On the long-range interactions and non-extensive systems

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In the presence of long-range interactions some classical thermodynamical laws break down. For example the energy is no longer proportional to the number of particles, at constant density. Furthermore some states of the system that are unstable for a canonical situation at the equilibrium with a thermostat become stable for the insulated system (microcanonical situation). At the microcanonical equilibrium the specific heat can turn to negative values. In this report these paradoxal conditions are analyzed in simple terms.

1 Extensivity and non-extensivity

In the Landau-Lifshitz book [1] in statistical mechanics one reads “Energy and entropy are additive: this means that if the number \( N \) of particles varies, they are proportional to \( N \).”

This statement is valid for a macroscopic system with short-range interactions. At variance, when the two-particles interactions decay with the distance \( r \) as \( r^{-1} \) (as it occurs for Newtonian or Coulombian interactions) then the energy \( U \) at constant density, for large number \( N \) of particles, turns out

\[
U \propto R^3 \int_0^R r^2 dr/r = R^5 = N^{5/3}.
\]

This non-additive (or extensive) form of the energy resembles the Bethe-Weizsäcker equation for nuclei [2], where a long range Coulomb repulsive interaction is present.

One can define an interaction as being long-range when it decreases with the distance \( r \) less rapidly than \( \exp(-kr) \), possibly multiplied by an oscillating or an angle-dependent factor. In this framework a long-range interaction can respect the extensivity provided that the decrease with \( r \) is sufficiently fast. For example this is the case for the Van der Waals interaction, going as \( r^{-6} \).

In the earth, condensed matter can be considered extensive with good approximation; the Newton interaction among particles is negligible, while the Coulomb interaction, which is not negligible, is cancelled because the positive and negative charges are almost in equal number. In a star the newtonian interactions cause spectacular effects, that are mass and energy dependent. The classical texts in thermodynamics usually deal with physics in the earth and then attention is primarily devoted to short range interactions. A relevant exception involves the book by Thirring [3].

The interest towards long-range interactions goes back to the black holes predicted by Michell and Laplace in 1700. In the twentieth century, the discovery of general relativity obviously induced a very relevant progress. In this report, however, mainly devoted to statistical mechanics, it is appropriate to recall some works worthy of great interest, due to Lebowitz and Lieb [4], Thirring [5] and Lieb and Thirring [6].

In recent times statistical mechanics has become a popular issue, particularly in view of the discovery of somewhat strange properties as negative specific heat, under certain circumstances. A negative specific heat is surprising, in the framework of what is taught in the classical books. Are they wrong?

2 Canonical and microcanonical distribution

The specific heat

\[ C = dU/dT \quad (1) \]
is evidently positive if the internal energy

\[ U = \sum p_n E_n \]  

(2)

is defined on the basis of the canonical distribution

\[ p_n = (1/Z) \exp(-\beta E_n) \]  

(3)

where \( Z = \sum \exp(-\beta E_n) \) and \( \beta = 1/(k_B T) \).

The sum is over the states \( n \) of the system \( S \), each with energy \( E_n \), and probability \( p_n \). The canonical distribution applies to systems in thermal equilibrium with a thermostat yielding a negligible perturbation on \( S \). This situation is evidently appropriate to an experiment in a laboratory, but inappropriate to a star. For astronomical objects, where the gravitational interactions are essential, it may be more appropriate to refer to the microcanonical distribution, pertaining to systems at fixed energy \( E \) and defined by \( p_n = 1/g(E) \) for \( E_n = E \), being \( g(E) \) the number of states at energy \( E \) and \( p_n = 0 \) elsewhere.

For a large extensive system the two distributions are essentially equivalent. To show this, let us write the canonical average value of a quantity \( X \)

\[ \langle X \rangle_c = \frac{\sum_n X_n \exp(-\beta E_n)}{\sum_n \exp(-\beta E_n)} \]

as an integral over the energy \( E \) taking into account the average microcanonical value \( \langle X \rangle_{mc} \)

\[ \langle X \rangle_c = \frac{\int \langle X \rangle_{mc} e^{S(E) - \beta E dE}}{\int e^{S(E) - \beta E dE}} \]

where \( e^{S(E)} \) is the density of states, which defines the entropy \( S(E) \). In general, the exponential has a sharp maximum for a given value \( U_1 \) and \( \langle X \rangle_c \) is the same as \( \langle X \rangle_{mc} (U_1) \). Thus canonical and microcanonical distribution are equivalent. An exception is when a phase transition from energy \( U_1 \) to energy \( U_2 \) occurs at a given temperature, with a discontinuity. For the canonical configuration the values between \( U_1 \) and \( U_2 \) are not allowed. For the microcanonical case, at variance, they are possible by means of phase separation in two domains with a domain wall. As a function of the wall position, the energy at constant temperature ranges from \( U_1 \) to \( U_2 \). In Fig. 1 one sees a line connecting \( U_1 \) and \( U_2 \), while in the canonical case there is a discontinuity.

Both the two domains are in states that could be obtained at the thermal equilibrium with the reservoir, namely for a canonical framework. Therefore one could say that both the two distributions (the canonical and microcanonical ones) are substantially equivalent. This is locally true, not globally, since the discontinuity is substituted by a straight line.

The canonical specific heat is positive, as it is reported in the books. The microcanonical specific heat is the same of the canonical specific heat (and then positive) with the exception at the transition, where the specific heat is not defined. One should remark that the assumption is that the interactions are at short-range. This is crucial. In the case of long-range interactions a domain wall could perturb the whole sample and the straight line would modify its nature, as it will be shown in the following.

### 3 The search of a simple model with long-range interactions

In the presence of long-range interactions, one can expect that the difficulties are related to the occurrence of phase transitions. Let us start with a simple example concerning a fluid (at constant pressure). For long range interactions, the fluids will turn to a complicate system, possibly a black hole or a neutron star. It is appropriate to refer to a system with fixed particles. A possible candidate is the Ising model. In this case we can write the Hamiltonian as

\[ H = -(1/2) \sum_{ij} J_{ij} S_i S_j \]  

(4)
Fig. 1: Left: phase transition in a microscopic system when the two phases have different energies \( U_1 \) and \( U_2 \). For a canonical system thermal equilibrium with a reservoir the range \([U_1, U_2]\) is not allowed and the temperature \( T(U) \) does not exist in the range \([U_1, U_2]\). For short range interactions, the curve is a straight line, while in the non-extensive case one could have a step by step line, with parts having negative slopes, corresponding to negative microcanonical specific heat, as discussed in Section 3. Right: a system with the two domains in the states 1 and 2.

where the “spins” \( S_i, S_j = \pm 1 \) are localized to the lattice points \( R_i \), for instance a cubic lattice. Let us assume ferromagnetic-like interaction with the form proportional to \( \alpha \) power of the distance:

\[
J_{ij} = 1/r_{ij}^\alpha, \quad r_{ij} = |R_i - R_j|. \tag{5}
\]

The ground state \( S_i = 1 \) is characterized by the energy

\[
U = -Nu_0 - Nu_1 \int_a^L \frac{r^2 dr}{r^\alpha} = -Nu_0' - Nu_1' L^{3-\alpha} \tag{6}
\]

where \( u_0, u_1, u_0', u_1' \) are constant, \( L \) is the length of the reference lattice, with lattice step \( a \). According to Eq. 6, the energy per spin is not related to the size \( L \) of the sample for \( \alpha > 3 \). This is the condition of extensivity of the model. One notes that the Coulomb or the Newton interaction (with \( \alpha = 1 \)) is not extensive while the Van der Waals interaction (\( \alpha = 6 \)) it is.

In order to investigate the consequences of phase transitions, let us refer to the simple, although artificial case, of interactions independent on the distance, namely \( \alpha = 0 \). The Ising Hamiltonian with the addition of a magnetic field becomes

\[
H = -(J/2) \sum_{ij} S_i S_j - NH \sum_i S_i \tag{7}
\]

the equivalent of the energy \( U \). Eq. 6 can be written in the form

\[
U(m) = -(JN^2/2)(m - Nh)^2 + (Nh)^2 J/2 \tag{8}
\]

in terms of the magnetization \( m \) per spin

\[
m = \sum_i S_i/N.
\]

The entropy is \( S(m) = -k_B \ln g \), with \( k_B \) Boltzmann constant and \( g \) number of states corresponding to the magnetization \( Nm \). Combinatorial analysis and Stirling approximation yield

\[
S(m)/k_B = N \ln 2 - (N/2)[(1 - m) \ln (1 - m) + (1 + m) \ln (1 + m)] \tag{9}
\]

In the canonical approach the equilibrium value is obtained by minimizing the free energy \( F(m) = U(m) - TS(m) \). The well known solution is the mean-field one for the one-dimensional Ising model.
that for the Hamiltonian (7) is not an approximation. As a function of temperature, for a given value of \( h \), a continuous second-order transition occurs only for \( h = 0 \). For a given \( T \), a first order phase transition occurs for \( h = 0 \), with a discontinuity of \( m \) but \( U(m) \) is continuous, according to (8). In the light of section 2 the canonical and microcanonical distribution are equivalent. Therefore the specific heat is positive.

One should observe that in order to keep \( m \) fixed on varying \( N \), the temperature \( T \) must be proportional to \( N \), or more generally to \( N^{1-\alpha/3} \), according to Eq. (6). In order to find a case of inequivalence between the canonical and microcanonical situations, and perhaps a negative microcanonical specific heat, one must have discontinuity in the energy and therefore a model less symmetric than the Ising one. One possibility is to include three-spin interaction, again independent on the distance. Then the energy \( U \) is a function of \( m^3 \), according to the equation

\[
U(m) = -K N^3 m^3 - h N^3 J m
\]

while the entropy is still given by Eq. (9). The field \( h \) has to be weak and positive. Then \( U \) is a function decreasing on increasing \( m \) and if a discontinuity in \( m \) at constant field occurs at a certain temperature \( T_c \) one has a discontinuity of the energy, from \( U_1 \) to \( U_2 \). We are going to show that the microcanonical specific heat \( C \) can be negative. In the canonical case, the energy range between \( U_1 \) and \( U_2 \) is forbidden. Outside this range, the canonical and microcanonical case are equivalent, for a macroscopic system, according to our general argument. The range in between \( U_1 \) and \( U_2 \) implies a magnetization range from \( m_1 \) to \( m_2 \). In this range the energy \( U \) can be defined as well as the entropy \( S \), their derivatives \( U' = dU/dt \) and \( S' = dS/dm \) and consequently also the temperature \( T = dU/dS = U'/S' \) and the specific heat \( C = dU/dm \). We know that the temperatures corresponding to \( U_1 \) and \( U_2 \) are the same. The functions \( U(m), S(m), U'(m) \) and \( S'(m) \) are continuous. Therefore there are values of \( U \) for which \( dT/dU < 0 \) and then \( C < 0 \). We have considered an artificial model at the only purpose to understand how a specific heat can be negative and, more generally, how a microcanonical system can have states that are forbidden to the canonical one. A less academic case could be the Ising model with non extensive interaction dependent on the distance. A first order phase transition occurs at a certain temperature \( T_c \), according to (8). In the light of section 2 one has a black hole. The general relativity yields a similar result. The value \( 2GM/c^2 \) is known as Schwarzschild radius, from the scientist of the first half of the twentieth century. Other scientists expert in black holes are Chandrasekhar, Penrose and Hawking.

**4 Realistic long range interaction**

I will report only some stimulating examples and references:

**Example 1. Nuclei and electrons with Coulomb interaction**: The specific heat is positive (Lieb 1969 [4]).

**Example 2. Newtonian interaction (in stars and galaxies)**: A review paper of didactic character is the one from Balian and Blaizot [7].

**Black hole according to Laplace**: The escape velocity from a star at a mass \( M \) and radius \( R \) is given by \( \sqrt{2GM/R} \), being \( G \) the Newton constant. Therefore the light is trapped in for a radius \( R < 2GM/c^2 \), being the light speed. One has a black hole. The general relativity yields a similar result. The value \( 2GM/c^2 \) is known as Schwarzschild radius, from the scientist of the first half of the twentieth century. Other scientists expert in black holes are Chandrasekhar, Penrose and Hawking.

**Specific heat negative**: A star can release energy and meantime to increase its temperature. According to Chavanis [8]: “If radiation energy is extracted from a star whose nuclear fuel is exhausted, the star will contract and heat up. ...Black holes display the same phenomenon. Thus, ...astronomical
Fig. 2: The energy (Eq. 10) is the blue dotted line while the entropy $S$ (Eq. 9) is the red dotted dashed line. The free energy $F = U - TS$ (solid line) has two equivalent minima at the transition temperature $T_c$. The green line tracks the $U_1$ of the Ising model.

Fig. 3: Plots of $U' = dU/dm$ and of $S = dS/dm$ as a function of $m$ according to Eqs. 9 and 10. The black line tracks the temperature. The continuous line is common to the canonical and microcanonical formalism while the dotted line is valid only for the microcanonical formalism. In the range at negative slope the microcanonical specific heat is negative.

systems have negative specific heat”. The system exhibiting such a negative specific heat is not at the equilibrium. The specific heat we are dealing with is not canonical (obviously) but also is not microcanonical. On the other hand a more elaborate argument (Balian and Blaizot 1999 [7], Chavanis 2006 [8]) confirms the negative value of the microcanonical specific heat.

**Low density limit:** There is a limit to the infinite volume with $V^{1/3}T/N$ fixed (de Vega and Sanchez, 2006). For instance one can fix the density $N/V$ and then the temperature is proportional to $N^{1/3} = N^{1-\alpha/3}$ as at the section 3.
Example 3. Jupiter: This planet is fluid and it irradiates more energy than the amount received from the sun. Therefore it must have an internal source of energy, likely related to the gravitational contraction. Although being a planet and not a star (its mass is too small, eventhough is the biggest planet in the solar system), still it has some properties of a star. The physicists devoted to non-extensive systems (Robert and Sommerie, 1992 [10]) find the presence of a vortices and, as all the vortices, having long range interaction. Why looking to Jupiter to find vortices that are present also on the earth? The vortices on Jupiter have two dimensions turbulence, very different from the usual ones: in this system there is weak energy dissipation, so the vortices on Jupiter are very stable. The red spot (a giant vortex) discovered in 1665 is still present nowadays.

5 Controversial aspects

In the introduction I wrote: “are the classical texts wrong?”. Obviously the statement by London and Lifshitz, recalled at the beginning of this report, is not valid when certain interactions, for instance the gravitational ones, are taken into account. Evidently the specific heat the classical texts are referring to is the canonical specific heat (always positive). When one writes a book one has to accept a certain lack of rigorousness if he doesn’t want to be boring. Certain authors make almost provocative criticism of the classical texts. Thus Combes and Robert (2006) [11] wrote: “The Gibbs canonical formalism has a priori no theoretical justification...”. The same authors later on (2007) [12] write “For [non-extensive] systems,...the canonical formalism of Gibbs is no longer justified. The canonical distribution, which describes correctly any extensive system in equilibrium with a thermostat ... cannot be used here any more”.

Francoise Combes is a distinguished astrophysicist and her competency in cosmology is very high. Raoul Robert is one of the best experts in two-dimensional turbulence. However Eq. 3 is valid for any finite system, both extensive and non-extensive, in equilibrium with a thermostat. That equilibrium might be difficult to achieve in practice but this is something else. The aim of the above authors is possibly to point out that certain approximations usual for short range interactions can be dangerous if used in the present of long range interactions. For instance, the canonical formalism does not describe the fluctuations occurring in a small sub-system (Bouchet and Barré, 2005 [13]). I will mention a few other statement that in my opinion are excessive. For instance, from Gross (2006) [14]: “...a phase transition of first order ... is only treated correctly by microcanonical Boltzmann-Planck statistics...Conventional canonical statistics is insufficient to handle the original goal of Thermodynamics, phase separations...”.

To conclude this section on the controversies in non-extensive statistical mechanics it is appropriate to mention the Tsallis’ entropy. This is the equation proposed by Tsallis in 1988 [15]:

$$S_q = k_B \frac{1 - \sum p_i^q}{q - 1}$$  (11)

in order to generalize the Boltzmann entropy $S_1 = k_B \sum p_i \ln p_i$, which corresponds to $q = 1$. The above equation has been considered a great success and Tsallis has been invited in 2005 to write the introduction to the special issue of Europhysics News devoted to non-linear statistics (Sévenne, 2005 [16]). On the other hand the Tsallis entropy has strong opponents, for instance Balian and Nauenberg (2006) [17]. The conditions of applicability of the Tsallis entropy are not clear. Perhaps the best comment is the one from Chavanis (2006 [18]): “In general, [the Tsallis entropy and its generalizations] reflect the existence of ‘hidden constraints’... If the system does not ‘mix well’ there is no universal form of entropy to account for non-ergodicity. In many cases, the resemblance with a “generalized thermodynamical formalism” is essentially effective or formal. In some cases, there is no relation with thermodynamics at all.”
6 Conclusions

The long range interactions have noticeable peculiarities. When the interaction decays sufficiently slow with the distance, the energy is no longer proportional to $N$. In this non-extensive system the microcanonical specific heat can be negative and more generally the microcanonical statistical mechanics can have properties very different from the ones pertaining to the canonical statistical mechanics. When $N$ goes to infinite, catastrophes as the black holes can occur but a thermodynamical limit is also possible with a temperature going to infinite with $N$. Obviously the equilibrium with a thermostat does not exist for the astronomical systems that are the ideal laboratory for the gravitational interaction and the microcanonical distribution can be more adequate than the canonical distribution.

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References