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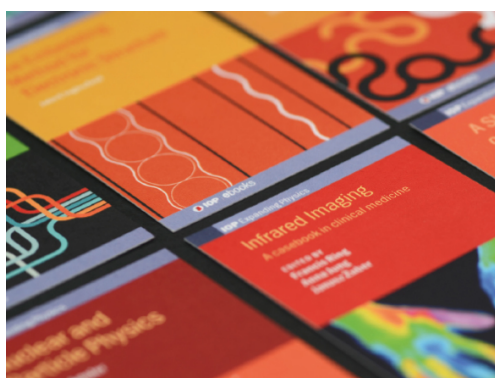
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A consistent description of fluctuations requires negative temperatures

Luca Cerino¹, Andrea Puglisi² and Angelo Vulpiani¹

¹ Dipartimento di Fisica, Università La Sapienza, and CNR—ISC,
p.le A. Moro 2, 00185 Rome, Italy

² CNR-ISC and Dipartimento di Fisica, Università La Sapienza,
p.le A. Moro 2, 00185 Rome, Italy

E-mail: luca.cerino@roma1.infn.it, andrea.puglisi@roma1.infn.it and angelo.vulpiani@roma1.infn.it

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Abstract. We review two definitions of temperature in statistical mechanics, T_B and T_G , corresponding to two possible definitions of entropy, S_B and S_G , known as surface and volume entropy respectively. We limit our attention to a class of systems with bounded energy, and such that the second derivative of S_B , with respect to energy, is always negative. The second condition holds in systems where the number N of degrees of freedom is sufficiently large (examples are shown where $N \sim 100$ is sufficient) and without long-range interactions. We first discuss the basic role of T_B , even when negative, as the parameter describing fluctuations of observables in a sub-system. Then, we focus on how T_B can be measured dynamically, i.e. averaging over a single long experimental trajectory. The same approach cannot be used in a generic system for T_G , since the equipartition theorem may be impaired by boundary effects due to the limited energy. These general results are substantiated by the numerical study of a Hamiltonian model of interacting rotators with bounded kinetic energy. The numerical results confirm that the kind of configurational order realized in the regions at small S_B , or equivalently at small $|T_B|$, depends on the sign of T_B .

Keywords: fluctuations (theory)

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1. Introduction

Two different definitions of temperature in equilibrium statistical mechanics have recently been the subject of an intense debate [1–10], after the publication of experimental measurements of a negative absolute temperature [11, 12]. In [11] the possibility of preparing a state was demonstrated where the observed distribution of the modified kinetic energy *per atom* appeared to be inverted, i.e. with the largest population in the high energy states, yielding a *de facto* negative absolute temperature.

The possibility of a negative absolute temperature is well known since the theoretical work by Onsager on the statistical hydrodynamics of point vortices [13] and the experimental and theoretical results on nuclear spin systems by Pound, Ramsey and Purcell (see [14–16] for a review and discussion). In those investigations, it was clear that an inverse temperature parameter β ranging over the full infinite real line $(-\infty, \infty)$ did not lead to any inconsistency or paradox. Ramsey in 1956 already realised that ‘the Carathéodory form of the second law is unaltered.’ [14]

A negative absolute temperature appears whenever the microcanonical entropy is non-monotonic in the energy, a condition which can be realized when the total energy has a global maximum, which may happen when the phase space is bounded. There are also cases where the phase space is bounded but the energy diverges: again this

may lead to a non-monotonic entropy; an important example is given by point vortices [13, 17–21]. It is crucial to highlight that the lack of monotonicity (for entropy versus energy) is realised if one adopts the simplest definition of microcanonical entropy, which is related to the logarithm of the number of states with a given energy. Since such a definition appears in the so-called ‘tombstone formula’ written on Boltzmann’s grave, ‘ $S = k \log W$ ’, it is often referred to as Boltzmann’s definition of entropy. Even if not historically precise [8], we adopt the same convention (but setting $k = 1$) and call ‘Boltzmann entropy’ in a system with Hamiltonian $H(\mathbf{Q}, \mathbf{P})$, where \mathbf{Q} and \mathbf{P} are vectors in \mathbb{R}^{dN} , d being the dimension of the system, the function

$$S_B(E, N) = \log \omega(E), \quad (1)$$

$\omega(E)$ being the density of states, i.e.

$$\omega(E) = \int \delta(H - E) d^{dN} Q d^{dN} P = \frac{\partial \Sigma(E)}{\partial E}, \quad (2)$$

and $\Sigma(E)$ the total ‘number’ of states with energy less than or equal to E , that is

$$\Sigma(E) = \int_{H < E} d^{dN} Q d^{dN} P. \quad (3)$$

In definition (1) we have ignored an additive constant which is not relevant in our discussion. In [8] it is stated that the validity of the second principle of thermodynamics depends on the value of this arbitrary constant. Nonetheless such an arbitrariness, and the consequent paradox, can be removed if all the quantities (energies, positions, momenta, time etc...) are considered adimensional. When propagating the denomination, it is customary to define the ‘Boltzmann temperature’ through

$$\beta_B = \frac{1}{T_B} = \frac{\partial S_B(E, N)}{\partial E}. \quad (4)$$

Some authors [1, 8] have argued that a different definition of microcanonical entropy, proposed by Gibbs, should be used in statistical mechanics, in order to be consistent with a series of ‘thermodynamic’ requirements and to avoid unpleasant paradoxes. The Gibbs entropy, which is always monotonically increasing, reads

$$S_G(E, N) = \log \Sigma(E), \quad (5)$$

and leads to the Gibbs temperature definition, which is always positive:

$$\beta_G = \frac{1}{T_G} = \frac{\partial S_G(E, N)}{\partial E} \geq 0. \quad (6)$$

We note that, since T_B is defined directly on the surface of interest (i.e. that at constant energy E), from the point of view of the ergodic approach its use appears to be rather natural. The Gibbs temperature, on the other hand, enters through an ensemble average in the equipartition formula common in textbooks [22]:

$$\left\langle x_i \frac{\partial H}{\partial x_j} \right\rangle = \delta_{ij} T_G, \quad (7)$$

where x_i is any of the components of the vector (\mathbf{Q}, \mathbf{P}) and the average is carried out in the microcanonical ensemble. In section 3, we will discuss the limits in the application of the formula (7) when the energy is bounded. We also mention that T_G appears in the theory of Helmholtz monocycles (which had an important role in the development of the Boltzmann's ideas for the ergodic theory), for one-dimensional systems [23, 24].

In spite of the fact that, in our opinion, the basic features of the different definitions of temperature do not present particular technical or conceptual subtleties, there is a certain confusion in the literature; therefore a general discussion on the topic can be useful. In this paper we present a line of reasoning where the Boltzmann temperature T_B (positive or negative) is the (unique) proper parameter for understanding the statistical properties of the energy fluctuations, as well as for determining the flux of energy between two systems at different temperatures. In addition to these it is measurable, without the appearance of inconsistencies. We remark that the systems discussed in [8], from which the authors try to show that only T_G is the 'good' temperature, are small ($N = \mathcal{O}(1)$) and/or with long interactions.

In section 2, after presenting the class of physically relevant systems which are the subject of our study, we describe how the Boltzmann temperature T_B naturally describes fluctuations of observables in subsystems, in analogy with the derivation of the canonical ensemble from the microcanonical one. In section 3 we discuss dynamical ('ergodic') measurements, which can reproduce T_B but are in general unsuited to measure T_G ; in particular we show a possible failure of the equipartition theorem. In section 4 we outline a series of numerical results with a model of interacting rotators with bounded kinetic energy, discussing the many practical uses of Boltzmann temperature. The summary and conclusions are drawn in section 5, together with a critique of some of the arguments used, in [8], to rule out the thermodynamic meaning of T_B .

2. The relevance of the Boltzmann temperature

In this section we show, following the standard approach that can be found even in some textbooks, the unavoidable role of T_B in many statistical mechanics problems.

2.1. Systems of physical relevance

In the paper we consider systems made of a finite but large number $N \gg 1$ of particles with local interactions, i.e. we exclude long-range potentials or mean-field models. It should be understood that long-range interactions widen the phenomenology of statistical mechanics and may lead to complicated functional dependences for $S_B(E, N)$, e.g. with several maxima or minima, even for large N . Nevertheless they are not necessary for the discussion on negative temperature and, most importantly, they represent a peculiar case where even thermodynamics is not obvious. For instance, there is no evidence that the typical *Gedankenexperiment* of putting in contact two—previously isolated—systems can be realized, as the isolation condition is prevented by the long-range interaction.

We also assume that $S_B(E, N)$ is always convex, i.e. $d^2 S_B(E, N)/dE^2 \leq 0$. This is certainly true in the limit of vanishing interaction and in short-range-interacting systems for large N , since S_B is strictly related to the large deviation function associated with the density of states³. Let us stress that these large values of N are not necessarily ‘thermodynamic’ ($N \rightarrow \infty$): for instance in section 4 we will introduce a system that possesses all the required features already at $N = 100$. In general such a value of N will depend on the specific system, corresponding to situations in which some common approximations (e.g. Laplace approximation for exponential integrals) can be safely applied. In section 2.3 we discuss in detail the origin of the convexity of $S_B(E, N)$. It is easy to understand that this assumption implies the validity of the second principle of thermodynamics, as discussed in the next subsection.

2.2. Second law and energy flux between two systems in contact

We consider a system \mathcal{A} of N_A particles described by the variables $\{\mathbf{Q}_A, \mathbf{P}_A\}$ and Hamiltonian $H_A(\mathbf{Q}_A, \mathbf{P}_A)$, a system \mathcal{B} of N_B particles described by the variables $\{\mathbf{Q}_B, \mathbf{P}_B\}$ and Hamiltonian $H_B(\mathbf{Q}_B, \mathbf{P}_B)$ and a small coupling among the two, so that the global Hamiltonian is

$$H = H_A(\mathbf{Q}_A, \mathbf{P}_A) + H_B(\mathbf{Q}_B, \mathbf{P}_B) + H_c(\mathbf{Q}_A, \mathbf{Q}_B). \quad (8)$$

If the two Hamiltonians have the same functional dependencies on the canonical variables (i.e. they correspond to systems with same microscopic dynamics, with possibly different sizes N_A and N_B), for large N , we can introduce the (Boltzmann) entropy per particle

$$S_B(E, N) = NS(e) \quad , \quad e = \frac{E}{N}, \quad (9)$$

with $S(e)$ a convex function, identical for systems \mathcal{A} and \mathcal{B} . Let us now suppose that systems \mathcal{A} and \mathcal{B} have, respectively, energy $E_A = N_A e_A$ and $E_B = N_B e_B$ and the corresponding inverse Boltzmann temperatures $\beta_B^{(A)}$ and $\beta_B^{(B)}$.

When the two systems are put in contact, a new system is realized with $N = N_A + N_B$ particles. Let us call $a = N_A/N$ the fraction of particles from the system \mathcal{A} . We know that the final energy is $E_f = E_A + E_B = N e_f$, where $e_f = a e_A + (1 - a) e_B$ and final entropy

$$S_B(E_f, N) = NS(e_f) \geq N_A S(e_A) + N_B S(e_B) = N[a S(e_A) + (1 - a) S(e_B)]. \quad (10)$$

The previous inequality follows from the convexity assumption for $S(e)$ which implies

³ It is interesting to note that Kubo in [34] uses the adjective ‘normal’ for systems satisfying $\Sigma(E, N) \sim e^{N\phi(E/N) + o(N)}$. It is easy to verify that for such systems one has $\beta_G = \beta_B + O(1/N)$. However our assumption is different: we ask that, in the large N limit, $\omega(E, N) \sim e^{N\psi(E/N) + o(N)}$. Since $\Sigma(E, N) = \int^E \omega(E') dE'$, a simple steepest descend computation shows that, if $d\psi(E'/N)/dE' > 0$ for $E' < E$, then $\psi(E/N) = \phi(E/N)$: this is equivalent to say that $T_B = T_G$ in the thermodynamic limit (i.e. up to $O(1/N)$) whenever $T_B > 0$ (see figure 1 for an example). On the other hand if ψ has a maximum at E^* then $\Sigma(E, N)$ is roughly constant for $E > E^*$. In summary, for ‘normal’ systems the temperatures must coincide, while with our assumption, one can have different temperatures in the region $E > E^*$. Note also that normal systems also satisfy our assumption, while the opposite is not true. Moreover, even if not all the systems satisfying our assumption could be named ‘normal’, all of them satisfy the equivalence of ensembles (as discussed below).

$$S(ae_A + (1 - a)e_B) \geq aS(e_A) + (1 - a)S(e_B). \quad (11)$$

The final inverse temperature $\beta_B^{(f)}$ is intermediate between $\beta_B^{(A)}$ and $\beta_B^{(B)}$, e.g. if $e_B > e_A$ —that is $\beta_B^{(A)} > \beta_B^{(B)}$ —then

$$\beta_B^{(B)} < \beta^{(f)} < \beta_B^{(A)}. \quad (12)$$

The energy flux obviously goes from smaller β_B (hotter) to larger β_B (colder). The consequence of convexity is that $\beta_B(E)$ is always decreasing and a negative value does not lead to any ambiguity. Confusion may arise from the fact that $T_B < 0$ is, for the purpose of establishing the energy flux, hotter than $T_B > 0$. However if β_B is used, the confusion is completely removed [14].

We also briefly discuss a particularly interesting case with different Hamiltonians. Suppose that for the system \mathcal{A} negative temperatures can be present, whereas system \mathcal{B} has only positive temperatures; it is quite easy to see that the coupling of the system \mathcal{A} at negative temperature with the system \mathcal{B} at positive temperature always produces a system with final positive temperature. Indeed, at the initial time the total entropy is

$$S_I = S^{\mathcal{A}}(E_A) + S^{\mathcal{B}}(E_B), \quad (13)$$

while, after the coupling, it will be

$$S_F = S^{\mathcal{A}}(E'_A) + S^{\mathcal{B}}(E'_B), \quad (14)$$

where $E'_A + E'_B = E_A + E_B$ and, within our assumptions, E'_A is determined by the equilibrium condition [22] that S_F takes the maximum possible value, i.e.

$$\beta_A = \frac{\partial S^{\mathcal{A}}(E'_A)}{\partial E'_A} = \beta_B = \frac{\partial S^{\mathcal{B}}(E'_B)}{\partial E'_B}. \quad (15)$$

Since β_B is positive for every value of E'_B , the final common temperature must also be positive. The above conclusion can also be found, without detailed reasoning, in some textbooks [25, 26].

2.3. Subsystems

We consider a vector \mathbf{X} in \mathbb{R}^{2dN_1} (with $N_1 < N$), that is a subsystem of the full phase space (\mathbf{Q}, \mathbf{P}) , and we indicate with $\tilde{\mathbf{X}}$ in $\mathbb{R}^{2d(N-N_1)}$ the remaining variables. We have

$$H = H_1(\mathbf{X}) + H_2(\tilde{\mathbf{X}}) + H_I(\mathbf{X}, \tilde{\mathbf{X}}) \quad (16)$$

with an obvious meaning of symbols.

We then consider the case $N \gg 1$ and $N_1 \ll N$. In the microcanonical ensemble with energy E , the probability density function (pdf) for the full phase space (\mathbf{Q}, \mathbf{P}) is

$$P(\mathbf{Q}, \mathbf{P}) = \frac{1}{\omega(E, N)} \delta(H(\mathbf{Q}, \mathbf{P}) - E). \quad (17)$$

The pdf of \mathbf{X} can be obtained from the latter, by integrating over $\tilde{\mathbf{X}}$. If the Hamiltonian $H_I(\mathbf{X}, \tilde{\mathbf{X}})$ is negligible (a consequence of our assumption for non long-range interaction) then we have

$$P(\mathbf{X}) \simeq \frac{\omega(E - H_1(\mathbf{X}), N - N_1)}{\omega(E, N)}. \quad (18)$$

It is now possible to exploit the definition of S_B and get

$$\omega(E, N) = e^{S_B(E, N)} \quad (19)$$

$$\omega(E - H_1(\mathbf{X}), N - N_1) = e^{S_B(E - H_1(\mathbf{X}), N - N_1)} \propto e^{S_B(E, N - N_1) - \beta_B(E) H_1(\mathbf{X})}, \quad (20)$$

which, together with (18) leads to

$$P(\mathbf{X}) \propto e^{-\beta_B H_1(\mathbf{X})}. \quad (21)$$

When H_1 is bounded (as in our assumptions), the previous simple derivation can be carried out irrespective of the sign of β_B . It is immediately clear from the above argument that T_B is the temperature ruling the statistics of fluctuations of physical observables in a subsystem. For instance, the pdf of the subsystem (i.e. in the canonical ensemble) energy E_1 reads

$$P(E_1, N_1) \propto \omega(E_1, N_1) e^{-\beta_B E_1} \propto e^{[S_B(E_1, N_1) - \beta_B E_1]}. \quad (22)$$

Of course the above result holds in the (important) case where the two subsystems are weakly interacting and $H_1 \ll E$. For $e_1 = E_1/N_1$, one has

$$P(e_1, N_1) \propto e^{N_1[S(e_1) - \beta_B e_1]}, \quad (23)$$

which is a large deviation law where the Cramer's function $C(e_1)$ is $C(e_1) = \beta_B e_1 - S(e_1) + \text{const}$. From general arguments of the theory of probability, we know that, if a large deviation principle holds, $\frac{d^2 C(e_1)}{de_1^2} \geq 0$ so $\frac{d^2 S(e_1)}{de_1^2} \leq 0$. The validity of the large deviation principle can be easily shown for non-interacting systems. For weakly interacting systems it is quite common and reasonable, and can be stated under rigorous hypothesis [27, 28].

2.4. The generalised Maxwell–Boltzmann distribution

The extreme case of the above discussions is when $N_1 = 1$, that is to say the fluctuations of a single degree of freedom (e.g. a momentum component of a single particle) are observed. This becomes interesting when the Hamiltonian has the form

$$H = \sum_{n=1}^N g(p_n) + \sum_{n,k}^N V(q_n, q_k) \quad (24)$$

where the variables $\{p_n\}$ are limited and the same happens for the function $g(p)$.

Repeating the arguments in the previous subsection, one may compute the probability density for the distribution of a single momentum p , obtaining

$$P(p) \simeq \frac{\omega(E - g(p), N - 1)}{\omega(E, N)} \propto e^{-\beta_B g(p)}, \quad (25)$$

which, again, is valid for both positive and negative β_B . We mention that in the experiment in [11], the above recipe has been applied to measure both positive and negative system's temperatures.

From equations (22) and (25) the true meaning of the (Boltzmann) temperature is quite transparent: it is a quantity which rules the pdf of the energy of a subsystem (or the momentum of a single particle). Let us note that since T_B is associated with the large microcanonical system (in physical terms the reservoir) it is a non-fluctuating quantity [29] also for each sub-system and, in general, for non-isolated systems. In the conclusions, we discuss again this aspect which is not always fully understood, see e.g. [8]

2.5. Temperature and order

In usual statistical mechanics, low temperatures—or, better, high values of inverse temperature—are usually associated with the possibility of some kind of order, the most noticeable example given by phase transitions. Intuitively, one would expect such a situation whenever $\omega(E)$ is relatively small, which usually corresponds to regions where $|\beta_B|$ is large irrespective of the temperature's sign. A famous example where such an order at negative (small) temperatures was observed is that of pointlike vortices discussed by Onsager in [13]. The system, obtained as a particular limit from two-dimensional Euler equations, describes N points of vorticities $\{\Gamma_1, \dots, \Gamma_N\}$ in a two-dimensional domain Ω : the equation of motions of the coordinates (x_n, y_n) of the n -th point vortex are shown to be (see for instance [30])

$$\Gamma_i \frac{dx_i}{dt} = \frac{\partial H}{\partial y_i}, \quad \Gamma_i \frac{dy_i}{dt} = -\frac{\partial H}{\partial x_i} \quad (26)$$

with Hamiltonian

$$H = \sum_{i \neq j} \Gamma_i \Gamma_j \mathcal{G}(r_{i,j}) \quad (27)$$

where $\mathcal{G}(r)$ is the Green function of the Laplacian in Ω : in the infinite plane one has $\mathcal{G}(r) = -1/4\pi \ln r$ where $r_{i,j} = \sqrt{(x_i - x_j)^2 + (y_i - y_j)^2}$. The canonical variables in this case are

$$q_i = \sqrt{|\Gamma_i|} x_i, \quad p_i = \sqrt{|\Gamma_i|} \text{sign}(\Gamma_i) y_i. \quad (28)$$

Onsager showed that if the domain of Ω is bounded, then negative T_B are achieved at large values of the energy. At large energies a particular spatial order appears too: clusters of vortices with the same sign of the vorticity are the unique possible structures. It is interesting to note that $T_B < 0$ (and the corresponding clusterization) is not a peculiarity of the divergence of $\mathcal{G}(r)$ in $r = 0$, nor of the long range nature of the interaction: indeed, it can be obtained with any arbitrary $\mathcal{G}(r)$ having a maximum (even finite) in $r = 0$, and vanishing at large r , provided that the domain is bounded. The presence of spatial order at high values of energy, in the form of discrete breathers, has also been observed in the discrete non-linear Schrödinger equation and analogous systems [10, 31]. In section 4 we introduce a different, in a way simpler, model which still exhibits its spatial order at small negative temperatures.

3. How to measure T_B and T_G

The definitions of β_B and β_G given in equations (4) and (6) are based on the functional dependence of the phase space occupations $\omega(E)$ and $\Sigma(E)$ upon the energy. In a real or numerical experiment it may be cumbersome or even impossible to make use of those definitions to measure the two temperatures: for instance, an empirical estimate of $\omega(E)$ (and therefore of $\Sigma(E)$) will always be limited by the available statistics (number of independent measurements of E) and therefore cannot provide a clear answer, for both β_B and β_G , in the interesting regimes where $\omega(E) \sim 0$.

On the other hand it has been shown [32] that β_B can be obtained as a microcanonical average of a certain observable. The recipe is the following

$$\beta_B = \langle R(\mathbf{X}) \rangle, \quad R(\mathbf{X}) = \nabla \cdot \frac{\nabla H}{|\nabla H|^2} \quad (29)$$

where ∇ stands for the vector of derivative operators along the degrees of freedom in the full phase space $\mathbf{X} \equiv (\mathbf{Q}, \mathbf{P})$. From (29) one has, assuming the ergodicity, that β_B can be computed with a molecular dynamics simulation, and, at least in principle, by a long-time series from an experiment. It is interesting to notice that such a kind of recipe does not exist for $S_B(E, N)$ or $S_G(E, N)$ [32]. It is clear that, in view of the considerations in sections 2.3 and 2.4, one may always measure fluctuations of appropriate observables, such as subsystem's energy or single particle momentum, to get an estimate of T_B .

A method to approach the problem of β_G measurement is via the equipartition theorem and has previously been discussed in textbooks and considered important [8]. It states

$$\left\langle x_i \frac{\partial H}{\partial x_j} \right\rangle = \delta_{ij} T_G. \quad (30)$$

However the usual derivation of equation (30) implies the possibility to neglect boundary terms in an integration by parts. Such a possibility is challenged in the class of systems with bounded energy and phase space that we are considering.

In particular it is easy to show that (30) does not hold under the simultaneous realization of the following conditions:

- bounded space of the canonical variables;
- bounded derivatives of the Hamiltonian $\frac{\partial H}{\partial x_j}$;
- bounded energy from above and below: $E_m \leq E \leq E_M$;
- vanishing density of states at the boundaries, i.e. $\omega(E_M) = 0$.

Given such conditions, one has that, on one side,

$$T_G(E) = \frac{\Sigma(E)}{\omega(E)} \quad (31)$$

diverges when $E \rightarrow E_M$. On the other side, $\langle x_i \frac{\partial H}{\partial x_j} \rangle$ is limited, resulting in a contradiction.

A failure of the equipartition formula equation (30) is also possible in systems where there are no negative temperatures, i.e. $T_G \simeq T_B > 0$ for all E . Consider, for instance, the following Hamiltonian

$$H = \sum_{n=1}^N \frac{p_n^2}{2} + \epsilon \sum_{n=1}^N (1 - \cos(\phi_n - \phi_{n-1})) \quad (32)$$

where $\phi_n \in [-\pi, \pi)$. For large E , i.e. $E \gg \epsilon N$, the contribution to $\Sigma(E)$ of the variables $\{\phi_n\}$ does not depend too much on the value of E , so that

$$\Sigma_\epsilon(E) \simeq \Sigma_0(E) \propto E^{N/2}, \quad (33)$$

and $T_G \simeq 2E/N$ and, for large N , $T_B = T_G + O(1/N)$.

On the other hand it is easy to see that

$$\left| \phi_n \frac{\partial H}{\partial \phi_n} \right| \leq 2\pi\epsilon, \quad (34)$$

and, therefore, the equipartition formula $\langle \phi_n \frac{\partial H}{\partial \phi_n} \rangle = T_G$ does not hold for large value of E and N .

4. Numerical results for a system with negative temperature

In this section we present a detailed study of a system composed of N ‘rotators’ with canonical variables $\phi_1, \dots, \phi_N, p_1, \dots, p_N$ with all ϕ_i and p_i defined in $[-\pi, \pi)$, and with Hamiltonian

$$H(\phi_1, \dots, \phi_N, p_1, \dots, p_N) = \sum_{n=1}^N [1 - \cos(p_n)] + \epsilon \sum_{n=1}^N [1 - \cos(\phi_n - \phi_{n-1})]. \quad (35)$$

We choose, as boundary condition, $\phi_0 = 0$ and this guarantees that the only conserved quantity by the dynamics is the total energy E . The equations of motion for the rotators can be readily obtained by applying Hamilton’s equations to equation (35):

$$\begin{aligned} \dot{\phi}_n &= \sin(p_n), \\ \dot{p}_n &= -\epsilon(\sin(\phi_n - \phi_{n-1}) + \sin(\phi_n - \phi_{n+1})). \end{aligned} \quad (36)$$

It is immediate to verify that the energy has a maximum value $E_M = 2N(1 + \epsilon)$ which is realised when $p_n = \pi$ and $\phi_n - \phi_{n-1} = \pi$ for every n .

When $\epsilon = 0$ it is immediately clear to see that the Hamiltonian in equation (35) implies negative Boltzmann temperatures. Indeed at low energy one has $1 - \cos(p_n) \simeq p_n^2/2$ so that

$$\Sigma(E) \simeq C_N E^{N/2}, \quad \omega(E) \simeq \frac{N}{2} C_N E^{N/2-1} \quad (37)$$

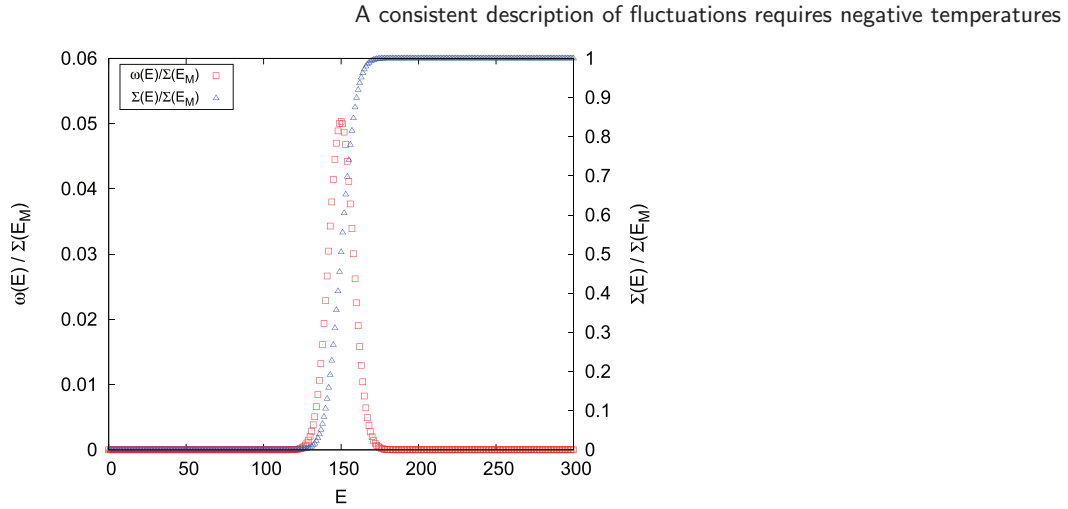


Figure 1. Phase space sampling: we report the reconstruction of the density of states $\omega(E)$ and its integral $\Sigma(E) = \int_0^E dE' \omega(E')$. The two functions are normalized with $\Sigma(E_M = 2N(1 + \epsilon))$. The parameters of the system are: $N = 100$ and $\epsilon = 0.5$.

with $C_N = (2\pi)^N \frac{\pi^{N/2}}{\Gamma(N/2 + 1)}$. Close to $E_M = 2N$ one has $1 - \cos(p_n) \simeq (\pi - p_n)^2/2$, therefore when E approaches E_M it is

$$\begin{aligned} \Sigma(E) &= \Sigma(E_M) - (2\pi)^N \int_{E < H < E_M} \prod_{n=1}^N dp_n \simeq \Sigma(E_M) - (2\pi)^N \int_{\sum_n \frac{(\pi - p_n)^2}{2} < (E_M - E)} \prod_{n=1}^N dp_n = \Sigma(E_M) \\ &\quad - C_N (E_M - E)^{N/2} \end{aligned} \quad (38)$$

and therefore

$$\omega(E) \simeq \frac{N}{2} C_N (E_M - E)^{N/2-1}. \quad (39)$$

In conclusion $\omega(E) = 0$ if $E = 0$ and $E = E_M$, which implies a maximum inbetween and a region (at high energies) with negative β_B . The previous scenario is expected to hold also in the prescence of a small interaction among the rotators and can be numerically confirmed with a sampling of the phase-space (see figure 1): random configurations of the system are extracted with an uniform distribution over the phase space and $\omega(E)$ is reconstructed by counting the number of configurations lying in a small interval of width δE around the energy E . It is clear from figure 1 that: the density of states $\omega(E)$ has a maximum in $\tilde{E} \approx E_M/2$; it is an increasing function for $E < \tilde{E}$ whence $T_B > 0$; it decreases for $E > \tilde{E}$ whence $T_B < 0$. Unfortunately, such a sampling is reliable only in a narrow region around \tilde{E} : indeed, there are very few configurations with energies much larger or smaller than \tilde{E} and, therefore, there is an extremely small probability such configurations can be extracted with this procedure.

For this reason, we have performed dynamical measures through numerical simulations of the motion of the system: the integration of equations (36) is carried out with the usual Verlet scheme with a time step $\Delta t = 10^{-3}$.

A consistent description of fluctuations requires negative temperatures

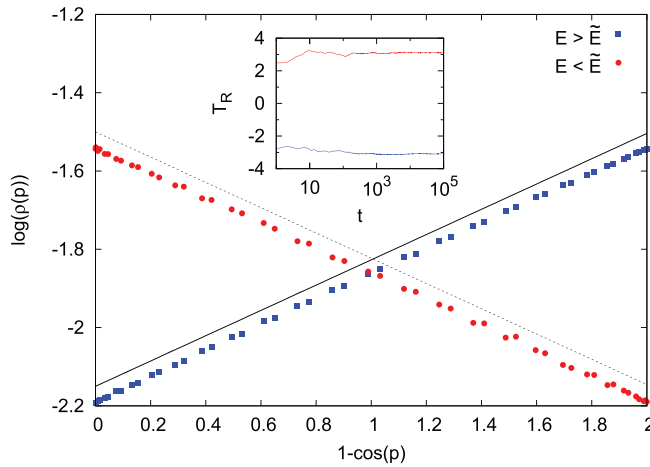


Figure 2. Measure of the Boltzmann temperature in the rotators chain for $N = 100$ and $\epsilon = 0.5$. Probability distribution function of the momentum of the rotators as a function of their ‘kinetic energy’ $g(p) = 1 - \cos(p)$ at energy $E = E_- = 170$ (blue squares) and $E = E_+ = 130$. The slopes of the two black straight lines are $1/T_R^\infty(E)$, where $T_R^\infty(E)$ is the asymptotic value of the corresponding curve in the inset. Inset: The T_R obtained from the cumulated average of the observable $R(\mathbf{X}(t))$ over a trajectory up to time t at $E = 170$ (blue line) and $E = 130$ (red line).

4.1. Measure of T_B

Measurements of the Boltzmann temperature are taken using the two methods discussed in the previous sections. In particular, by computing the following average (over a single trajectory of the system)

$$\rho(p) = \lim_{\tau \rightarrow \infty} \frac{1}{N\tau} \int_0^\tau dt \sum_{i=1}^N \delta(p_i(t) - p), \quad (40)$$

for different values of p , and assuming that the system is ergodic, we recover the single-particle-momentum probability density function $P(p)$, equation (21). The result of such a measure is reported in figure 2: for two different values of energy $E_+ < \tilde{E}$ and $E_- > \tilde{E}$ the measured $\rho(p)$ is plotted as a function of the ‘kinetic energy’ of the individual rotator $g(p) = 1 - \cos(p)$. The presence of a negative temperature at $E = E_-$ can be readily identified by means of the consideration in section 2.4. On one hand, the exponential behaviour of $\rho(p)$ guarantees that the approximation used to obtain equation (25) is already valid (for every value of $g(p)$) at $N = 100$. On the other hand, the clear positive slope of the function at $E = E_-$ is a direct consequence of the fact that $T_B(E_-) < 0$: the opposite situation is encountered at $E = E_+$, where the decreasing behavior of $\rho(p)$ indicates a temperature $T_B(E_+) > 0$. These conclusions can also be drawn by measuring the time average of the function $R(X)$, equation (29): in the inset of figure 2 we report the temperature obtained with the cumulated average of $R(\mathbf{X})$ up to time t , namely

$$\frac{1}{T_R(t)} = \frac{1}{t} \int_0^t dt' R(\mathbf{X}(t')), \quad (41)$$

for $E = E_+$ and $E = E_-$. These two quantities converge, for large t , to an asymptotic value representing an estimate of the inverse Boltzmann temperature β_B of the system. This value, as expected, is positive for $E = E_+$ and negative for $E = E_-$: moreover, the values are in very good agreement with the slopes of the single particle distribution function, as shown by the dashed and solid lines in figure 2.

4.2. Equivalence of ensembles and the equipartition formula

We briefly discuss the problem of the equivalence of ensembles. In the usual textbook approach one starts from equation (23): assuming that $S(e)$ is convex and performing a steepest descent analysis, for large N , one obtains the canonical functions from the (Boltzmann) microcanonical ones, e.g.:

$$T_B(e)S(e) = e - f(T_B(e)), \quad (42)$$

where $f(T)$ is the free energy per particle in the canonical ensemble. In addition the energy fluctuations are negligible. In such a derivation, the relevant point is only the convexity of $S(e)$ and nothing about its first derivative is required. Therefore, the equivalence of ensembles naturally holds under our hypothesis even for negative T_B . Since T_B and T_G can be different even for large N , as in our model defined with equation (35), it is evident that T_G is not relevant for the ensemble equivalence.

A common way [8] to measure the Gibbs temperature is by the equipartition formula, equation (30): for the Hamiltonian in equation (35) one should get

$$\langle p_k \sin p_k \rangle_E = T_G(E), \quad (43)$$

for every $1 \leq k \leq N$. In the present subsection, we use the notation $\langle \rangle_E$ to denote the average in the microcanonical ensemble, in order to distinguish it from a canonical average $\langle \rangle_\beta$ which is useful to get some analytic expressions and better investigate the validity of equation (43). The canonical probability density reads

$$\rho(\phi_1, \dots, \phi_N, p_1, \dots, p_n) = \frac{1}{Z(\beta)} e^{-\beta H(\phi_1, \dots, \phi_N, p_1, \dots, p_n)}, \quad (44)$$

where $Z(\beta)$ is the partition function and β the (external) inverse temperature, that can be either positive or negative: if such a distribution is derived from a larger isolated system, as already discussed in section 2.3, the temperature in the canonical ensemble is precisely the Boltzmann temperature of the whole system. A simple explicit expression (see details of analogous calculations in [33]) can be derived for the mean energy

$$U(\beta) = \langle H \rangle_\beta = N \left(1 + \epsilon - \frac{I_1(\beta)}{I_0(\beta)} - \frac{\epsilon I_1(\beta\epsilon)}{I_0(\beta\epsilon)} \right), \quad (45)$$

where $I_0(x)$ and $I_1(x)$ are, respectively, the zeroth and the first modified Bessel function of the first kind. Analogously, one can get an analytic formula for the equipartition function

$$\langle p \sin(p) \rangle_\beta = \frac{1}{\beta} - \frac{e^{-\beta}}{\beta I_0(\beta)}. \quad (46)$$

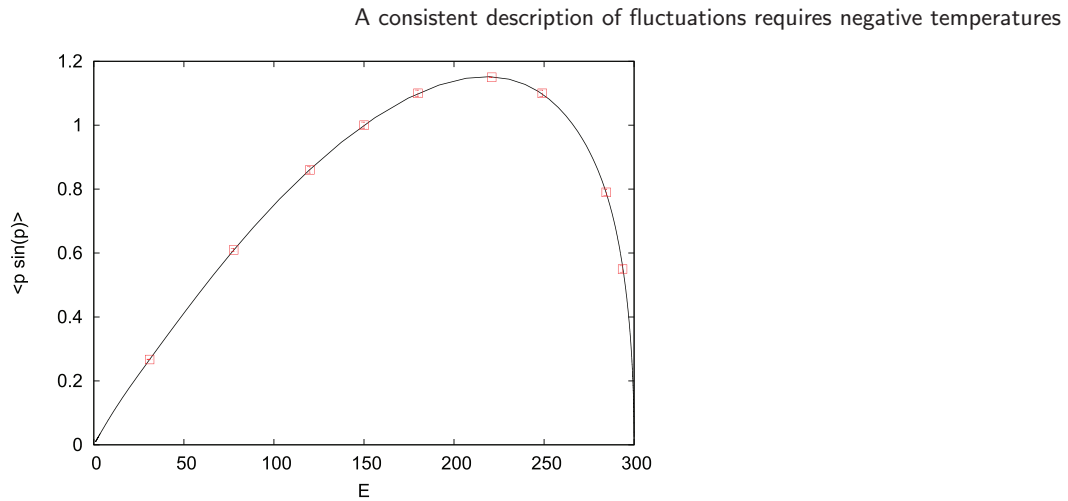


Figure 3. Black line: $\langle p \sin(p) \rangle_\beta$ versus $U(\beta)$ in the canonical ensemble (equations (45) and (46)) as parametric functions of $\beta \in (-\infty, \infty)$. Red squares: time averages of the equipartition function in molecular dynamics simulations at fixed energy E (microcanonical ensemble). The values for the parameters of the model are $N = 100$ and $\epsilon = 0.5$.

Equations (45) and (46) hold for both positive and negative β . In figure 3 we report the plot of the parametric curve $(U(\beta), \langle p \sin(p) \rangle_\beta)$ obtained by varying β both in the positive and in the negative region of the real axis.

This curve is then compared with the measurements of $\langle p \sin(p) \rangle_E$ computed from molecular dynamics simulations in the microcanonical ensemble at different values of the energy E (figure 3). This comparison clearly shows that the results obtained in the two different ensembles are identical, a transparent evidence that the equivalence of ensemble already exists for this system quite far from the thermodynamic limit ($N = 100$).

Figure 3 also shows that the equipartition formula cannot be used to measure the Gibbs temperature: as previously discussed in section 3, the equipartition theorem can fail if the density of states $\omega(E)$ vanishes. This is the case of our system (figure 1), where $T_G = \Sigma(E)/\omega(E)$ should diverge for $E \rightarrow 2N(1 + \epsilon)$: on the other hand the results obtained in the canonical and in the microcanonical ensemble clearly indicate that $\langle p \sin(p) \rangle_E \rightarrow 0$ as $E \rightarrow 2N(1 + \epsilon)$.

4.3. Spatial coherence

By analogy with systems of point vortices discussed in section 2.5, the rotator model in equation (35) possesses a spatially ordered phase at large values of E : this can be easily understood by noting that the density of states $\omega(E)$ vanishes in $E = E_M$, i.e. there is a small number of microscopic configurations corresponding to large values of E . In particular, the maximum of the energy $E_M = 2N(1 + \epsilon)$ is attained by the unique microscopic state where, for every n , $p_n = \pi$ and $\phi_n - \phi_{n-1} = \pi$; that is, where all the rotators are fixed ($\dot{\phi} = \sin \pi = 0$) and the distance among two consecutive rotators is $\Delta\phi = \pi$. As a consequence, since $\phi_0 = 0$, all the particles with even index ($n = 0, 2, 4, \dots$) must be at $\phi = 0$ and the others ($n = 1, 3, \dots$) in $\phi = \pi$. At smaller values of $E \lesssim E_M$, see

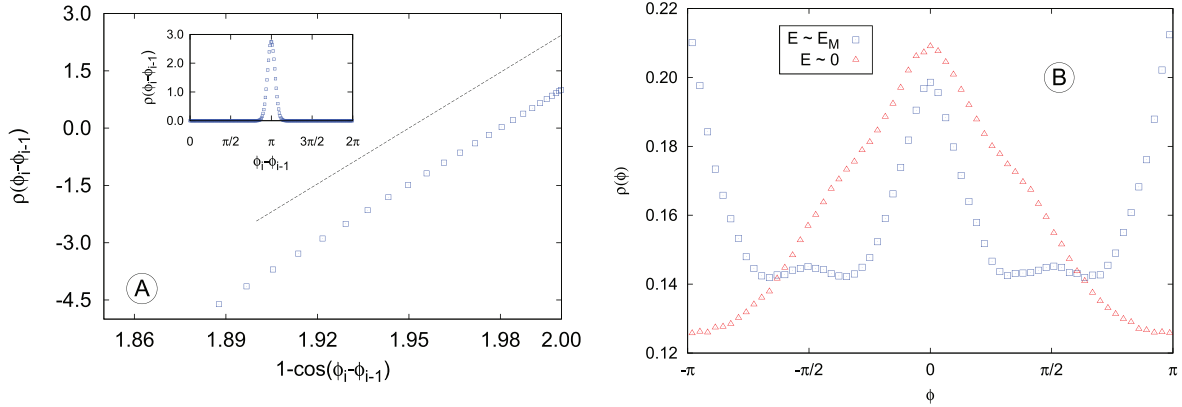


Figure 4. (A): Probability distribution function of angular distance between two consecutive rotators at high energy $E = 298.96$. (B): Probability distribution function of rotators' positions ϕ in the high energy case $E = 298.96$ (blue squares) and in the low energy case $E = 6.79$ (red triangles). The two maxima of the high energy distribution correspond to the clusters around $\phi = 0$ and $\phi = \pi$ discussed in the text. The other parameters are $N = 100$ and $\epsilon = 0.5$.

figure 4(B), such considerations can be extended, yielding a very similar situation: even and odd rotators must be close, respectively, to $\phi = 0$ or $\phi = \pi$.

We note that an ordered phase exists whenever, at a given energy E , the number of corresponding configurations is small, i.e. when $\omega(E)$ vanishes: for instance, the clustering can also be observed at small energies, when the rotators accumulate around $\phi = 0$, in order to minimize the interaction energy, see figure 4(B). The sign of the Boltzmann temperature plays a crucial role in this context, defining the features of the coherent phase. Indeed, in analogy with the single-particle-momentum distribution, it is easy to show that

$$\rho(\phi_i - \phi_{i-1}) \propto \exp\{-\beta_B[1 - \cos(\phi_i - \phi_{i-1})]\}. \quad (47)$$

When $E \rightarrow E_M$ or $E \rightarrow 0$, the inverse temperature β_B diverges and, depending on the sign of β_B , the distribution equation (47) peaks around $\phi_i - \phi_{i-1} = 0$ or $\phi_i - \phi_{i-1} = \pi$, see figure 4(A).

We stress that not every state with negative temperature is spatially ordered: the necessary condition is a small corresponding phase space volume, which implies a very high energy or, equivalently, a very small negative temperature. The same argument applies to small positive temperatures. Of course, if negative temperatures appear, they signal a reduction of phase space with increasing energy, and therefore announce a more ordered structure at higher energy.

5. Conclusions

In this paper we have given a series of arguments to support the thesis of the Boltzmann temperature T_B as a useful parameter to describe the statistical features of a system with many particles and short-range interactions, even when it takes negative values.

We draw our conclusions with a series of remarks on the role of the negative temperature and some comments on recent papers.

We have shown that the temperature T_B is the proper quantity for describing the distribution of the energy fluctuations in the canonical ensemble. It enters an immediate generalization of the Maxwell–Boltzmann distribution in the case of ‘kinetic energy’ which is not a quadratic function of momentum. For a particular model we have also demonstrated that at small $|T_B|$ (for both positive and negative values) a spatial order induced by interactions appears, whose qualitative traits depend upon the temperature’s sign.

If the microcanonical entropy $S(e)$ is a convex function, independent of the sign of T_B , there is no ambiguity in determining the flux of energy as it always goes from the hotter system, i.e. with smaller β_B to the colder one (with larger β_B). It should be remembered that the convexity of $S(e)$ can be violated only for very small systems or systems with long range interaction, both cases being very well known examples that can violate thermodynamic requirements.

From a physical point of view it is possible to obtain the canonical ensemble from the microcanonical one only for large systems with short range interactions. In such a class of systems, if $N \gg 1$, the $S(e)$ is convex and it is easy to obtain the equivalence of the ensembles. This is a fundamental requirement to obtain equilibrium thermodynamics, where there is no difference between thermostatted and isolated macroscopic systems. It is worth emphasizing that the equivalence of the ensembles only holds if one adopts the Boltzmann definition of entropy: for this reason, in systems exhibiting negative temperatures, where S_B and S_G are no longer equivalent in the large N limit, thermodynamic can be recovered for $N \rightarrow \infty$ only through the Boltzmann formalism.

In systems with few components and/or with long-range interactions, one can still define a canonical ensemble at a formal level (i.e. assume that the phase space distribution is $\propto e^{-\beta H}$), and then consider the equivalence of the ensembles. However such a formal mathematical approach, in our opinion, has no physical meaning. Since in the presence of long-range interactions (or equivalently a system with $N = O(1)$) it is not possible to make a clear distinction between the system and the reservoir, it is not possible to construct systems following a canonical distribution. For the same reason the question of the flux of energy among two systems appears to be meaningless in those cases.

Following Rugh [32], T_B can be computed via a molecular dynamics simulation, and (at least in principle) from the data of an experiment. The microcanonical formula (30), which, in most cases, allows for a practical definition of T_G , can fail in systems with negative T_B , therefore, as far as we know, at a variance with T_B , there is no general method to compute T_G in an experiment.

We emphasise that the counterexamples used in [8] to support the claimed inconsistency in the use of T_B are based on systems with very few degrees of freedom and non-convex $S(e)$. We note that the system in equation (71) of [8] is nothing but the system considered in our section 4, equation (35), with $N = 1$ and $\epsilon = 0$: the claimed strange behavior of T_B is present only if $N = O(1)$. On the contrary for $N \gg 1$ as a consequence of the convexity of $S(e)$ one has a quite natural scenario, as discussed above. In a similar way we have shown that the consistency of T_G with the microcanonical formula fails for large N .

In the microcanonical ensemble the temperature T_B is a function of the total energy E . In the canonical ensemble the temperature T_B is a mere property of the reservoir and does not depend on the microscopic configuration of the system. In [8], see section 3.4, the wrong concept of temperature (in non-isolated (sub)-systems) depending upon the energy of the microscopic configuration, see their equation (31), is used to explain this inconsistency of T_B . Such confusion seems to be persistent, see [29] for a discussion of the topic of the (non existing) fluctuations of temperature.

In conclusion our analysis, that applies to a large class of systems with many degrees of freedom and short-ranged interactions, shows that the Boltzmann temperature has the following properties: (i) it is the proper quantity ruling the fluctuations of energy in a sub-system; (ii) it can be measured by means of time-averages of a suitable observable; (iii) it rules the direction of the fluxes of energies between two coupled systems at different initial temperatures. For the Gibbs temperature, we observe that: (i) the Gibbs entropy is an adiabatic invariant (although to the best of our knowledge a mathematically rigorous proof exists only for one-dimensional systems); (ii) the microcanonical formula for equipartition in general is not valid therefore—at variance with T_B —a simple way to measure T_G is not available. We note that the differences between T_B and T_G can survive for large N , even when the ensembles are equivalent in the thermodynamic limit.

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