The microcanonical entropy is multiply differentiable
No dinosaurs in microcanonical gravitation:
No special ”microcanonical phase transitions”

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The microcanonical entropy $S = \ln[\mathcal{W}(E)]$ is the geometrical measure of the microscopic redundancy or ignorance about the N-body system. Even for astronomical large systems is the microcanonical entropy everywhere single valued and multiply differentiable. Also the microcanonical temperature is at all energies single valued and differentiable. It is further shown that the recently introduced singularities of the microcanonical entropy like ”microcanonical phase transitions”, and exotic patterns of the microcanonical caloric curve $T(E)$ like multi-valuednes or the appearance of ”dinosaur’s necks” are inconsistent with Boltzmann’s fundamental definition of entropy.

I. INTRODUCTION

In a recent paper Barré[1] introduced a special class of ”microcanonical” phase transitions. These are defined by singularities of the microcanonical entropy or the microcanonical temperature. However, such singularities do not exist in the microcanonical thermodynamics based on Boltzmann’s principle [2] neither for small systems nor for the really large self-gravitating ones.

We will show in the next section, the entropy as defined by Boltzmann’s principle

$$S(E) = \ln[\mathcal{W}(E)]$$

as also the inverse temperature

$$\beta(E) = T^{-1}(E) = \frac{dS}{dE} > 0$$

are single valued, smooth, and multiple differentiable ($\frac{18N-7}{2}$ times) for any finite, especially so for astronomically large $N$. This, obviously, means that $S(E)$ as well $\beta(E)$, and consequently $T(E) = 1/\beta$ are everywhere single valued and multiply differentiable.

Here $\mathcal{W}(E)$ is the $(6N-1)$ folded integral i.e. the geometric area of the microcanonical many-fold of points with the energy $E$ in the $6N$-dim. phase space. It measures the number (in units of $2\pi\hbar$) of points in the $6N$-dim phase space which are consistent with all known and dynamically conserved constraints of the system. If no other conservation law, i.e. time independent constrain, exists, the usual assumption is, the phase-space point of the system moves as time passes over the whole remaining sub-manifold (here the microcanonical energy shell) of the $6N$-dim. phase space. The dynamics is ”mixing”. In some cases like nuclear collisions, mixing may even not be needed. As we don’t have any further control every point of the manifold can be the initial point of the system. Here we assume with Boltzmann, there is no preference of any initial region of the allowed manifold compared to any other. This does not necessarily imply that a single trajectory touches during its move in time any equal sized patch in phase space equally often (ergodicity). An example is the erratic trajectory of a ball on Galton’s nail board which does not touch every nail. Repeated very often the final distribution is binomial, i.e. ruled by a simple statistical law. The microcanonical entropy thus measures our ignorance about the microscopic 6N-degrees of freedom (dof’s) needed to completely determine the system.
II. S(E) IS MULTIPOLY DIFFERENTIABLE

The microcanonical partition sum of N particles interacting via the two-body potential \( U(r - r') \), for simplicity assumed to be bound from below and confined within the volume \( V \), is defined as:

\[
W(E) = \frac{1}{N!(2\pi\hbar)^{3N}} \int_{V^N} d^{3N} \vec{r}_i \int d^{3N} \vec{p}_i \delta \{ E - \sum_i \frac{\vec{p}_i^2}{2m_i} - \Phi(\{ \vec{r}_i \}) \} \delta^3 \{ \sum_i \vec{p}_i \} \quad (3)
\]

\[
\Phi(\{ \vec{r}_i \}) = \sum_{i<j} U(\vec{r}_i - \vec{r}_j) = \frac{1}{2} \sum_{i,j} (U_{i,j} - \delta_{i,j} U_{i,i}) \quad (4)
\]

\[
W(E) = \int_{V} d^{3N} \vec{r}_i \Theta(E - \Phi(\{ \vec{r}_i \})) F_N(E - \Phi(\{ \vec{r}_i \})) \quad (5)
\]

\[
F_N(E_{\text{kin}}(\{ \vec{r}_i \})) := \frac{1}{N!(2\pi\hbar)^{3N}} \int d^{3N} \vec{r}_i \delta(E_{\text{kin}}(\{ \vec{r}_i \}) - \sum_i \frac{\vec{p}_i^2}{2m_i}) \delta^3 \{ \sum_i \vec{p}_i \} \quad (6)
\]

\[
\frac{\partial^3}{\partial E^3} \Theta(E - \Phi) \left( \frac{2E - \Phi}{3N - 5} \right) \Rightarrow T_{\text{thd}} = \frac{1}{\beta} = \left( \Theta(E - \Phi) \left( \frac{2E - \Phi}{3N - 5} \right) \right)^{-1} \quad (11)
\]

The entropy: \( S = \ln(W) \) and the inverse temperature

\[
\frac{\partial S}{\partial E} = \beta(E) = \frac{\partial S}{\partial E} = \frac{1}{W} \frac{\partial W}{\partial E} = \frac{1}{W} \int_{V} d^{3N} \vec{r}_i \Theta(E - \Phi(\{ \vec{r}_i \})) F_N(E - \Phi(\{ \vec{r}_i \})) \frac{3N - 5}{2(E - \Phi)} \quad (9)
\]

\[
\left( \Theta(E - \Phi) \frac{3N - 5}{2} \frac{1}{2} \left( \frac{1}{E - \Phi} \right)^2 \right) - \left( \Theta(E - \Phi) \frac{3N - 5}{2} \left( \frac{1}{E - \Phi} \right)^2 \right) \quad (13)
\]

is in any case finite.

III. CONSEQUENCES

For really large \( N \), e.g. for a star,

\[
\frac{dT(E)}{dE} = -\frac{\beta'}{\beta^2} = \frac{1}{cN} \quad (14)
\]

can never be infinite and leading to jumps or loops in \( T(E) \) like the ones claimed by [1] and [3]. Here \( c(e) \) is the microcanonical heat capacity of a star per atom:

\[
e = \frac{E}{N} \quad (e)
\]

\[
s(e) = S(E)/N
de/dT = c(e)
c(e) = -\frac{(ds/de)^2}{d^2s/de^2} \quad (15)
\]
As $\beta = \partial S / \partial E > 0$ as well as $\beta' = \partial^2 S / \partial E^2 \neq \pm \infty$, $c(e)$ can be positive or negative but never $= 0$ [2]. $T(E)$ is a single valued differentiable function at all energies. This clearly excludes all "hysteretic cyclings", -zones, or "dinosaur's necks" as introduced by [3]. These exotic forms of the microcanonical caloric curves must be artifacts of the mean-field approximation for the entropy (equation 5 in ref. [3]).

Not only is the microcanonical entropy everywhere multiple differentiable especially for astronomical numbers of particles, but also the interpretation of the entropy as being the geometrical measure of our ignorance about the possible initial values of the N-body system is the most fundamental and by far simplest definition for $S$ of all proposed so far.

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