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The third law of thermodynamics and the fractional entropies

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ABSTRACT

We consider the fractal calculus based Ubriaco and Machado entropies and investigate whether they conform to the third law of thermodynamics. The Ubriaco entropy satisfies the third law of thermodynamics in the interval $0 < q \leq 1$ exactly where it is also thermodynamically stable. The Machado entropy, on the other hand, yields diverging inverse temperature in the region $0 < q \leq 1$, albeit with non-vanishing negative entropy values. Therefore, despite the divergent inverse temperature behavior, the Machado entropy fails the third law of thermodynamics. We also show that the aforementioned results are also supported by the one-dimensional Ising model with no external field.

1. Introduction

The recent progress in the use of information-theoretic entropies to construct a generalized statistical mechanics follows two main routes: the former approach uses the definitions of Tsallis [1], Rényi [2], Kaniadakis [3] entropies so that the non-equilibrium stationary metastable cases are also considered within the context of the statistical mechanics [4]. Along this direction, many important applications were reported in the fields of quantum information [5–8], econophysics [9,10], high energy phenomenology [11], black hole thermodynamics [12,13] and the rigid rotators in modeling the molecular structure [14,15]. All these entropy definitions share the common feature that they yield distributions of inverse power law form under the entropy maximization [1,3,16,17]. The latter approach consists of using the Shannon entropy with time-dependent probabilities thereby forming the field of stochastic thermodynamics [18], opening up the possibility for the treatment of the physical systems at the nanoscale [19–21].

A third alternative was recently presented by relying on the fractional calculus so that Ubriaco [22] and Machado [23] provided two alternative definitions. The approach of Ubriaco [22] is based on replacing the ordinary derivative yielding Shannon entropy with the fractional Riemann–Liouville derivative. Machado [23] on the other hand introduces his entropy through a fractional generalization of the information content whose average yields the Machado entropy [23]. These novel entropy expressions are then applied to numerous cases including the study of the financial time series and stock market index [23,24], the disclosing of the relation between DNA and the fractional Brownian motion [25], image splicing [26], and a new metrics of the emergence in the field of complexity [27].

However, whether these new entropy definitions based on fractional calculus is valid for a generalized statistical mechanics have not been tested yet apart from the thermodynamic stability of the entropy introduced by Ubriaco [22]. In this context, the third law of thermodynamics has been introduced as a test for the generalized entropies [28], since it should be satisfied for any suitable entropy expression independent of the Hamiltonian. The methodology in Ref. [28] is to express the third law in terms of micro-probabilities by assuming that the physical system has ordered microscopic energies E_λ where $\lambda = 0, 1, \ldots, N$ with no degeneracy. The state with $\lambda = 0$ is then the ground state. The probability of the system to be in the state λ is given by p_λ where $\sum_\lambda p_\lambda = 1$ i.e., assuming that the normalization is carried out. Since $p_0 = 1 - \sum_n p_n$ due to the normalization with $n = 1, \ldots, N$, any function f of the micro-probabilities satisfies the relation $\frac{\partial f(p_0)}{\partial p_n} = -\frac{\partial f(p_0)}{\partial p_0}$. Then, by setting the ground state probability p_0 to unity, one realizes the situation that only the ground state is populated while all the remaining probabilities p_n's are null. The contribution of the nth energy level to the inverse temperature β as β_n is given by

$$\beta_n = \frac{\partial S}{\partial p_n}\left(\frac{\partial U}{\partial p_n}\right)^{-1}, \tag{1}$$

where $\beta = \sum_n \beta_n$. Then one checks whether this inverse temperature attains infinity when $\{p_n\} \to 0$ as $p_0 = 1$ showing that only the ground state is occupied while all the other states are not. Note that the third law dictates that the diverging temperature occurs if and only if when the entropy vanishes [28]. Before considering the Ubriaco and Machado entropies, we also note that the Tsallis entropy has recently been shown to conform to the third law for its

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whole interval of convergence while the Renyi entropy satisfies the third law of thermodynamics only in the region where it is neither concave nor convex [29].

2. The third law of thermodynamics: Ubriaco and Machado entropies

The Shannon entropy (having set the Boltzmann constant to unity) can be defined through

$$S=\lim_{t\to -1}\frac{d}{dt}\sum_{\lambda}p_{\lambda}^{-t}=-\sum_{\lambda}p_{\lambda}\ln p_{\lambda}. \tag{2}$$

Considering this equality as the point of departure, Ubriaco introduced the fractional entropy by relying on the Riemann–Liouville definition of the fractional derivative as

$$S_q=\lim_{t\to -1}\frac{d}{dt}\left({}_{-\infty}D_t^{q-1}\sum_{\lambda}e^{-t\ln p_{\lambda}}\right), \tag{3}$$

where the integro-differential operator ${}_aD_t^{q-n}$ reads

$${}_aD_t^{q-n}f(t)=\frac{1}{\Gamma(n-q)}\int_a^t dt'\frac{f(t')}{(t-t')^{1+q-n}} \tag{4}$$

so that

$$S_q=\lim_{t\to -1}\frac{d}{dt}\frac{1}{\Gamma(1-q)}\sum_{\lambda}\int_{-\infty}^{t}dt'\frac{e^{-t'\ln p_{\lambda}}}{(t-t')^{q}}. \tag{5}$$

Performing the integration and taking the limit $t\to -1$ [22], one obtains the fractal entropy as

$$S_q=\sum_{\lambda}(-\ln p_{\lambda})^q\,p_{\lambda}, \tag{6}$$

where $0\le q\le 1$. In the limit $q\to 1$, the fractal entropy S_q approaches the Shannon entropy S. We also note that the fractal entropy S_q is non-additive and thermodynamically stable for $0<q\le 1$ [22].

Using Eq. (6), we can calculate the following expression

$$\frac{\partial S_q}{\partial p_n}=(-\ln p_n)^q-q(-\ln p_n)^{q-1}-(-\ln p_0)^q+q(-\ln p_0)^{q-1}. \tag{7}$$

Since the system energy is given through $U=\sum_{\lambda}p_{\lambda}E_{\lambda}$, we have

$$\frac{\partial U}{\partial p_n}=E_n-E_0, \tag{8}$$

which is independent of the index q. Using Eqs. (7) and (8), one can then calculate β_n in Eq. (1) as

$$\beta_n=\frac{(-\ln p_n)^q-q(-\ln p_n)^{q-1}-(-\ln p_0)^q+q(-\ln p_0)^{q-1}}{(E_n-E_0)}. \tag{9}$$

Having substituted $p_0=1$, we obtain

$$\lim_{p_n\to 0}\beta_n=\lim_{p_n\to 0}\frac{(-\ln p_n)^q-q(-\ln p_n)^{q-1}}{(E_n-E_0)}+\infty=\infty \tag{10}$$

for the interval $0<q\le 1$. This result shows that the fractal entropy of Ubriaco satisfies the third law of thermodynamics exactly in the region where it is thermodynamically stable i.e. $0<q\le 1$ [22].

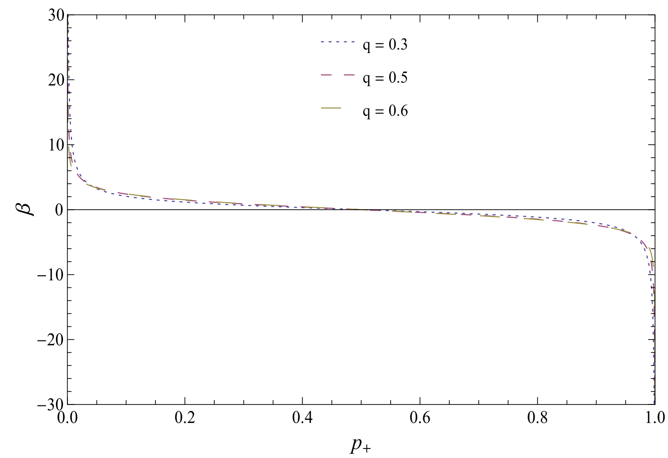

Fig. 1. The Ubriaco inverse temperature β versus p_+ for the one-dimensional Ising model with $q=0.3$, $q=0.5$ and $q=0.6$.

To illustrate our results, we consider one dimensional Ising model with periodic boundary conditions, namely, $\sigma_i=\sigma_{i+1}$, with no external field

$$H=-J\sum_i\sigma_i\sigma_{i+1} \tag{11}$$

where J is the interaction strength and the summation is taken over the number of spins whose values are ± 1. The mean energy is given by $U=J(p_+-p_-)$ where p_+ (p_-) denotes the probability of the random pair of neighboring spins being anti-parallel (parallel). Note that the mean energy can also be written as $U=Jp_+-J(1-p_+)$ due to the normalization. The energies of the anti-parallel and parallel cases are $E_1=+J$ and $E_0=-J$, respectively. In terms of the notation adopted before, the ground state probability p_0 corresponds to p_- while the excited state p_1 (with $n=1$) corresponds to p_+. Then, $\frac{\partial U}{\partial p_n}$ i.e. $\frac{\partial U}{\partial p_+}$ in Eq. (1) is equal to $2J$ for the one-dimensional Ising model. One can then calculate the entropy using only the probability p_+, since $p_+=1-p_-$ due to the normalization. Setting $2J=1$ without loss of generality, we plot the inverse temperature β and the Ubriaco entropy S_q in Figs. 1 and 2, respectively. From these figures, one can see that the Ubriaco entropy S_q is zero when $p_+\to 0$ (i.e. when $p_-\to 1$ implying that only the ground state is populated) exactly at the point where the inverse temperature β attains the limit $+\infty$. Moreover, just like the Boltzmann–Gibbs entropy, the Ubriaco entropy S_q is also zero when $p_+\to 1$ (i.e. when $p_-\to 0$ implying that only the excited state is populated) where $\beta\to -\infty$. In accordance with the third law of thermodynamics, the Ubriaco entropy is non-zero everywhere else.

Next, we now consider the Machado entropy [23] which is given by

$$S_q=\sum_{\lambda}-\frac{p_{\lambda}^{1-q}}{\Gamma(1+q)}\left[\ln p_{\lambda}+\Psi(1)-\Psi(1-q)\right] \tag{12}$$

for $-1\le q\le 1$ where the gamma and digamma functions are defined as $\Gamma(x)\equiv\int_0^{\infty}t^{z-1}e^{-t}dt$ and $\Psi(x)\equiv\frac{\frac{d\Gamma(x)}{dx}}{\Gamma(x)}$, respectively. When the parameter q in the Machado entropy is set to zero, one recovers the ordinary Shannon entropy. One can then calculate its partial derivative as

$$\frac{\partial S_q}{\partial p_n}=\frac{p_n^{-q}}{\Gamma(1+q)}\left[-1+(q-1)(\ln p_{\lambda}+\Psi(1)-\Psi(1-q))\right] \tag{13}$$

so that we obtain