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Inverse temperature in Superstatistics

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Abstract. In this work, it is shown that there are (at least) three alternative definitions of the inverse temperature for a non-canonical ensemble. These definitions coincide in expectation but, in general, not in their higher moments. We explore in detail the application to the recent formalism of Superstatistics (C. Beck, 2003), and, in particular, to the configurational probability distribution in the microcanonical ensemble.

1. Introduction
In Statistical Mechanics the canonical ensemble is the ubiquitous probabilistic model. This is the correct model for a system immersed in a thermal bath at temperature $T$, and it is given by

$$P(\vec{r}, \vec{p} | \beta) = \frac{\exp(-\beta \mathcal{H}(\vec{r}, \vec{p}))}{Z(\beta)}$$

with $\beta = 1/k_B T$ and $\mathcal{H}$ the Hamiltonian of the system. Despite its undisputed utility, there are systems (for instance, out of equilibrium systems and also in the so called non-extensive systems) for which predictions using the canonical ensemble are not verified. For these cases, the idea of Superstatistics [1] has been recently proposed. Superstatistics assumes the correct ensemble is not canonical, but a superposition of canonical ensembles at different (inverse) temperatures, weighted by a factor $f(\beta)$,

$$\exp(-\beta E) \rightarrow \int d\beta f(\beta) \exp(-\beta E)$$

In a Bayesian interpretation, Superstatistics is nothing but marginalization over the $\beta$ parameter, thus

$$P(\vec{r}, \vec{p} | I) = \int_0^\infty d\beta P(\beta | I) P(\vec{r}, \vec{p} | \beta) = \int_0^\infty d\beta P(\beta | I) \frac{\exp(-\beta \mathcal{H}(\vec{r}, \vec{p}))}{Z(\beta)}$$

which means we have to make the identification

$$f(\beta) = \frac{P(\beta | I)}{Z(\beta)}.$$

Above, $I$ represents our state of knowledge with respect to the system, which leads to the particular assignment of $f(\beta)$ against other possible distributions.
2. Temperature in non-canonical ensembles

For an arbitrary probabilistic model $P(\vec{x}|I)$ of continuous variables $\vec{x}$ based upon a state of knowledge $I$, it can be shown [2], by using the divergence theorem that the following identity holds,

$$\langle \nabla \cdot \vec{v}(\vec{x}) \rangle_I = -\langle \vec{v}(\vec{x}) \cdot \nabla \ln P(\vec{x}|I) \rangle_I,$$

(4)

where $\vec{v}(\vec{x})$ is an arbitrary (differentiable) vector field. Let us assume now a model whose dependence on $\vec{x}$ is given only through a function $F(\vec{x})$ by

$$P(\vec{x}|I) = p(F(\vec{x})).$$

(5)

In this case, we have $\nabla P(\vec{x}|I) = (dp/dF)\nabla F$ and therefore, the identity in Eq. 4 takes the form

$$\langle \nabla \cdot \vec{v}(\vec{x}) \rangle_I = \langle \hat{\lambda}(F(\vec{x})) \vec{v}(\vec{x}) \cdot \nabla F(\vec{x}) \rangle_I,$$

(6)

where we have defined the quantity

$$\hat{\lambda}(f) = -\frac{d}{df} \ln p(f).$$

(7)

In the case of the canonical ensemble, the function $p(f)$ is simply $p(f) = \exp(-\lambda f)/Z(\lambda)$ and we recover $\hat{\lambda}(f) = \lambda$, a constant. This suggests that $\hat{\lambda}$ is a generalization of the idea of inverse temperature in the case of a physical system with $F$ corresponding to the Hamiltonian $\mathcal{H}$ and $\lambda$ to the inverse temperature $\beta = 1/k_B T$. We will call $\hat{\lambda}(f)$ the fundamental inverse temperature, in order to distinguish it from similar functions we will present shortly.

This quantity has been previously used by Velázquez and Curilef [3] as an effective inverse temperature in the particular case of Superstatistics.

Let us take Eq. 6 and use $\vec{v} = \vec{\omega}/(|\vec{\omega}| \cdot \nabla F)$, this leads to

$$\langle \nabla \cdot \left[ \frac{\vec{\omega}(\vec{x})}{|\vec{\omega}(\vec{x})| \cdot \nabla F(\vec{x})} \right] \rangle_I = \langle \hat{\lambda}(F) \rangle_I,$$

(8)

where we recognize the quantity in the left hand side as Rugh’s inverse temperature [4, 5],

$$\hat{\lambda}_R(\vec{x}) = \nabla \cdot \left[ \frac{\vec{\omega}(\vec{x})}{|\vec{\omega}(\vec{x})| \cdot \nabla F(\vec{x})} \right].$$

(9)

For the kind of ensemble defined by the condition $P(\vec{x}|I) = p(F(\vec{x}))$ we see that the probability of observing a particular value $f$ of the function $F(\vec{x})$ is

$$P(F(\vec{x}) = f|I) = \langle \delta(F(\vec{x}) - f) \rangle_I = \int d\vec{x} \delta(F(\vec{x}) - f)p(F(\vec{x})) = p(f)\Omega(f)$$

(10)

where we have introduced the density of states of $F$,

$$\Omega(f) = \int d\vec{x} \delta(F(\vec{x}) - f).$$

(11)

The equivalent of the identity in Eq. 4 for the probability distribution of the values of $F$ is

$$\langle \frac{dg(f)}{df} \rangle_I = \langle g(f) \left[ \hat{\lambda}(f) - \hat{\lambda}_R(f) \right] \rangle_I,$$

(12)
with
\[ \hat{\lambda}_\Omega(f) = \frac{d}{df} \ln \Omega(f). \] (13)

We will call this quantity the microcanonical inverse temperature, given that it coincides with the traditional definition of temperature in the microcanonical ensemble,
\[ \frac{1}{T} = \frac{dS(E)}{dE} = \frac{d}{dE} k_B \ln \Omega(E). \] (14)

If we choose \( g(f) = 1 \) in Eq. 12 we immediately see that, taking also into account Eq. 8,
\[ \langle \hat{\lambda}_\Omega(f) \rangle_I = \langle \hat{\lambda}(f) \rangle_I = \langle \hat{\lambda}_R(\vec{x}) \rangle_I, \] (15)
i.e., all three alternative definitions of temperature (fundamental, Rugh’s and microcanonical) given by Eqs. 7, 9 and 13, are equivalent on expectation.

3. The particular case of Superstatistics
In the case of Superstatistics, \( p(f) \) has the form
\[ p(f) = \int d\lambda P(\lambda|I) \frac{\exp(-\lambda f)}{Z(\lambda)} \] (16)
therefore the fundamental inverse temperature is given by
\[ \hat{\lambda}(f) = \frac{d}{df} \ln p(f) = \frac{\int d\lambda \cdot \lambda P(\lambda|I) \exp(-\lambda f)}{p(f) Z(\lambda)}. \] (17)

We can gain further understanding of this expression if we write \( P(\lambda|\vec{x}) \) using Bayes’ theorem, as
\[ P(\lambda|\vec{x}) = \frac{P(\lambda|I) P(\vec{x}|\lambda)}{P(\vec{x}|I)} = \frac{1}{p(F(\vec{x}))} P(\lambda|I) \frac{\exp(-\lambda F(\vec{x}))}{Z(\lambda)} \] (18)
which allows us to write \( \hat{\lambda}(f) \) as
\[ \hat{\lambda}(F(\vec{x})) = \int d\lambda \cdot \lambda P(\lambda|\vec{x}) = \langle \lambda \rangle_{\vec{x}}. \] (19)

This means the fundamental estimator \( \hat{\lambda}(F(\vec{x})) \) in this case is the expectation of the “genuine” Superstatistical inverse temperature given that the system is in a known microstate \( \vec{x} \). Taking expectation on both sides under a state of knowledge \( I \), we see that
\[ \langle \hat{\lambda} \rangle_I = \langle \lambda \rangle_I, \] (20)
i.e., the expectation of any of the three inverse temperatures is equal to the Superstatistical expectation of \( \lambda \). In order to relate to the fluctuations of the superstatistical parameter \( \lambda \), we differentiate \( \langle \lambda \rangle_{\vec{x}} \) with respect to \( F(\vec{x}) \), obtaining
\[ \frac{d}{dF} \langle \lambda \rangle_{\vec{x}} = -\langle \lambda^2 \rangle_{\vec{x}} + \langle \lambda \rangle_{\vec{x}}^2 \] (21)
Taking expectation on both sides under \( I \) we see that
\[ \langle \hat{\lambda} \rangle_I = \langle \lambda \rangle_I. \] (22)
i.e., the expectation of any of the three inverse temperatures is equal to the expectation of the superstatistical parameter $\lambda$. In order to connect the fluctuations of the superstatistical parameter $\lambda$ with the fluctuations of the estimators, we differentiate $\langle \lambda \rangle_{\vec{x}}$ with respect to $F(\vec{x})$, obtaining

$$\frac{d}{dF} \langle \lambda \rangle_{\vec{x}} = -\langle \lambda^2 \rangle_{\vec{x}} + \langle \lambda \rangle_{\vec{x}}^2$$

Taking expectation on both sides under the state of knowledge $I$ we see that

$$\langle (\delta \lambda)^2 \rangle_I = \langle (\delta \hat{\lambda})^2 \rangle_I - \langle \frac{d \hat{\lambda}}{dF} \rangle_I,$$

which tells us that the fundamental inverse temperature does not necessarily have the same fluctuations of the parameter $\lambda$.

4. Application to the microcanonical coordinate distribution

For a physical system with Hamiltonian

$$\mathcal{H}(\vec{r}, \vec{p}) = \frac{1}{2m} (\vec{p})^2 + \Phi(\vec{r}),$$

it can be shown [6] that the correct probability distribution for the coordinates at constant energy (microcanonical ensemble) is

$$P(\vec{r}|E) = \frac{1}{\eta(E)} \Theta(E - \Phi(\vec{r})) \sqrt{E - \Phi(\vec{r})}^{3N-2}$$

where $\eta(E)$ is proportional to the density of states $\Omega(E)$. For this distribution, the condition in Eq. 5 holds, with $F = \Phi$, and therefore

$$p(\phi) = \frac{1}{\eta(E)} \Theta(E - \phi) \sqrt{E - \phi}^{3N-2}.$$  

The fundamental inverse temperature is then given by

$$\hat{\beta}(\phi) = -\frac{d}{d\phi} \ln p(\phi) = \frac{d}{d\phi} \ln \Theta(E - \phi) + \frac{3N - 2}{2(E - \phi)}.$$  

This leads to

$$\langle \nabla \cdot \vec{v} \rangle_E = \left\langle \frac{3N - 2}{2(E - \Phi)} \vec{v} \cdot \nabla \Phi \right\rangle_E,$$

given that the first term on the right hand side of Eq. 28 vanishes in expectation. We can take the fundamental inverse temperature to be, without loss of generality,

$$\hat{\beta}(\phi) = \frac{3N - 2}{2(E - \phi)},$$

which, interestingly, coincides with the kinetic inverse temperature, as $E - \Phi = \frac{p^2}{2m}$ is the kinetic energy.

We have, finally, the equality of all three temperatures,

$$\langle \nabla \cdot \left[ \frac{\vec{\omega}}{\omega} \nabla \Phi \right] \rangle_E = \left\langle \frac{3N - 2}{2(E - \Phi)} \right\rangle_E = \left\langle \frac{d}{d\Phi} \ln \Omega(\Phi) \right\rangle_E.$$
5. Conclusions
We have shown that, for ensembles which are dependent of a Hamiltonian but are not canonical, at least three different definitions of inverse temperature are admissible. A particular case of this is Superstatistics, and consequently the $q$-exponential (Tsallis) distributions. All three estimators agree in expectation but their fluctuations are not necessarily equal. These results reveal a possible conceptual ambiguity in the definition of temperature for superstatistical systems, which must be resolved in order to construct an internally consistent theory of these systems.

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