Cent. Eur. J. Phys. • 7(3) • 2009 • 401-404
DOI: 10.2478/s11534-008-0149-3

VERSITA

Central European Journal of **Physics**

Conditional approach to thermo-superstatistics

Research Article

Sumiyoshi Abe*

Department of Physical Engineering, Mie University, Mie 514-8507, Japan†
Institut Supérieur des Matériaux et Mécaniques Avancés, 44 F. A. Bartholdi, 72000 Le Mans, France
Inspire Institute Inc., McLean, Virginia 22101, USA

Received 30 September 2008; accepted 22 October 2008

Abstract: A conditional approach is developed for establishing a generalized thermodynamic-like formalism for superstatistical systems. In this framework, the existence of two largely-separated time scales is explicitly taken into account. A generalization of Einstein's relation for fluctuations is derived based on the restricted conditional maximum-entropy method.

PACS (2008): 05.20.-y, 05.40.-a, 05.70.-a, 89.75.-k

Keywords: conditional thermodynamics • superstatistics • time-scale separation • generalization of Einstein's relation for fluctuations

1. Introduction

Superstatistics, which was anticipated in Refs. [1, 2] and formulated in Ref. [3], turned out to offer a highly general framework for describing statistical mechanical properties of complex systems in nonequilibrium quasi-stationary states. There, a fundamental premise is the existence of two largely-separated time scales: one is a short time scale concerning relaxation of a system to local equilibrium and the other is a long one associated with temperature variations on a large spatial scale.

Our purpose here is to construct the thermodynamic-like formalism for superstatistics. This issue has an obvious importance, since it may offer a macroscopic description of superstatistical systems. To do so, we base our consideration on the conditional concepts in probability theory. In this way, we shall explicitly take into account the existence of two separated time scales. Moreover, we show how the restricted conditional maximum entropy method can give rise to the distribution of temperature variations, which turns out to be a generalization of Einstein's relation for fluctuations [4, 5].

2. Hyperensemble and conditional concepts

Consider a system in a nonequilibrium quasi-stationary state. As the common first step, we divide it into a lot of cells. Each cell is small so that its state is characterized by a representative value of temperature (*i.e.*, local temperature) but still contains an enough number of elements. In other words, the system is composed of a collection of local canonical ensembles.

*E-mail: suabe@sf6.so-net.ne.jp
†Permanent address

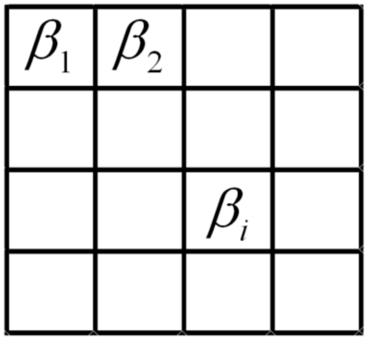

Figure 1. Each cell is in a local equilibrium state characterized by the value of inverse temperature, β.

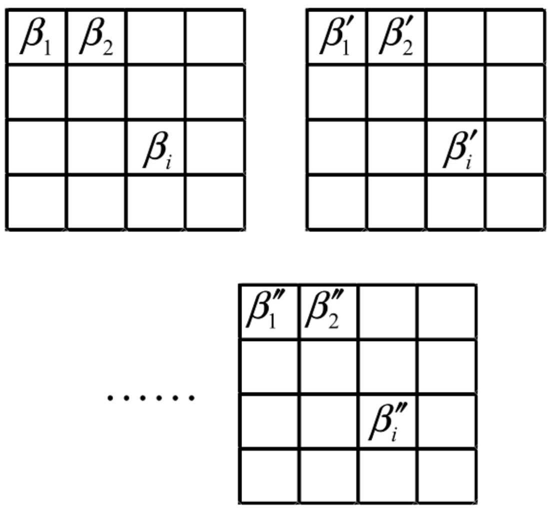

Figure 2. Hyperensemble.

Thus, there is temperature gradient between neighboring cells, and heat flows among them. Accordingly, the local temperature may vary (the other intensive variables, the pressure and chemical potential, may also vary, in general, but here only the temperature variations are considered for the sake of simplicity). To express this situation, we construct replicas of the system illustrated in Fig. 1 with different values of local temperature of the cell under consideration. The resulting ensemble is referred to as *hyperensemble* [6], and superstatistics is a theory of it (Fig. 2).

As mentioned earlier, in a superstatistical complex system, relaxation to local equilibrium is fast, whereas variation of temperature is slow. Its statistical-mechanical state in the hyperensemble picture is mathematically given by

$$p(\varepsilon_i) = \int d\beta\, f(\beta)\, Z^{-1}(\beta) \exp(-\beta\,\varepsilon_i), \qquad (1)$$

where the canonical factor, $Z^{-1}(\beta)\exp(-\beta\,\varepsilon_i)$ with $Z(\beta) = \sum_i \exp(-\beta\,\varepsilon_i)$, represents local equilibrium.

Eq. (1) can be viewed as follows. In a superstatistical system, both energy and temperature are random variables: the former is fast and the latter is slow. The joint distribution is given by $P(\varepsilon_i, \beta)$, which satisfies the Bayesian rule

$$P(\varepsilon_i, \beta) = P(\varepsilon_i|\,\beta)\, f(\beta), \qquad (2)$$

where $f(\beta) = \sum_i P(\varepsilon_i, \beta)$ is a marginal distribution describing the temperature variations and $P(\varepsilon_i|\,\beta)$ is a conditional distribution describing local equilibrium with a given value of the inverse temperature, β, which is of the canonical form:

$$P(\varepsilon_i|\,\beta) = Z^{-1}(\beta)\exp(-\beta\,\varepsilon_i). \qquad (3)$$

Since we are interested in the energy distribution, we calculate the marginal

$$p(\varepsilon_i) = \int d\beta\, P(\varepsilon_i, \beta), \qquad (4)$$

which is, in fact, identical to Eq. (1).

3. Generalized thermodynamics

We need consider the entropy to formulate a generalized thermodynamic-like formalism. Since we are concerned with local equilibria, what we should evaluate is the Boltzmann-Gibbs-Shannon entropy

$$S[E, B] = -\int d\beta \sum_i P(\varepsilon_i, \beta)\, \ln P(\varepsilon_i, \beta). \qquad (5)$$

Here, E and B are the random variables, the values of which are $\{\varepsilon_i\}_i$ and $\{\beta\}$, respectively, and the Boltzmann constant, k_B, is set equal to unity for the sake of simplicity. Substituting Eq. (2) into Eq. (5), we have

$$S[E, B] = S[E|\,B] + S[B], \qquad (6)$$

where$S[B]$ and $S[E|\,B]$ are the marginal and conditional entropies given by

$$S[B] = -\int d\beta\, f(\beta)\, \ln f(\beta), \qquad (7)$$

$$S[E|\,B] = \int d\beta\, f(\beta)\, S[E|\,\beta], \qquad (8)$$

with

$$S[E|\,\beta) = -\sum_i P(\varepsilon_i|\,\beta)\ \ln\ P(\varepsilon_i|\,\beta). \qquad (9)$$

Eq. (6) is nothing but Khinchin's second axiom for the Shannon entropy [7].

Using Eq. (3) in Eqs. (7) and (8), we obtain

$$S[E,\ B] = \overline{\beta\, U(\beta) + \ln Z(\beta)}\ + S[B]. \qquad (10)$$

In this expression, the over-bar denotes the average over the varying inverse temperature, $\overline{Q(\beta)} \equiv \int d\beta\, f(\beta)\, Q(\beta)$, and $U(\beta)$ is the "local" internal energy defined by

$$U(\beta) = \sum_i \varepsilon_i\, P(\varepsilon_i|\,\beta). \qquad (11)$$

Regarding Eq. (10), we notice the following point. The summation over the fast degree of freedom, E, is taken first, and subsequently the slow degree of freedom, B, is averaged over. In other words, the randomness of B is *quenched* when E is summed up. Thus, the existence of two largely-separated time scales in superstatistics is explicitly taken into account in this way.

From Eq. (10), it follows that the conditional entropy can be rewritten as

$$S[E|\,B] = \overline{\beta\,[U(\beta) - F(\beta)]}\,, \qquad (12)$$

where

$$F(\beta) = -\frac{1}{\beta}\ \ln Z(\beta) \qquad (13)$$

is the "local" free energy. Eq. (12) shows how the ordinary thermodynamic Legendre-transformation structure is modified in thermo-superstatistics. In particular, we notice that what is relevant here is the conditional entropy and not the total entropy.

To see how ordinary thermodynamics is modified, it may be of interest to consider a case when $f(\beta)$ is sharply peaked around a certain fixed representative value of β. In such a case, it is possible to systematically evaluate the superstatistical corrections to ordinary thermodynamics. This kind of discussions can be found in a recent work in Ref. [8].

4. Conditional maximum entropy method and determination of temperature variations

The present conditional approach also enables one to calculate the distribution, $f(\beta)$, describing temperature variations in a given superstatistical system. The basic idea is to make use of the maximum entropy method only for the slow degree of freedom, B, (recalling that the fast degree of freedom, E, was already summed up).

The simplest situation is the case when there is no *a priori* information available. In this case, we maximize the total entropy in Eq. (6) with respect only to $f(\beta)$ under the constraint on normalization alone:

$$\delta_f\ \left\{ S[E,\ B] - \alpha \left(\int d\beta\, f(\beta) - 1 \right) \right\} = 0, \qquad (14)$$

where α is a Lagrange multiplier and δ_f denotes the variation with respect to $f(\beta)$. The solution of Eq. (14) is given by

$$f(\beta) = \text{const} \cdot \exp\ S[E|\,\beta), \qquad (15)$$

where

$$S[E|\,\beta) = \beta\, U(\beta) + \ln Z(\beta)\ , \qquad (16)$$

which is a function only of β.

Eq. (15) has an interesting similarity with Einstein's theory of fluctuations [4, 5], which is based on the reversal of Boltzmann's relation: $W = e^S$. We notice however that the entropy appearing in Eq. (15) is not the ordinary thermodynamic entropy, S, but a conditional quantity given in Eq. (9). If there exists no correlation between E and B, then $P(\varepsilon_i|\,\beta) = P(\varepsilon_i)$, and accordingly $S[E|\,\beta)$ becomes reduced to the thermodynamic entropy. This means that the correlation between energy (E) and inverse temperature (B) is essential in superstatistics, and thus Eq. (15) is seen to be a generalization of Einstein's relation.

In the above, we have imposed only the constraint on normalization of $f(\beta)$. If additional information is available on averages of some physical quantities, say $Q^{(a)}(\beta)$ $(a = 1,\ 2,\ 3,\ \ldots)$, then the corresponding constraints can be included in Eq. (14). Accordingly, Eq. (15) is changed into the following form:

$$f(\beta) = \text{const} \cdot \exp\ \left\{ S[E|\,\beta) - \sum\nolimits_a \lambda^{(a)}\, Q^{(a)}(\beta) \right\}, \qquad (17)$$

where λ's are Lagrange multipliers.

5. Superstatistical gas

To illustrate the above formulation, let us consider a simple model of a superstatistical gas, which consists of n mutually noninteracting Brownian particles with unit mass in the spatial cells of a fluid that is subject to large-scale temperature variations such as those in turbulence. The conditional probability of a given value of the inverse temperature, β, is of the Maxwellian form:

$$P\left(\mathrm{v}_1, \mathrm{v}_2, \ldots, \mathrm{v}_n \middle| \beta\right) = \frac{1}{Z(\beta)} \exp\left[-\frac{\beta}{2}\left(\mathrm{v}_1^2 + \mathrm{v}_2^2 + \cdots + \mathrm{v}_n^2\right)\right], \tag{18}$$

$$Z(\beta) = \frac{V_0}{n!}\left(\frac{2\pi}{h^2\beta}\right)^{3n/2}, \tag{19}$$

where V_0 and h^3 are the volumes of the spatial cells in the fluid and those in phase space, respectively. The local internal energy is given by

$$U(\beta) = \frac{3n}{2\beta}. \tag{20}$$

Therefore, the quantity in Eq. (16) is calculated to be

$$S[E|\,\beta) = n\left(-\frac{3}{2}\ln\beta + c_0\right), \tag{21}$$

where $c_0 = -(3/2)\ \ln[h^2/(2\pi)] + \ln(V_0/n) + 5/2$. Accordingly, Eq. (15) yields the following distribution:

$$f(\beta) = \mathrm{const}\cdot\beta^{-3n/2}. \tag{22}$$

This is purely a power-law distribution and therefore is normalizable only over finite intervals of nonvanishing β. Eq. (22) is obtained without imposing any *a priori* constraint. Now, if we impose a constraint on the average internal energy, $\overline{U(\beta)}$, then we obtain from Eq. (17) that

$$f(\beta) = \mathrm{const}\cdot\beta^{-3n/2}\exp\left(-\lambda\frac{3n}{2\beta}\right), \tag{23}$$

where λ is a Lagrange multiplier. This is the inverse χ^2-distribution [9] peaked at $\beta = \lambda$ and is normalizable in the whole range of $\beta \geqslant 0$.

Finally, we wish to emphasize the following difference between the present approach and those in Refs. [6, 9]. The authors in Refs. [6, 9] derive the temperature distribution, $f(\beta)$, also by using the maximum entropy method by imposing three constraints: the normalization, the internal energy, and the average entropy. On the other hand, in the present approach, we impose only two constraints: the normalization and the internal energy; the quantity $S[E|\,\beta)$ automatically appears in $f(\beta)$ as in Eq. (15). Therefore, we have one Lagrange multiplier less compared to the discussions in Refs. [6, 9].

6. Conclusion

We have developed a conditional approach to thermo-superstatistics, in which the existence of two largely-separated time scales is explicitly taken into account. We have proposed a way of consistently deriving the distribution of temperature variations based on the restricted conditional maximum entropy method. We have found that this approach offers a generalization of Einstein's relation for fluctuations. These concepts and ideas are illustrated by employing a simple example of the superstatistical gas.

Acknowledgements

The present article is based on the author's invited talk at the International Conference on Statistical Mechanics ΣΦ2008 (14-18 July, 2008, Kolympari, Crete, Greece). The author would like to thank Giorgio Kaniadakis for the invitation to the conference. He also acknowledges the support by a Grant-in-Aid for Scientific Research from the Japan Society for the Promotion of Science.

References

[1] G. Wilk, Z. Wlodarczyk, Phys. Rev. Lett. 84, 2770 (2000)
[2] A. G. Bashkirov, A. D. Sukhanov, J. Exp. Theor. Phys. 95, 440 (2002)
[3] C. Beck, E. G. D. Cohen, Physica A 322, 267 (2003)
[4] A. Einstein, Ann. Phys. 33, 1275 (1910)
[5] L. D. Landau, E. M. Lifshitz, Statistical Physics, 3rd edition (Pergamon Press, Oxford, 1980)
[6] G. E. Crooks, Phys. Rev. E 75, 041119 (2007)
[7] A. I. Khinchin, Mathematical Foundations of Information Theory (Dover, New York, 1957)
[8] S. Abe, C. Beck, E. G. D. Cohen, Phys. Rev. E 76, 031102 (2007)
[9] J. Naudts, AIP Conf. Proc. 965, 84 (2007)