Comment on "Consistent thermostatistics forbids negative absolute temperatures"

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In their paper [1], Dunkel and Hilbert argue that negative absolute temperatures, a well-established thermodynamic concept, are inconsistent with thermodynamics. They claim to "prove that all previous negative temperature claims and their implications are invalid as they arise from the use of an entropy definition that is inconsistent both mathematically and thermodynamically". Here we point out that, on the contrary, negative temperatures are not only thermodynamically consistent for systems with bounded spectra $(|\langle \hat{H} \rangle|/N \leq \epsilon)$ with N the number of constituents and $\epsilon < \infty$), such as spin systems or Hubbard models, but are in fact necessary to describe equilibrated states of these systems in the high-energy regime, where the density of states, and thereby the conventional entropy, drops as a function of energy. Recently, we have successfully predicted [2] and experimentally observed [3] negative absolute temperatures using ultracold atoms in optical lattices.

To show how thermodynamically consistent negative temperatures can be used for bounded Hamiltonians, we start from conventional (not inverted) thermal states of a given bounded Hamiltonian \hat{H} , described by density matrices ρ , entropies S and positive absolute temperatures $T \geq 0$. For the inverted Hamiltonian $\hat{H}' = -\hat{H}$ with the same density matrix $\rho' = \rho$ we define the entropy S' according to S' = S. As E' = -E, it directly follows that the resulting temperature has to be negative, since $T' = (dS'/dE')^{-1} = -(dS/dE)^{-1} = -T$. With this definition, namely S' = S, all thermodynamic relations are trivially fulfilled for the \hat{H}' system if they have been fulfilled for \hat{H} . The simplest example for such a construction is a canonical ensemble, where

$$\rho = e^{-\hat{H}/(k_B T)}/Z = e^{-(-\hat{H})/(-k_B T)}/Z = e^{-\hat{H}'/(k_B T')}/Z = \rho'.$$

Combined with the usual definition of entropy, $S = -k_B \text{Tr}(\rho \ln \rho)$, the canonical ensemble therefore fulfills all conditions demanded by Dunkel and Hilbert for a consistent thermodynamics (see Eq. (4-6) in [1]), as can be checked straightforwardly and is acknowledged by Dunkel and Hilbert in [4]. Thus, the only remaining issue is the question of the equivalence of ensembles for inverted systems. In the above situation with $\hat{H}' = -\hat{H}$ and $\rho' = \rho$, however, any proof given for the conventional case of T > 0 and Hamiltonian \hat{H} can be directly translated to T' < 0 for Hamiltonian \hat{H}' . Therefore the main claim of Ref. [1] is not valid.

In the remainder of this comment, we discuss advantages and disadvantages of the alternative point of view advocated by Dunkel and Hilbert in [1]: The authors choose a non-standard

definition of the entropy of microcanonical ensembles using the so-called Hertz entropy (unfortunately named Gibbs entropy in Ref. [1]), $S_G = k_B \ln \Omega$, where $\Omega = \text{Tr }\Theta(E - \hat{H})$ counts all states up to energy E, starting from the bottom of the spectrum. With this definition, the entropy by construction always increases monotonically as a function of energy and therefore temperatures calculated from this definition are always positive, $T_G = (dS_G/dE)^{-1} > 0$. As pointed out by Dunkel and Hilbert, S_G and T_G have some advantages in case that one does insist on defining temperatures for small microcanonical systems. While temperature is a very powerful and useful concept in the thermodynamic limit and for small (canonical) ensembles in contact with a thermal bath, its usefulness for small microcanonical systems is limited: Dunkel and Hilbert correctly point out that for such systems the second part of their Eq. (6) in [1] is not valid when the standard Boltzmann entropy is used. This does, however, by no means imply that standard microcanonical thermodynamics is "thermodynamically inconsistent", it is rather one of several problems that can arise when one tries to define thermodynamics for small microcanonical systems. For example, an infinitesimal coupling of two small microcanonical systems with formally identical initial T typically induces a heat flow changing T [5, 6].

It is furthermore interesting to note that, for systems with bounded spectra, one can equally well consider an inverted version of the microcanonical Hertz entropy by defining $S_{G'} = k_B \ln \Omega'$ with $\Omega' = \text{Tr }\Theta(-E+\hat{H})$, in which the number of states is counted from the top instead of the bottom of the spectrum. The resulting temperature $T_{G'}$ is always negative and has, in contrast to T_G , the correct thermodynamic limit for inverted states.

To show the disadvantages of the postulates used by Dunkel and Hilbert, in the following we list a number of severe problems of their approach:

- (i) The entropy S_G is unphysical in the sense that it cannot be computed from the density matrix alone. It furthermore depends on states that are energetically inaccessible to the system.
- (ii) S_G cannot be connected to foundational concepts of modern statistical physics based on information theory: The highest Hertz entropy would, for example, be associated to the ensemble at the highest possible energy, which typically consists of only one non-degenerate state such as, e.g., all spins up in a spin system. The highest S_G therefore corresponds to a pure state with zero entropy in conventional approaches.
- (iii) In inverted situations the thermodynamic limit of the approach of Dunkel and Hilbert is completely ill defined [7].
- (iv) S_G violates the second law of thermodynamics in the formulation that entropy cannot decrease in an isolated system. Consider a many-body system with a unique highest excited state: the microcanonical ensemble at this energy has zero conventional entropy S but maximal S_G . If one perturbs this system by, e.g., a quantum quench, it can undergo transitions to lower energy states such that the density matrix becomes mixed and S increases. In the formalism of Dunkel and Hilbert, however, this would correspond to a decreasing entropy S_G [8].
- (v) T_G violates that heat should always flow from the hotter (smaller 1/T) into the colder (larger 1/T) system. Consider a finite microcanonical system with bounded spectrum and inverted population, where the energy is larger than that of the $T=\infty$ canonical ensemble. The use of S_G ascribes a finite positive T_G to this state. Next we bring this system into weak thermal contact with an unbounded and infinitely large thermal bath at $T=T_G=\infty$. Once the system has equilibrated with the bath, it is described by a canonical density matrix at $T=\infty$ and has thereby lowered its energy. Therefore heat has flowed from the inverted system with $T_G<\infty$ into the $T=\infty$ bath.

(vi) T_G is inconsistent with T defined for canonical ensembles. Consider the microcanonical ensemble of an infinitely large system with inverted population. The reduced density matrix of a finite subsystem can accurately be described by a canonical ensemble with T < 0 while $T_G > 0$. In contrast, microcanonical and canonical temperatures coincide when the usual Boltzmann entropy is used.

Although the vast majority of physical systems have no upper bounds in energy (e.g. the kinetic energy $p^2/2m$ is unbounded) and can therefore sustain only positive T, for systems with bounded spectra negative absolute temperatures are a well-established concept, which is not only consistent with thermodynamics, but unavoidable for a consistent description of the thermal equilibrium of inverted populations.

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