Temperature fluctuations and mixtures of equilibrium states in the canonical ensemble

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Abstract. It has been suggested recently that ‘\(q\)-exponential’ distributions which form the basis of Tsallis’ non-extensive thermostatistical formalism may be viewed as mixtures of exponential (Gibbs) distributions characterized by a fluctuating inverse temperature. In this paper, we revisit this idea in connection with a detailed microscopic calculation of the energy and temperature fluctuations present in a finite vessel of perfect gas thermally coupled to a heat bath. We find that the probability density related to the inverse temperature of the gas has a form similar to a \(\chi^2\) density, and that the ‘mixed’ Gibbs distribution inferred from this density is non-Gibbsian. These findings are compared with those obtained by a number of researchers who worked on mixtures of Gibbsian distributions in the context of velocity difference measurements in turbulent fluids as well as secondaries distributions in nuclear scattering experiments.

1. Introduction

Most if not all textbooks on thermodynamics and statistical physics define temperature as being a quantity which, contrary to other thermodynamic observables like energy or pressure, does not admit fluctuations. Because of that, it is somewhat surprising to see papers with the expression ‘temperature fluctuations’ in their titles appearing from time to time in serious scientific journals on subjects as various as particle physics and fluid dynamics (see, e.g., [1, 2, 3, 4]). Indeed, how can the temperature of a system, however small, fluctuate if one defines it ‘as equal to the temperature of a very large heat reservoir with which the system is in equilibrium and in thermal contact’ [5]? Also, in the case of the reservoir, how can temperature be a fluctuating parameter if its definition requires one to assume the thermodynamic limit, i.e., to assume that the system acting as a reservoir is composed of an infinite number of particles or degrees of freedom? Presumably, the thermodynamic limit should rule out any fluctuations of thermodynamic quantities like the mean energy or the pressure, so that if temperature is related to these quantities, how can it fluctuate?

The solution to this conundrum is quite simple. First, the standard definition of temperature found in textbooks is too restrictive: there is not one but many definitions of temperature and of quantities analogous to temperature, as well as many physical (non-equilibrium) situations in the context of which these different definitions admit fluctuations [6]. Second, the standard definition of temperature involving the thermodynamic limit is only an idealization, a “purist” definition. Real physical bodies are always composed of a finite number of particles or degrees of freedom, which means that the concept of temperature must be applicable...
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outside the idealized realm in which it is defined if experimentalists are indeed able to measure the temperature of real bodies in real laboratories. Physically, this means also that there must be a threshold number of particles or degrees of freedom (more or less precisely defined) above which a system can be measured or “felt” to have a temperature [7]. Well above this number, temperature is assured to be defined and likely to be constant, while close to this number it may be well-defined, but may change in time or vary in space; that is, it may fluctuate!

All the studies concerned with temperature fluctuations exploit one of the above ‘indents’ to the standard definition of temperature. That is, they either consider alternatives to the standard definition of temperature which do admit fluctuations or apply the ‘thermodynamic-limit’ definition of temperature in situations where the thermodynamic limit is assumed to be “effectively” reached without being reached “formally”, so to speak. Our aim in this paper is to review a number of these alternative definitions and situations, and to dispel, in doing so, some of the misunderstanding and misconceptions surrounding the notion of temperature fluctuations. We will be particularly interested in giving a detailed calculation of temperature fluctuations present in a system which is commonly thought to be at constant temperature, namely a system composed of a finite number of independent particles (basically a finite volume of perfect gas) thermally coupled to an infinite-size heat reservoir at constant temperature. In the following, we will show that if instead of defining the temperature of the particle system simply as being equal to the temperature of the reservoir we apply the statistical definition of temperature to the finite-size system of particles (provided that the number of particles is sufficiently large), then we must come to the conclusion that the system’s temperature is fluctuating, just as its internal energy is fluctuating because of the thermal coupling with the heat reservoir. The temperature of the particle system, in this case, is precisely related to its internal energy, and can be seen as a ‘microcanonical temperature’ associated with the microscopic configurations of a system whose internal energy is held fixed during a period of time shorter than the energy fluctuations time scale.

Our motivation for studying the temperature fluctuations of a system of particles in a canonical ensemble setting, and for presenting moreover this study in a book about non-extensive statistical mechanics is threefold. First, a system composed of a bunch of independent particles coupled to a heat bath is one of the few thermodynamic systems for which the probability density describing the temperature fluctuations can be calculated directly using ‘first-principle’ or ‘microscopic’ arguments. Second, for this specific system, the probability density of the temperature happens to be very similar to a class of $\chi^2$ densities of temperature fluctuations recently introduced by Wilk and Włodarczyk [8, 9, 10], as well as by Beck [11, 12, 13], in the context of non-extensive statistical mechanics [14, 15]. Finally, the models of non-extensive behavior proposed by these authors are all based on the idea of ‘mixed equilibrium states,’ i.e., near-equilibrium states of systems characterized by fluctuating temperatures. In the context of the present study, this idea, as we will see, arises very naturally.

2. Phenomenology of temperature fluctuations

One can imagine many different systems exhibiting temperature fluctuations. The common characteristic of all of these systems is that they are non-equilibrium systems. Below, we list and briefly comment four systems or, more precisely, four generic situations for which temperature can be defined and be thought to fluctuate. The list is far from being exhaustive: the first three situations are presented to give an idea of the physical phenomena involving temperature fluctuations which have been discussed from the point of view of non-extensive
Temperature fluctuations recently. The fourth and last case of the list, the particles and heat bath system, is the focus of this paper (see Section 3).

- **Temperature fluctuations in a gas.** A system with fluctuations of temperature ‘spread’ over space can be constructed simply in the following way. Take a vessel of gas, and divide it in some number of compartments thermally insulated from one another. Bring the content of each compartment at different temperatures, and then remove the insulating partition. From the moment where the partition is removed, a process of temperature relaxation will take place, whereby the particles forming the gas will collide and exchange energy until a state of uniform temperature is achieved.

The details of the relaxation process are quite complicated at the microscopic level, and depend on the nature and properties of the gas considered. But, at the macroscopic level, the net result of this experiment is simply described: between the time where the partition is removed and the time where the gas’ temperature is completely uniform, the temperature field of the gas will vary in space as well as in time. Thus, as a whole, the vessel of gas can be said to be in a state of fluctuating temperature. This is admittedly an expletive way to say that the temperature is not homogeneous in space, but the expression is nonetheless correct and widely used (e.g., when referring to the spatial temperature fluctuations of the cosmic background radiation).

Experimentally, there are various ways by which one can reconstruct the temperature field of the gas, apart from plunging a thermometer into it at different places. A simple method (conceptually, not experimentally) consists in measuring the momenta (along a fixed direction) of many particles of the gas at one point in space or, equivalently, sample the momentum of a single particle over some period of time, and construct from the measurements a histogram of the number of particles $L(x)$ having a momentum value between $x$ and $x + \Delta x$. ($\Delta x$ is the coarse-graining scale at which two particles are considered to have different momentum values.) If the sample of measurements is large enough, then it is expected that the form of $L(x)$ should approximately be Gaussian, as predicted by Maxwell and Boltzmann, with a variance proportional to the temperature $T$. Hence, fitting $L(x)$ with a Gibbs distribution proportional to $\exp(-\beta x^2)$ or calculating its variance or its half-width all constitute operational procedures for probing the temperature $T = (k_B \beta)^{-1}$ of the gas. It should be noted that the accuracy of any of these methods for obtaining $\beta$ depends on (i) the number of measurements used to construct $L(x)$, which should be large, but not necessarily infinite!, and (ii) the assumption that the gas is non-interacting (perfect) or weakly interacting. These two points are necessary to assume that the momenta of the particles are Gaussian distributed.

- **Velocity temperature in turbulent fluids.** It is common in turbulent flow experiments to define an analog of temperature by looking at the distribution $L(x)$ of particle velocity differences in a restricted region of a fluid using anemometry or interferometry equipments. Just as in the case of the gas, temperature is defined for a fluid by fitting $L(x)$ with a Gibbs distribution of the form $e^{-\beta u(x)}$, where $u(x)$ is the one-particle energy function taken to be a quadratic or a nearly quadratic function of the velocity variable. This defines a local inverse temperature $\beta$ which, it is important to note, does not represent the physical inverse temperature of the fluid. Rather, it is a correlate of the local rate of energy dissipation that takes place at the microscopic level over a time scale known as the Kolmogorov time. The Gibbsian character of $L(x)$ and the fluctuations of the velocity temperature in space, related to the spatial fluctuations of the local energy dissipation rate, have been observed in many experiments of weakly turbulent fluids (see, e.g., and references cited...
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therein). However, for fluids at high Reynolds number, i.e., highly turbulent fluids, a totally different behavior of $L(x)$ is observed. Indeed, recent experiments have demonstrated that $L(x)$ in strong turbulence regimes is not Gibbsian; instead, it takes the form of a power-law which appears to be well-fitted by a so-called $q$-exponential function

$$e_q^{-\beta u(x)} = [1 - (1 - q)\beta q u(x)]^{1/(1-q)}, \quad (1)$$

where $\beta^{-1}$ is a fitting parameter analogous to temperature [11, 18, 19]. To account for this non-Gibbsian behavior, Beck has suggested to interpret $q$-exponential distributions as ‘mixed’ distributions arising from an ensemble of exponential distributions $e^{-\beta u(x)}$ parameterized by a fluctuating inverse temperature $\beta$ [11, 12, 13]. That is to say, if one assumes that what is probed in those experiments is not one velocity distribution $L(x)$ characterized by a fixed temperature, but a continuum of distributions $L(x)$ having different temperatures, then what should be observed physically is an average Gibbs distribution, the average being performed over the temperature fluctuations. In this context, the essential point made by Beck (see [11] for the details) is that, if the probability density $f(\beta)$ ruling the temperature fluctuations has the following form:

$$f(\beta) = \frac{1}{\Gamma (\frac{1}{q-1})} \left[ \frac{1}{(q-1)\beta_0} \right]^{\frac{1}{q-1}} \beta^{-\frac{1}{q-1}-1} \exp \left[ -\frac{\beta}{(q-1)\beta_0} \right], \quad (2)$$

where $\beta \geq 0$ and $q > 1$, then the mixed distribution obtained by averaging the Gibbs kernel $e^{-\beta u(x)}$ with $f(\beta)$ is $q$-exponential. Indeed, one can readily verify that

$$e_q^{-\beta_0 u(x)} = \int_{0}^{\infty} e^{-\beta u(x)} f(\beta) d\beta \quad (3)$$

using the above variant of the $\chi^2$ or gamma density [27] for $f(\beta)$. This integral representation of the $q$-exponential function is sometimes referred to as Hilhorst’s formula [20, 21].

- **Nuclear collision temperature.** The basic idea involved in the definition of temperature in nuclear scattering experiments is to consider the set of particles produced during a collision (called the products) as forming a gas of particles which, at a first level of approximation, can be treated as being non-interacting (perfect gas approximation). From this point of view, a concept of ‘collision temperature’ is defined essentially in the same way that temperature was defined for turbulent fluids except that the precise physical property to look at in scattering experiments is not the shape of the momenta distribution itself, but the so-called exponential dependence of the distribution of secondaries with respect to transverse momentum [4, 13].

Since the number of particles probed during one scattering experiment is never very large ($\sim 10 - 1000$), one must sometimes collect the momenta of particles over many scattering experiments before the exponential shape of the secondaries distribution reveals itself. However, this is not always the case: in heavy-ion experiments at very high energy, for example, it is often observed that a single event, i.e., only one scattering experiment is sufficient for a thermostatistical analysis to be effective [4]. Also, what is often seen is that scattering events of same nature repeated over time yield different collision temperatures, making obvious that temperature is a fluctuating parameter.

Observations of ‘non-extensive’ behavior in relation to this thermodynamic picture of scattering experiments have been reported so far on two different fronts. The first is related to the distribution of secondaries, and, more precisely, to observed deviations of this distribution from its expected exponential form. Due to the limited space available here, we will not discuss this case as it is quite involved. Let us only mention that Wilk
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and Włodarczyk have advanced in [9] a ‘mixed exponential distribution’ model of these deviations analogous to the one suggested by Beck.

The second case of ‘non-extensive’ behavior concerns the absorption of cosmic ray particles in lead chambers [8, 9, 10]. This case was also studied by Wilk and Włodarczyk who suggested for its explanation yet another variant of the $\chi^2$ temperature fluctuations model (actually before Beck applied similar ideas to the study of turbulent fluids). The physics explained by their model is the following. The number $N$ of hadronic particles absorbed in lead chambers is usually measured to be distributed as a function of the depth $l$ according to

$$\frac{dN}{dl} \propto e^{-l/\lambda},$$

where $\lambda$ is the mean free path parameter or mean penetration depth (an analog of temperature). This exponential distribution is, at least, what is observed at small penetration depths ($\sim 60$ cm of lead); beyond that, what is observed is that $dN/dl$ changes to a power-law which can be fitted by a $q$-exponential with $q \simeq 1.3$. To account for this crossover, Wilk et al. simply conjectured that the $\lambda$ parameter characterizing the long flying components (i.e., the deep penetration events) is subject to fluctuations, and, thus, that the $q$-exponential penetration profiles observed experimentally for these components are mixtures of exponential distributions. By assuming that the probability density of $\lambda$ is a $\chi^2$ density, they were effectively able to reproduce the non-exponential distributions measured in laboratories [8,9,22].

- **System coupled to a heat bath.** Our last example in the panorama of thermodynamic systems characterized by temperature fluctuations is the prototypical system defining the canonical ensemble: that is, a small system $S$ in thermal contact with a larger system $R$ acting as a heat reservoir. Following the standard textbook definition of the canonical ensemble, one should say that the temperature of system $S$ at equilibrium is constant, and is equal to the temperature of system $R$; after all, this is how thermal equilibrium is defined. However, such a statement does not do justice to one important property of $S$ which is that the energy density of $S$ fluctuates (because of its finiteness) while the energy density of $R$ does not (by definition of a heat bath).

To make this statement more precise, suppose that $S$ consists of $n$ independent particles whose energy density or mean total energy is given by

$$U_n = \frac{1}{n} \sum_{i=1}^{n} u_i,$$

Since the particles are coupled to $R$, the $u_i$’s above are random variables, which means that $U_n$ is also a random variable. Moreover, observe that $U_n$, for any finite $n$, has a non-negligible probability to assume many different values because, in this case, the probability density $g_n(u)$ of $U_n$ is not a Dirac-delta function. The Dirac density, formally, is only a limiting density which “attracts” $g_n$ as $n \to \infty$. (This basically follows from the law of large numbers.) Thus, if we can associate an inverse temperature $\beta(u)$ to all energy states such that $U_n = u$, e.g., by applying the equipartition theorem or by fitting a distribution of energy levels with a Gibbs distribution as described earlier, then we must conclude that there are different values of $\beta$ effectively realized ‘in’ or ‘by’ the particle system, so to speak. That is to say, the probability density $f_n(\beta)$ for $\beta$, obtained from $g_n(u)$ by a change of variables $u \to \beta(u)$, cannot be a Dirac-delta function if $g_n(u)$ is not itself a delta function. It is to be expected that $f_n(\beta) \to \delta(\beta - \beta_0)$, where $\beta_0$ is the inverse temperature of heat bath, only in the thermodynamic limit where $n \to \infty$. These points are discussed in more mathematical details in the next sections.
3. Energy and temperature fluctuations in the canonical ensemble

Our analysis of energy and temperature fluctuations of a system coupled to a heat bath will be presented in the context of the following model. Let a vessel of gas containing \( n \) independent (classical) particles be thermally coupled to a heat reservoir characterized by a fixed inverse temperature \( \beta_0 \). The state of each particle is represented by a random variable \( X_i \), \( i = 1, 2, \ldots, n \), to which is associated a (one-particle) energy \( u(X_i) \). The set of outcomes of each of the \( X_i \)'s (the one-particle state space) is denoted by \( \mathcal{X} \). With these notations, the energy density or mean energy of the gas is written as

\[
U_n(x^n) = \frac{1}{n} \sum_{i=1}^{n} u(x_i) = \sum_{x \in \mathcal{X}} L_n(x) u(x),
\]

where \( x^n = x_1, x_2, \ldots, x_n \) is the joint state of the system, i.e., the state of the system as a whole. Note that in the above expression we have defined \( L_n(x) \) as the relative number of particles which are in state \( x \), i.e., as

\[
L_n(x) = \frac{\#(\text{particles} : X_i = x)}{n}.
\]

It should be noted that the vector \( L_n \) is nothing but the histogram of one-particle states referred to as previously when we discussed temperature fluctuations. Indeed, in the case where \( x \) represents a momentum variable, the quantity \( nL(x) \) precisely counts the number of particles having a momentum value equal to \( x \). (We assume throughout that the \( X_i \)'s are discrete random variables; the continuous case can be treated with minor modifications.)

Now, owing to the fact that the gas is treated in the canonical ensemble, in the sense that it is coupled to a heat bath, we have

\[
P_n(x^n) = P_n(X_1 = x_1, X_2 = x_2, \ldots, X_n = x_n) = \frac{e^{-\beta_0 nU_n(x^n)}}{Z_n(\beta_0)}
\]

as the joint probability distribution over the states \( x^n \), where

\[
Z_n(\beta_0) = \sum_{x^n \in \mathcal{X}^n} e^{-\beta_0 nU_n(x^n)}
\]

is the \( n \)-particle partition function. Of course, since all the particles are assumed to be independent (perfect gas assumption), as well as all individually coupled to the same heat bath, we can also write

\[
P_n(x^n) = p(x_1)p(x_2) \cdots p(x_n) = \frac{e^{-\beta_0 u(x_1)}}{Z(\beta_0)} \frac{e^{-\beta_0 u(x_2)}}{Z(\beta_0)} \cdots \frac{e^{-\beta_0 u(x_n)}}{Z(\beta_0)}
\]

with \( Z(\beta_0) = Z_1(\beta_0) \) (one-particle partition function). These equations make obvious the fact that what we are dealing with is a system of independent and identically distributed (IID) random variables.

The first quantity that we are interested to calculate at this point is the probability distribution or probability density \( g_n(u) \) associated with the outcomes \( U_n = u \). A priori, finding an exact expression for \( g_n(u) \) is not an easy task, even though \( U_n \) is the simplest sum of random variables that one can imagine, i.e., one involving IID random variables. Fortunately, there exists a general method by which one can obtain a very accurate approximation of \( g_n(u) \) for \( n \gg 1 \) without too much efforts. This method is based on the theory of large deviations \cite{23}, and proceeds by observing that probability densities of normalized sums of IID random variables, such as the one defining \( U_n \), satisfy two basic properties: (i) they decay exponentially with the number \( n \) of random variables involved; and (ii) the rate of decay is a function of the
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value (outcome) of the sum alone. In the present context, this means specifically that \( g_n(u) \) has the form

\[
g_n(u) \asymp e^{-nD(u)}.
\]  

(11)

The sign ‘\( \asymp \)’ above is there to emphasize that the large deviation approximation of the density \( g_n(u) \) is ‘exponentially tight’ with \( n \), i.e., that it is exact up to \( O(n^{-1} \ln n) \) marginal corrections to the rate of decay \( D(u) \). This rate of decay or rate function is itself calculated as the Legendre transform of the quantity

\[
\lambda(k) = \ln E[e^{ku(X)}] = \ln \sum_{x \in X} p(x)e^{ku(x)}
\]  

(12)

which is the cumulant generating function of the probability distribution \( p(x) \) associated with the IID random variables. The result of this transform is

\[
D(u) = uk(u) - \lambda(k(u)),
\]  

(13)

\[
\beta(u) = dH(u)\bigg|_{k(u)} = u.
\]  

(14)

A proof of this result can be found in [23, 24, 25, 26] (see also the notes contained in [23] for a historical account of the developments of the theory of large deviations together with a list of the founding papers of this theory).

Physicists who are not familiar with the formalism of large deviations will probably look at the above formulae for calculating \( g_n(u) \) as being quite formal if not fancy (in a pejorative way). For them, we offer the following alternative derivation of \( g_n(u) \). Consider the density \( \Omega_n(u) \) of states \( x^n \) having the same energy \( U_n(x^n) = u \). Following the thermostatistics of Gibbs and Boltzmann, this density of states must be an exponential function of \( n \) taking the form

\[
\Omega_n(u) \asymp e^{nH(u)},
\]  

(15)

where \( H(u) \) is the entropy of the system at energy density \( u \). As is well-known, the function \( H(u) \) is also obtained by a Legendre transform, this time involving the logarithm of the one-particle partition function or free energy. Now, using the above approximation for \( \Omega_n(u) \), and the fact that all states \( x^n \) such that \( U_n(x^n) = u \) have the same probability

\[
P_n(x^n : U_n(x^n) = u) = \frac{e^{-\beta_n u}}{Z(\beta_0)},
\]  

(16)

we can write

\[
g_n(u) = \Omega_n(u)P_n(x^n : U_n(x^n) = u) \asymp e^{-n[U_n + \ln Z(\beta_0) - H(u)]}.
\]  

(17)

Thus, we arrive at

\[
D(u) = u\beta_0 + \ln Z(\beta_0) - H(u).
\]  

(18)

One can verify that the above expression for the rate function is totally equivalent to the one found in the context of large deviation theory. Both expressions are, in fact, related by the transformation \( \beta(u) = \beta_0 - k(u) \), where

\[
\beta(u) = \frac{dH(u)}{du}
\]  

(19)
is the usual thermostatistical definition of the inverse temperature. The proof of this equivalence result follows, essentially, by noting that

\[ \lambda(k) = \ln \sum_{x \in \mathcal{X}} e^{-\beta_0 u(x)} Z(\beta_0) e^{ku(x)} = \ln Z(\beta_0 - k) - \ln Z(\beta_0), \]  

(20)

and by using the familiar expression \( H(u) = u \beta(u) + \ln Z(\beta(u)) \) for the entropy. (The complete verification of the result is left as an exercise to the reader.)

Let us now turn to the matter of defining an inverse temperature \( \beta \) for our system of IID particles, and to the complement matter of inferring the probability density \( f_n(\beta) \). Following our discussion of temperature fluctuations, it should be expected that there are many ways by which one can assign a temperature to the microcanonical set of states defined by

\[ M_n(u) = \{ x^n : U_n(x^n) = u \}. \]  

(21)

Also, it is to be expected that one definition of temperature may not necessarily coincide with another in the case of finite-size \((n < \infty)\) systems. We illustrate this possibility by comparing below four different definitions or ‘flavors’ of temperature.

- **Derivative of entropy or free energy.** An obvious way to associate a temperature to the states in \( M(u) \) is to take the energy derivative of the microcanonical entropy \( H(u) \) as in Eq. (19). Equivalently, one can solve the equation

\[ - \frac{d \ln Z(\beta)}{d \beta} = u \]  

(22)

for \( \beta \), or compute the function \( k(u) \) from Eq. (14) and use the relation \( \beta(u) = \beta_0 - k(u) \). The inverse temperature obtained by any of these methods will be denoted by \( \beta_{th}(u) \) to emphasize that it is based on *intensive* thermodynamic potentials which do not depend on \( n \).

- **Derivative of the density of state.** A slightly different definition of inverse temperature is obtained by taking the ‘logarithmic derivative’ of \( \Omega_n(u) \) with respect to the total energy \( nu \)

\[ \beta_{th}(u) = \frac{1}{\Omega_n(u)} \frac{d \Omega_n(u)}{d (nu)} = \frac{d \ln \Omega_n(u)}{d (nu)} \]  

(23)

in lieu of the derivative of the entropy exponent as in Eq. (19). This defines another inverse temperature \( \beta_{th}(u) \) which differs from \( \beta_{th}(u) \) by a term of order \( O(n^{-1} \ln n) \) which vanishes as \( n \to \infty \).

- **Gibbsian distribution of states.** An inverse temperature \( \beta_L(u) \) can be defined from a phenomenological point of view by fitting a given distribution of states \( L_n(x) \) of mean energy \( U_n = u \) with a Gibbs distribution of the form

\[ L^n(x) = \frac{e^{-\beta_L(u)u(x)}}{Z(\beta_L(u))}. \]  

(24)

We have described this definition of temperature earlier (see Section 2), and have noted that it is accurate when \( n \) is large. To be more precise, it is accurate in a probabilistic sense because, in theory, there is always a possibility that non-Gibbsian distributions \( L_n(x) \) of mean energy \( U_n = u \) can be observed. However, the probability associated with such a possibility is very small and vanishes rapidly as \( n \to \infty \). To see why, let us consider all the states \( x^n \) and their corresponding distributions \( L_n \) present in the energy ‘box’ \( M(u) \). What we want to show is that the probability \( P_n(L^n) \) that \( L^n \) is observed in \( M(u) \) is overwhelmingly large compared to the probability \( P_n(L) \) to observe any
other distribution $L \neq L^n$. To show this, we use another result of the theory of large
deviations [24, 25, 26] which states that
\[
\frac{P_n(L)}{P_n(L^n)} \approx e^{-n[H(L^n) - H(L)]} = e^{-n\Delta H},
\]
where
\[
H(L) = -\sum_{x \in \mathcal{X}} L(x) \ln L(x)
\]
is the Boltzmann-Gibbs-Shannon entropy, and $\Delta H = H(L^n) - H(L)$. Using the fact
that $L^n$ is a maximum entropy distribution under the constraint $U_n = u$, it is easy to
see that $\Delta H \geq 0$ with equality if and only if $L = L^n$, so that $P_n(L)/P_n(L^n) \to 0$ as
$n \to 0$. Moreover, the discrepancy between the two probabilities is exponentially large
in $n$. Thus, for $n$ large it can be said that any distribution $L_n$ picked at random in $M(u)$
will be such that $L_n \simeq L^n$. As this holds for any $M(u)$, this implies that any measured
distribution related to some randomly chosen state $x^n$ with $n \gg 1$ ought to be a Gibbs
distribution or be very close to a Gibbs distribution with a probability nearly equal to 1.

The preceding paragraphs show that there is some arbitrariness in defining the concept
of temperature for systems composed of a finite number of particles or degrees of freedom.
In theory, there is some indeed; however, if $n$ is large, then defining the temperature in any
of the ways described above should have little effect on the actual value of the temperature
inferred. Thus, for all practical purposes, we can assume that $\beta_{th}(u) \simeq \beta_{Q}(u) \simeq \beta_L(u)$
for $n \gg 1$. In view of what was said in Section 2, it should be noted that the particular
approximation $\beta_{th}(u) \simeq \beta_L(u)$ is of deep consequences: if we look at the distributions
$\tilde{L}_n(x)$ associated to the states $x^n \in \mathcal{X}^n$, then we are likely to realize that the majority of
these distributions, i.e., those which have the most probability to be observed, form a set of
Gibbs distributions $L^n$ parameterized by a fluctuating inverse temperature $\beta(u)$ (from now
on we do not distinguish between the different flavors of inverse temperature). This means
that for $1 \ll n < \infty$ all the statistical and thermodynamic properties of our system can be
described, in an effective manner, using an ensemble of Gibbs distributions with a fluctuating
temperature. The probability density $f_n(\beta)$ ruling the inverse temperature fluctuations must,
in this case, be given by
\[
f_n(\beta) = g_n(u(\beta)) \left| \frac{du(\beta)}{d\beta} \right|,
\]
where $u(\beta)$ is the inverse function of $\beta(u)$. Using this density, one then defines a ‘mixed’ or
‘average’ Gibbs distribution of one-particle states as follows:
\[
\tilde{L}(x) = \int L^u(\beta) f_n(\beta) d\beta = \int \frac{e^{-\beta u(x)}}{Z(\beta)} f_n(\beta) d\beta.
\]
This integral is a definite integral which must be evaluated over the range of definition of $\beta$.
Equivalently, the average can be taken over the energy coordinate:
\[
\tilde{L}(x) = \int L^u g_n(u) du = \int \frac{e^{-\beta u(x)}}{Z(\beta(u))} g_n(u) du.
\]
In the above equation, be sure to distinguish the energy function $u(x)$ from the value $u$ of the
mean energy $\bar{U}_n$. Also note the slight difference between these mixed distributions and those
proposed by Wilk et al. and Beck: in our version of mixed distributions, we take the average
over the Gibbs factor $e^{-\beta u(x)}$ normalized by the partition function which is itself a function
of $\beta$ (compare Eqs. (23) and (28)).
4. The case of the perfect gas

As an application of the large deviation formalism, we carry out in this section the complete calculation of $g_n(u)$ and $f_n(\beta)$ for $u(x) = x^2/2$. By using this form of energy, we assume that the particles composing the gas have a unit mass, and that their momentum $x_i$, $i = 1, 2, \ldots, n$, is confined to one dimension ($X$ is the real line extending from $-\infty$ to $+\infty$). We also abstract out the position of the particles from the analysis, since the mean energy $U_n$ of the $n$ particles does not depend on the position degree of freedom.

To find $g_n(u)$, we first calculate the rate function $D(u)$ using the Legendre transform method. The cumulant generating function associated with the quadratic energy function is calculated to be

$$
\lambda(k) = \ln \int_{-\infty}^{\infty} \frac{e^{-\beta_0 x^2/2}}{Z(\beta_0)} e^{kx^2/2} dx = \frac{1}{2} \ln \frac{\beta_0}{\beta_0 - k}. \tag{30}
$$

From this equation, we find the ‘translated’ inverse temperature $k(u)$ by solving

$$
d\lambda(k) \bigg|_{k(u)} = \frac{1}{2} \frac{1}{\beta_0 - k(u)} = u \tag{31}
$$

The solution is $k(u) = \beta_0 - (2u)^{-1}$, so that

$$
D(u) = uk(u) - \lambda(k(u)) = u\beta_0 - \frac{1}{2} \ln 2\beta_0 u. \tag{32}
$$

Thus,

$$
g_n(u) \propto u^{n/2} e^{-nu\beta_0}. \tag{33}
$$

This form of density is a variant of the $\chi^2$ or gamma density mentioned previously with $n$ as the number of degrees of freedom [23]. Note that this density for the mean energy can be derived directly by noting that $U_n$, for $u(x) = x^2/2$, is a normalized sum of squares of $n$ Gaussian random variables. In statistics, this is usually how the $\chi^2$ density is introduced [27].

At this point, the density $f_n(\beta)$ describing the fluctuations of $\beta$ is readily deduced from the expression of $g_n(u)$ found above by calculating the physical inverse temperature $\beta(u)$. To this end, we can use the fact that $\beta(u) = \beta_0 - k(u)$ or use the equipartition theorem to find in both cases that $\beta(u) = (2u)^{-1}$. Hence, following Eq.(27), $f_n(\beta)$ must have the form

$$
f_n(\beta) \propto \frac{1}{\beta^{n/2}} e^{-\frac{\beta\beta_0}{2}}. \tag{34}
$$

Normalizing this expression for $\beta \in [0, \infty)$ yields

$$
f_n^ld(\beta) = \frac{\beta_0}{\Gamma(n/2)} \left( \frac{n\beta_0}{2} \right)^{n/2} \beta^{-n/2-2} e^{-\frac{\beta_0}{\beta}} \tag{35}
$$

as the large deviation (ld) approximation of $f_n(\beta)$. A plot of this density for two values of $n$ (10 and 100) is shown in Fig. [1] with $\beta_0 = 1$. The plot corresponding to $n = 10$ has no real physical significance, since the large deviation approximation is not expected to be effective in this case. However, it is presented to illustrate the skewness (to the right) of $f_n(\beta)$ which disappears as $n \to \infty$. The maximum value of $f_n(\beta)$ is given by $\beta_{\text{max}} = \beta_0 n/(4 + n)$. As expected, $f_n(\beta)$ converges (in a uniform sense) to the thermodynamic-limit density $f_\infty(\beta) = \delta(\beta - \beta_0)$ when $n \to \infty$; this is partially seen by looking at Fig. [1]. By virtue of the law of large numbers, $g_n(u)$ must also converge in the same limit to a $\delta$ density taking this time the form $g_\infty(u) = \delta(u - u(\beta_0))$ where

$$
u(\beta_0) = E[u(X)] = \int_{-\infty}^{\infty} \frac{e^{-\beta_0 x^2/2}}{Z(\beta_0)} \frac{x^2}{2} dx = \frac{1}{2\beta_0}. \tag{36}
$$
Temperature fluctuations

Figure 1. Probability densities $f_n^l(\beta)$ characterizing the $\beta$ fluctuations of $n = 10$ and $n = 100$ free particles thermally coupled to a heat bath with $\beta_0 = 1$. Each density is defined for $\beta > 0$, and shows a maximum at $\beta_0 n/(4 + n)$.

Figure 2. Comparison of the $\chi^2$ $\beta$-density proposed by Beck (B) [11] and the one proposed in this work (T) for $n = 10$ (left) and $n = 100$ (right) particles (see text). For $n = 100$, the two densities are quasi-indistinguishable. The maximum value of the $\beta$-density, in the case of Beck, is located at $\beta_0(n - 2)/n$.

We now come the main point of our study which is to compare the $f_n(\beta)$ density obtained here and the $\chi^2$ probability density of Eq. (3) which was ‘postulated’ by Wilk et al. and Beck in their studies of mixed distributions (see Section 2). To establish this comparison, we present in Fig. 2 two plots of $f_n^l(\beta)$ for two different values of $n$ and a variant of the $\chi^2$ $\beta$-density proposed by Beck

$$f_n^B(\beta) = \frac{1}{\Gamma\left(\frac{n}{2}\right)} \left(\frac{n}{2\beta_0}\right)^{n/2} \beta^{n/2-1} e^{-\frac{n\beta}{2\beta_0}},$$

(37)
Temperature fluctuations

which results from identifying $1/(q-1)$ in Eq. (2) with $n/2$. The plots are presented again for $n = 10$ and $n = 100$. A rapid inspection of the expressions of $f_n^{ld}$ and $f_n^B$ reveals that these densities are not at all the same. The density $f_n^B$ can in fact be viewed as emerging from the sum of the squares of $n$ Gaussian random variables, whereas, in our case, the sum of squared Gaussian random variables arises as the mean energy, and so as $\beta^{-1}$ modulo some constant. This explains why performing the change of variables $\beta \to \beta^{-1}$ in $f_n^{ld}$ yields $f_n^B$ modulo some constant and a Jacobian term arising from the change of variables. In spite of this important difference, the second plot of Fig. 2 shows that both densities are remarkably similar as $n$ gets large. This, at first, does not seem surprising as both densities converge to the delta density $f_\infty^B(\beta)$ in the thermodynamic limit $n \to \infty$. However, it is to be noted that each of them gives totally different mixed distributions when they are used in Eq. (28). Indeed, it can be shown that the mixed distribution associated with $f_n^{ld}$ has the asymptotic form

$$\tilde{L}_n^{ld}(x) \sim e^{-|x|}$$

(38)

for $|x| \gg 1$, instead of

$$\tilde{L}_n^B(x) \propto e^{-x^2},$$

(39)

where $q = 1 - 2/n$. Both of these results should be compared with the (pure) Gibbsian distribution

$$L_n^G(x) \propto e^{-x^2}$$

(40)

which is the limiting distribution of $\tilde{L}_n^{ld}$ and $\tilde{L}_n^B$ in the thermodynamic limit ($n \to \infty$).

The above scaling relationships clearly indicate that choosing between $f_n^{ld}(\beta)$ or $f_n^B(\beta)$ has a dramatic consequence on the functional form of the mixed distribution calculated even for $n \gg 1$. Does that imply that our model of temperature fluctuations cannot serve as a model of the non-Gibbsian distributions which have been observed in turbulent fluid experiments as well as in nuclear scattering experiments? The answer is not as straightforward as one would think. First, it is not at all clear that turbulent fluids can actually be treated in the canonical ensemble and/or that the perfect gas assumption is a valid approximation in this case. These points call for further justifications. Second, the extreme events $|x| \gg 1$ needed to validate either one of the two temperature densities compared in this work are often very difficult to detect experimentally in a reliable way. Surely, additional calculations and experimental data would be welcome in order to test the validity of our approach, and to confront it with that of the authors mentioned in the present study. This seems to be especially true for nuclear scattering experiments which are usually thought to fit perfectly well into the canonical ensemble picture.

5. Concluding remarks

Our treatment of the energy and temperature fluctuations of a system coupled to a heat bath has focused mainly on the perfect gas. However, it is worth noting that the large deviation approach presented in this paper for calculating the energy and temperature probability densities in the canonical ensemble is very general. It can be applied independently of the form of the energy function $u(x)$ which defines the mean energy $U_n$, and can also be generalized without too much difficulties to cases involving other forms of probability distribution for $P_n(x^n)$ (e.g., $q$-exponential distributions). In this context, an obvious extension of our work could be to consider different forms for $u(x)$, and to look at the mixed distributions which result from the corresponding temperature fluctuations. This line of thought has been followed recently by Beck and Cohen who derived a number of ‘superstatistical’ mixed distributions (sometimes unphysical ones) by assuming different forms of temperature fluctuations.
Another problem could be to solve the following ‘inverse problem’: for which \( u(x) \) is \( f_n(\beta) \) the same \( \chi^2 \) density as the one suggested by Beck? Finally, note that a large deviation calculation of \( g_n(u) \) and \( f_n(\beta) \) can also be carried out for systems involving dependent random variables. Unfortunately, the calculations leading to the specific forms of \( g_n(u) \) and \( f_n(\beta) \) in this case are likely to be tedious. Also, the concept of mixed distribution does not generalize easily to the case of interacting particles because the Eqs. (25) and (26) which were used to prove that Gibbs distributions are the only distributions likely to be observed in large systems are valid for sequences of IID random variables only. It is, in fact, a long-standing open problem of large deviation theory to generalize these equations to sequences of dependent random variables. Solving this problem would have direct consequences in statistical physics, for it implies ipso facto a generalization of the maximum entropy principle to systems of interacting particles.

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