

A non-extensive thermodynamic theory of ecological systems

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Abstract. After almost 30 years of development, it is not controversial issue that the so-called Tsallis entropy provides a useful approach to studying the complexity where the non-additivity of the systems under consideration is frequently met. Also, in the ecological research, Tsallis entropy, or in other words, q -entropy has been found itself as a generalized approach to define a range of diversity indices including Shannon–Wiener and Simpson indices. As a further stage of development in theoretical research, a thermodynamic theory based on Tsallis entropy or diversity indices in ecology has to be constructed for ecological systems to provide knowledge of ecological macroscopic behaviors. The standard method of theoretical physics is used in the manipulation and the equivalence between phenomenological thermodynamics and ecological aspects is the purpose of the ongoing research.

The present work is in the line of the authors research to implement Tsallis non-extensivity approach to obtain the most important thermodynamic quantities of ecological systems such as internal energy U_q and temperature T_q based on a given modeled truncated Boltzmann distribution of the Whittaker plot for a dataset. These quantities have their own ecological meaning, especially the temperature T_q provides the insight of equilibrium condition among ecological systems as it is well-known in 0th law of thermodynamics.

1. Introduction

In the history of science, the applications of thermodynamics and statistical physics, and their methods on research of complex systems, especially biological and ecological systems is not a new trend in interdisciplinary science [1–3]. The basic of these branches of physics brings new methodologies, new ideas and new understanding into ecological science [3–7]. In its birth, thermodynamics was considered as a phenomenological and experimental science trying to describe the macroscopic states of many-body physical systems with minimal sets of observable macroscopic variables. And only since the beginning of the last century, the nature of thermodynamical processes and properties were understood and explained from the points of view of kinetic theory and statistics which were pioneered by the works of Gibbs and Boltzmann. That statistical background requires to determine and to define a set of identical microscopic particles involving in physical processes within systems. These different basic principles have caused a lot of discussions in applicability of thermodynamics and statistical physics to complex



systems such as biological, ecological, social and others, where the definitions of macroscopic and microscopic objects are depending not only on systems themselves but also on the scales of observation. In despite of these differences in understanding the attempts of searching new applications of thermodynamics and statistical physics in the research of complex systems are always attracting the attention of many researchers in many aspects, from theory to practice.

To continue these great ideas, the present work as an extension of the previous work [8] focuses on finding the way of constructing a thermodynamic theory for ecological systems. However, instead of attempting to define the interacting individuals in a ecological system, the approach used in the present work tries to build up a thermodynamic consistent theory from the diversity index which is the most common ecological quantity obtained from ecological measurements, and within the proposed approach the most important thermodynamic quantities such as internal energy U and temperature T are explicitly defined and obtained. It would be expected that the results should cover in itself ecological meaning and also fulfill the thermodynamic consistence of physics.

2. Tsallis entropic approach to a thermodynamic theory

Thermodynamic is full of highly scientific and charming terms and concepts, giving an impression of philosophical and scientific profundity. Entropy, thermal death of the Universe, ergodicity, statistical ensemble—all these words sound very impressive posed in any order. But, placed in the appropriate order, they can help us to find the solution of urgent practical problems.

Unlike the most of traditional physical systems where the non-extensivity is very small, even gets zero in every experimental observations, ecological systems or in general, complex systems have visible non-extensivity, in some cases, very strong [8–12]. Furthermore, experimental observations in ecological systems are indirect in whole, and always in situations of information incompleteness. Due to these difficulties, a new physical and mathematical tool has to be developed to take into account of the non-extensivity, and the Tsallis entropy [13] would be the best nominee available in this scope of works [8].

2.1. Non-extensive statistical mechanics

A non-extensive statistical mechanics of a complex system will be built upon the Tsallis entropy [9, 13–16]

$$S_q = \frac{1}{q-1} \left(1 - \sum_{i=1}^W p_i^q \right), \quad (1)$$

where $q \in \mathbb{R}$ is some real parameter characterizing the non-extensivity, W is the number of possible microscopic states, and normalized constraint of statistical weight p_i

$$\sum_{i=1}^W p_i = 1. \quad (2)$$

To construct statistical mechanics from the above given entropy S_q , it has to be optimized with the normalized constraint (2) to statistical weight p_i and some constraint related to internal energy [11–13, 15]

$$\sum_{i=1}^W p_i E_i = U, \quad (3)$$

where $\{E_i\}$ are the eigenvalues of some Hamiltonian H with the appropriate boundary conditions, and the internal energy U is a finite fixed value. The constraint (3) would be generalized in non-extensive manner as

$$\langle \mathcal{H} \rangle_q = \left(\sum_{i=1}^W p_i^q \right)^{-1} \sum_{i=1}^W p_i^q E_i = U_q, \quad (4)$$

with $\langle \dots \rangle_1 = \langle \dots \rangle$ and $\left(\sum_{i=1}^W p_i^q \right)^{-1} p_i^q$ is referred to as the *escort distribution*. The optimization of the Tsallis entropy (1) with the constraints (2) and (4) straightforwardly yields

$$p_i = (\bar{Z}_q)^{-1} e_q^{-\beta_q(E_i - U_q)}, \quad (5)$$

with

$$\bar{Z}_q = \sum_{i=1}^W e_q^{-\beta_q(E_i - U_q)}, \quad (6)$$

and

$$\beta_q = \left(\sum_{i=1}^W p_i^q \right)^{-1} \beta, \quad (7)$$

where $\beta = (kT)^{-1}$ being the Lagrange parameter associated with constraint (4). Here to avoid confusion, the parameter k , which should be the Boltzmann constant k_B in the context of standard statistical mechanics, has been restored. And the q -exponential function e_q^x is defined as

$$e_q^x = (1 + (1 - q)x)^{\frac{1}{1-q}}, \quad (8)$$

that approaches to the exponential function when q goes to 1,

$$\lim_{q \rightarrow 1} e_q^x = e^x. \quad (9)$$

2.2. Connection to q -Thermodynamics

Following the standard routine of thermodynamics presented in original works and textbooks [13–15, 17, 18], it would be easy to define an abstract temperature T within q -thermodynamics as

$$\frac{1}{T} = \frac{\partial S_q}{\partial U_q}, \quad (10)$$

which is identical to physical temperature in normal situations when q approaches to 1. Other q -thermodynamic potentials such as free energy F_q

$$F_q = U_q - TS_q - kT \ln_q Z_q, \quad (11)$$

are also obtained in standard way of thermodynamics, where

$$\ln_q Z_q = \ln_q \bar{Z}_q - \beta U_q, \quad (12)$$

with the inverse of q -exponential function e_q^x

$$\ln_q x = \frac{x^{1-q} - 1}{1 - q}. \quad (13)$$

To the end of this section, it would be said that all above consideration of non-extensive statistical mechanics and corresponding derivative q -thermodynamics provides a sufficiently plain physical and mathematical tool to develop a thermodynamic theory for ecological systems where the diversity indices is well determined in the manner of real datasets in ecological measurements.

3. An application to ecological systems

3.1. Truncated exponential distribution and diversity index

In very recent research [8], the rank abundance curve of a given ecological dataset [19, 20] has been proposed to be modeled by a truncated exponential distribution

$$p_{(x,\lambda)} = p_i = \begin{cases} \frac{\exp\{\frac{C}{\lambda}\}}{\lambda(\exp\{\frac{C}{\lambda}\}-1)} \exp\left\{-\frac{x_i}{\lambda}\right\} & \text{for } 0 \leq x_i \leq C \\ 0 & \text{otherwise,} \end{cases} \quad (14)$$

where x_i is the i th species in the community, C is maximum value of species rank and λ is some rate parameter of the rank abundance curve under consideration. The model parameters C and λ are directly obtained from a given observed dataset by fitting techniques. The diversity index would be identified as the Tsallis entropy with respect to modeled truncated exponential distribution above, and has been analytically obtained in [8]

$$S_q = \frac{1}{q-1} \left(1 - \frac{\lambda}{q} \left(e^{\frac{Cq}{\lambda}} - 1 \right) \left(\lambda \left(e^{\frac{C}{\lambda}} - 1 \right)^{-q} \right) \right). \quad (15)$$

It is easy to verify the fallback of the Tsallis entropy (15) to Boltzmann entropy in statistical mechanics and to Shanon–Wiener diversity index when parameter C approaches to infinity and non-extensivity equals to one [8]. This ensures the validity of the proposed approach.

3.2. q -Thermodynamics of the truncated exponential distribution

The internal energy of the system under consideration is obtained by performing directly analytical manipulations on expression (3)

$$U_q = \frac{\lambda}{q} - C \left(e^{\frac{Cq}{\lambda}} - 1 \right)^{-1}. \quad (16)$$

And, the inverse of temperature (10) is, therefore, calculated by standard routine of thermodynamics as

$$\begin{aligned} \beta_q(\lambda, C) &= \frac{\partial S_q(\lambda, C)}{\partial U_q(\lambda, C)} \\ &= \frac{\partial S_q}{\partial \lambda} \left(\frac{\partial U_q}{\partial \lambda} \right)^{-1} + \frac{\partial S_q}{\partial C} \left(\frac{\partial U_q}{\partial C} \right)^{-1}. \end{aligned} \quad (17)$$

The resultant expression of the inverse of temperature (17) in above calculation is quite long and verbose to write down here. However, its limit when C approaches to infinity is subject of further interests, because of its simplicity and ease to compare to physical well-known consequences where the number of particle could be assumed to be infinity. In the interested limit, $C \rightarrow \infty$, the inverse of temperature reads

$$\lim_{C \rightarrow \infty} \beta_q = \lambda^{-q}. \quad (18)$$

The formula (18) provides the influence of non-extensivity on the physical temperature that leads to change the temperature as a q -power function of physical temperature. When the systems are extensive, or in other words, $q = 1$, the temperature (18) recovers real physical temperature as it is always in Gibbs-Boltzmann approach of thermodynamics, i.e. $k_B T = \lambda$.

In fact, the importance of (18) in ecological research is to determine a equilibrium parameter among systems based on their diversity indices, that satisfies thermodynamic consistence. This parameter is first obtained and introduced in ecological research.

4. Conclusions

Along with previous work [8], the present work is obviously an attempt to bring thermodynamics and statistical mechanics into the field of ecological research.

What has been done in this work is to obtain the internal energy U_q and the abstract temperature T_q of a ecological system in the context of Tsallis entropy which has been proved to be considered as diversity index of the corresponding ecological system. Once, the internal energy U_q and the abstract temperature T_q of a system are known, its thermodynamic theory would be well defined. The first introduced abstract temperature T_q in ecological research plays the role of new indicator for the equilibrium condition in ecology, which is similar to real physical temperature in the 0th law of thermodynamics defining the equilibrium among systems. The results in this work also confirm the thermodynamic fulfillment of newly constructed thermodynamical theory that early developed theories have been hardly achieved.

And, the derivative thermodynamic quantities such as other thermodynamic potentials, heat capacity, and many others will be implemented in next works, to evaluate the theory and to examine their ecological meaning.

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