^*\}$ becomes

$$P(p_i)=\alpha+\frac{\partial}{\partial p_i}Q(\{p_i\},\{\beta_\sigma\}), \tag{15}$$

where we put $f'(p_i)=P(p_i)$. Although the explicit form of the solution $\{p_i^*\}$ is not obtained from the above, we can pursue further discussion along the line of [10] by regarding the solution as $\{p_i^*(\{\beta_\sigma\}_{\sigma=1,\dots,N})\}$. Therefore, the S and the $\langle M^\sigma\rangle$ read

$$S=\sum_{i=1}^{W}f(p_i^*) \tag{16}$$

and

$$\langle M^\sigma\rangle=\sum_{j=1}^{W}g_j(p_1^*,\dots,p_W^*)M_j^\sigma \tag{17}$$

respectively. From this we immediately have

$$\frac{\partial S}{\partial\beta_\sigma}=\sum_{i=1}^{W}f'(p_i^*)\frac{\partial p_i^*}{\partial\beta_\sigma} \tag{18}$$

and

$$\frac{\partial\langle M^\mu\rangle}{\partial\beta_\sigma}=\sum_{j=1}^{W}\sum_{i=1}^{W}\frac{\partial g_j(p_1^*,\dots,p_W^*)}{\partial p_i^*}\frac{\partial p_i^*}{\partial\beta_\sigma}M_j^\mu. \tag{19}$$

We are considering the Legendre transform of the entropy S

$$\mathcal{L}[S]=S-\sum_{\sigma=1}^{N}\frac{\partial S}{\partial\langle M^\sigma\rangle}\langle M^\sigma\rangle. \tag{20}$$

To evaluate the above, let us calculate the derivatives of the general entropy S in equilibrium with respect to both β_σ and $\langle M^\sigma\rangle$. With equation (15) and equation (18), $\partial S/\partial\beta_\sigma$ becomes

$$\frac{\partial S}{\partial\beta_\sigma}=\sum_{i=1}^{W}(\alpha+\frac{\partial Q}{\partial p_i^*})\frac{\partial p_i^*}{\partial\beta_\sigma}=\sum_{i=1}^{W}\frac{\partial Q}{\partial p_i^*}\frac{\partial p_i^*}{\partial\beta_\sigma} \tag{21}$$

where we have used the relation arising from the normalization condition

$$\sum_{i=1}^{W}\frac{\partial p_i^*}{\partial\beta_\sigma}=\frac{\partial}{\partial\beta_\sigma}\sum_{i=1}^{W}p_i^*=0. \tag{22}$$

Then from equation (14), equation (21) immediately leads to

$$\begin{aligned}\frac{\partial S}{\partial\beta_\sigma}&=\sum_{\mu=1}^{N}\beta_\mu\left[\sum_{i=1}^{W}\sum_{j=1}^{W}M_j^\mu\frac{\partial g_j(p_1,\dots,p_W)}{\partial p_i^*}\frac{\partial p_i^*}{\partial\beta_\sigma}\right]\\&=\sum_{\mu=1}^{N}\beta_\mu\frac{\partial\langle M^\mu\rangle}{\partial\beta_\sigma}.\end{aligned} \tag{23}$$

Therefore we have

$$\begin{aligned}\frac{\partial S}{\partial\langle M^\sigma\rangle}&=\sum_{\nu=1}^{N}\frac{\partial S}{\partial\beta_\nu}\frac{\partial\beta_\nu}{\partial\langle M^\sigma\rangle}=\sum_{\nu=1}^{N}\sum_{\mu=1}^{N}\beta_\mu\frac{\partial\langle M^\mu\rangle}{\partial\beta_\nu}\frac{\partial\beta_\nu}{\partial\langle M^\sigma\rangle}\\&=\beta_\sigma.\end{aligned} \tag{24}$$

Thus, we again see that equation (23) and equation (24) maintain the same relations as equation (5) and equation (6), respectively, as expected. Equation (23) (Eq. (5)) expresses Euler's theorem in the general context [10,18]. Equation (24) (Eq. (6)) represents a general thermodynamical relation where the Lagrange multipliers and the mean values constitute conjugate variables with each other with respect to S. It should be noted that this thermodynamical relation (namely, reciprocity relation [10], which corresponds to the one relating the intensive parameters with the extensive parameters in ordinary thermodynamics) is seen to be independent of *both* the entropy functional and the mean energy form.

Since the entropy S can be described either with an entire set of $\langle M^\sigma\rangle$'s as $S(\{\langle M^\sigma\rangle\})$, or with β_σ's as $S(\{\beta_\sigma\})$ due to the reciprocity relation, if we regard S as $S(\{\langle M^\sigma\rangle\})$, the derivative of $\mathcal{L}[S]$ with respect to β_σ becomes

$$\begin{aligned}\frac{\partial\mathcal{L}[S]}{\partial\beta_\sigma}&=\sum_{\nu=1}^{N}\frac{\partial S}{\partial\langle M^\nu\rangle}\frac{\partial\langle M^\nu\rangle}{\partial\beta_\sigma}-\sum_{\nu=1}^{N}\beta_\nu\frac{\partial\langle M^\nu\rangle}{\partial\beta_\sigma}-\langle M^\sigma\rangle\\&=-\langle M^\sigma\rangle\end{aligned} \tag{25}$$

where we have used $\partial S/\partial\langle M^\nu\rangle=\beta_\nu$. In a similar way, if we regard the S as $S(\{\beta_\sigma\})$, that is,

$$\mathcal{L}[S]=S(\{\beta_\sigma\})-\sum_{\sigma=1}^{N}\beta_\sigma\langle M^\sigma\rangle(\{\beta_\sigma\}) \tag{26}$$

then the derivative of $\mathcal{L}[S]$ with respect to $\langle M^\sigma\rangle$ gives

$$\frac{\partial \mathcal{L}[S]}{\partial\langle M^\sigma\rangle} = \sum_{\nu=1}^{N} \frac{\partial S}{\partial \beta_\nu}\frac{\partial \beta_\nu}{\partial\langle M^\sigma\rangle} - \sum_{\nu=1}^{N}\frac{\partial \beta_\nu}{\partial\langle M^\sigma\rangle}\langle M^\nu\rangle - \beta_\sigma$$
$$= -\sum_{\nu=1}^{N}\frac{\partial \beta_\nu}{\partial\langle M^\sigma\rangle}\langle M^\nu\rangle$$
$$= -\sum_{\nu=1}^{N}\frac{\partial^2 S}{\partial\langle M^\sigma\rangle\partial\langle M^\nu\rangle}\langle M^\nu\rangle \tag{27}$$

where we have used

$$\sum_{\nu=1}^{N}\sum_{\mu=1}^{N}\beta_\mu\frac{\partial\langle M^\mu\rangle}{\partial\beta_\nu}\frac{\partial\beta_\nu}{\partial\langle M^\sigma\rangle} = \beta_\sigma \tag{28}$$

in the first term of the first line.
Further, from equation (24), equation (25) we have

$$\frac{\partial\langle M^\sigma\rangle}{\partial\beta_\sigma} = -\frac{\partial^2\mathcal{L}[S]}{\partial\beta_\sigma^2} = \frac{1}{\frac{\partial^2 S}{\partial\langle M^\sigma\rangle^2}}\,. \tag{29}$$

To guarantee the uniqueness of the LTS, that is, from a requisition that $\partial\mathcal{L}[S]/\partial\beta_\sigma$ and $\partial S/\partial\langle M^\sigma\rangle$ are to be monotonic functions, we assume

$$\frac{\partial^2\mathcal{L}[S]}{\partial\beta_\sigma^2} \neq 0, \quad \frac{\partial^2 S}{\partial\langle M^\sigma\rangle^2} \neq 0. \tag{30}$$

As indicated by equation (29), we see that when the S is convex, then the $\mathcal{L}[S]$ is concave, and *vice versa* in general context. From the equations (24, 25, 29), we can stress that the LTS is preserved *both* for an arbitrary form of the entropy and for the general definition of the mean value.

4 Gibbs' fundamental equation

We have found that the given mean values $\langle M^\sigma\rangle$ and the associated Lagrange multipliers β_σ are "thermally conjugated" [8] with each other in general context. This relation (Eq. (24)) for all σ can be written in the following form

$$\mathrm{d}S = \sum_{\sigma=1}^{N}\beta_\sigma \mathrm{d}\langle M^\sigma\rangle, \tag{31}$$

which is called Gibbs' fundamental equation [8,9]. The concrete expression for equation (31) in thermodynamics is well known as

$$\mathrm{d}S = \frac{1}{T}\mathrm{d}U + \frac{p}{T}\mathrm{d}V - \frac{\mu}{T}\mathrm{d}N. \tag{32}$$

We should notice that, in the conventional phenomenological thermodynamic picture, the entropy S, the internal energy U, the volume V and the particle number N are regarded as extensive parameters and the coefficients (T: temperature, p: pressure, μ: chemical potential) are intensive parameters, however, Gibbs' fundamental equation holds independently of the entropic form (extensive or nonextensive) and of the definition (linear or nonlinear) of the expectation value.

5 Summary and conclusion

We have derived the thermodynamical relation between the entropy and the energy in the most general circumstance (Eq. (24)) along the line of [10]. Furthermore, we have shown that the Legendre transform structure is a robust structure against the choice of the statistical entropic measure and the way of weighting for energy eigenstates of the system under consideration. As a necessary consequence of this structure, Gibbs' fundamental equation is also independent of the present extension into the arbitrariness. These results are supported by the ubiquitous property of the Jaynes maximum entropy principle. The construction of a statistical mechanics whose basis should be consistent with the conventional thermodynamics, therefore, is considered to be not adequate with the preservation of the LTS and Gibbs' fundamental equation alone, which of course are essential ingredients for realization. The present conclusion is considered to be consistent with results of reference [12] which took another route for discussing arbitrary thermostatistics.

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