Thermo-Statistics or Topology of the Microcanonical Entropy Surface

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Abstract. Boltzmann’s principle $S(E, N, V \cdots) = \ln W(E, N, V \cdots)$ allows the interpretation of Statistical Mechanics of a closed system as Pseudo-Riemannian geometry in the space of the conserved parameters $E, N, V \cdots$ (the conserved mechanical parameters in the language of Ruppeiner [1]) without invoking the thermodynamic limit. The topology is controlled by the curvature of $S(E, N, V \cdots)$. The most interesting region is the region of (wrong) positive maximum curvature, the region of phase-separation. This is demonstrated among others for the equilibrium of a typical non-extensive system, a self-gravitating and rotating cloud in a spherical container at various energies and angular-momenta. A rich variety of realistic configurations, as single stars, multi-star systems, rings and finally gas, are obtained as equilibrium microcanonical phases. The global phase diagram, the topology of the curvature, as function of energy and angular-momentum is presented. No exotic form of thermodynamics like Tsallis [2,3] non-extensive one is necessary. It is further shown that a finite (even mesoscopic) system approaches equilibrium with a change of its entropy $\Delta S \geq 0$ (Second Law) even when its Poincaré recurrence time is not large.

1 Introduction

Why this paper?
Since more than 100 years does thermo-statistics emphasize the canonical- or the grand-canonical ensemble in the thermodynamic limit as the appropriate microscopic description of an equilibrized system. Here a homogeneous, practically infinite, system is controlled by intensive parameters like the temperature. Though in textbooks the microcanonical ensemble is considered as the fundamental ensemble, due to mathematical difficulties it is quickly left in favor of the canonical ones. Intensive variables like temperature, pressure and chemical potential are used instead of the mechanical defined extensive energy, volume and particle number.

The intensive variables are even canonized to found the axiomatic definition of an orthode [4] from where Statistical Mechanics (at least its intensive or canonical form) is deduced. Lebowitz [5,6] considers the thermodynamic limit and Elliott Lieb [7] extensivity, which also needs the thermodynamic limit to ignore surface effects, as the condition sine-qua-non.
In the thermodynamic limit \( \lim_{V,N \to \infty} \frac{N}{V} = \rho \) all surface effects may be ignored. Usually, it is clear that this approach cannot do justice to phase separations. In fact, the gain in entropy when a system splits into different phases by interphase surfaces is the essence of phase transitions of first order. A liquid-gas transition is experimentally detected just by the interface between the liquid and the gas. Consequently, in the (grand)-canonical approach, phase-transitions are indicated by the Yang-Lee singularities [8] where the grand-canonical potentials are non-analytic in \( z = e^{\beta \mu} \) or singular. These indicate the break-down of the (grand)-canonical formalism. In remarkable contrast, the microcanonical ensemble has no problems at phase-separations and the microcanonical density of states remains single-valued and multiply differentiable in all conserved control parameters also here, see below. This is certainly the strongest argument in favor of the fundamental significance of the micro-ensemble.

At phase-separation the entropy \( S(E,N,\cdots) \) has a positive curvature. Ruppeiner’s Riemannian geometry of fluctuations [1] must be reformulated there as Pseudo-Riemannian. This leads to a negative heat capacity and a violation of Clausius’ formulation of the Second Law (“heat flows always from the hot to the cold system”). Phase-separations demand an essential, fundamental, change of conventional classical thermo-statistics. Thermodynamics, however, was invented in the 19. century to explain the working of steam engines. I.e. one of its primary issues were just phase-separations.

What was said applies to large systems with short-range forces. The largest systems in nature, self-gravitating astro-physical systems, are subjected to forces (gravitation) with a range comparable to the linear extension of the system. These systems are naturally inhomogeneous and non-extensive. A description of their equilibrium by intensive variables with a homogeneous spatial distribution misses these most interesting situations. Ironically, the thermodynamic limit does not apply to these really large systems. Tsallis [2] on the other hand addresses non-extensive systems explicitly but keeps the description in terms of intensive variables which fix the relevant conserved parameters only on average. However, non-extensive systems are usually not self-averaging. He believes the equilibrium statistics of Hamiltonians systems demands a new definition of entropy. This, is not so [9], see section 3.2.

It is well known that self-gravitating systems collapse to a star in a more or less void background at low energies, the “gravothermal catastrophe” [10,11]. This is of course quite interesting but outside of any homogeneous canonical thermodynamics. There is nothing peculiar with this in microcanonical thermodynamics. Certainly, angular-momentum can change this essentially. However, the microcanonical equilibrium configuration of a self-gravitating system under larger angular-momentum has not been investigated yet (exception [12]). I will show in section 3.2 how the competition between gravitational collapse and centrifugal disruption leads in a natural manner to a breaking of rotational symmetry and to multi-star configurations with a large variety of different but quite realistic configurations. In this section the global phase diagram of self-gravitating and rotating many-body systems as function of energy and angular-momentum.
is presented, c.f. [12]. It is for the first time that these various realistic stellar configurations are interpreted as global equilibrium configurations.

The thermodynamic limit is also invoked since Boltzmann to deduce the Second Law of Thermodynamics [6,13–15] from microscopic reversible dynamics. Then Zermelo’s [16] paradox becomes blunted as the Poincaré recurrence time \( t_{\text{rec}} \) is much longer than any physically relevant observation time. This is different for a finite, eventually small system.

By all these reasons a reinvestigation of the microscopic foundation of Statistical Mechanics starting from Newtonian reversible mechanics of the finite many-body system using a minimum of assumptions but avoiding the thermodynamic limit is highly needed. The “Geometric Foundation of Thermo-Statistics” proposed in [17] and further developed here offers a new, deeper, and much simpler understanding of the microscopic foundation of Thermodynamics.

2 The few essentials of Statistical Mechanics

2.1 Why does conventional statistics like the thermodynamic limit?

The relative fluctuations of a macroscopic observable \( A \) in pure phases of an extensive system vanish in the large \( N \) limit:

\[
\frac{\langle A^2 \rangle - \langle A \rangle^2}{\langle A \rangle^2} \propto \frac{1}{N}
\]

We call this behavior self-averaging. Then the probability aspect of statistics becomes unimportant.

Here we want to study also non-extensive situations, therefore, we are not allowed to go to the thermodynamic limit. Fluctuations must be taken seriously.

2.2 Obsolete gospels of conventional thermo-statistics

Then, most axioms which are mistaken to be fundamental for Statistical Mechanics even turn out to be violated:

- Phase transitions (do not) exist only in the thermodynamic limit
- Specific heat is (not) \( c \sim \langle (\delta E)^2 \rangle > 0 \) or \( dT/dE > 0 \)
- Heat does (not) always flow from hot to cold
- Thermodynamic stability does (not) necessarily imply the concavity of \( S(E,N,\ldots) \)
- (No) extensivity of \( S \), (no) scaling with \( N \)
- (No) unique Legendre mapping, \( T \rightarrow E \), etc.
- Rise of entropy is (not) necessarily connected to trend towards uniformization
- Second Law (not) only in infinite systems, i.e. second law (not) only when the recurrence time is much larger than the observation-time \( t_{\text{rec}} \gg t_{\text{obs}} \)
• A system at equilibrium is \( \text{(not)} \) necessarily an orthode in the sense of Gallavotti [4]. “Boltzmann’s heat theorem”, i.e.

\[
\frac{dE(T, P)}{T} + \frac{PdV(T, P)}{T}
\]

is \( \text{(not)} \) necessarily a total differential \( dS(T, P) \), because \( S(T, P) \) is not always a smooth, one valued, function of \( (T, P) \), see section 3.1, order parameter.

Violations of these gospels seem shocking statements: Lebowitz [5] and Lieb[18,14] believe these make thermo-statistics impossible to exist. Nevertheless these violations are valid building stones of statistics. They are even necessary for thermo-statistics to apply to the original goal of Thermodynamics, the description of phase-separation, the scenario in which steam engines do work. At closer inspection these violations are not so strange. Recapturing the main roots of statistical mechanics we will see that it makes a lot of sense to formulate it without invoking the above axioms and without using the thermodynamic limit. The only essential axiom needed to define equilibrium statistics is Boltzmann’s principle c.f. section 2.4, eq.(3), once we agree not to use the thermodynamic limit. To concentrate on this is a great advantage as this principle has a very simple geometrical meaning.

It is a benefit of the new, extended theory which I offer here, that by reducing its axiomatic basis to this single principle it applies also to Hamiltonian non-extensive systems and among them to the really large systems as astrophysical ones, which are far larger than the thermodynamic “limit” of any homogeneous system allows. A whole new world for applications of thermo-statistics opens. Of course, then one cannot separate volume from surface effects. This is anyhow dubious for non-extensive systems or at phase-separation.

Here however, I must make it very clear that in any cases where the thermodynamic limit of a homogeneous phase does exist, the geometrical theory is in complete agreement with conventional Thermodynamics and conventional extensive Statistical Mechanics.

### 2.3 Thermodynamics, a probabilistic theory; Control parameters

Thermodynamics is a macroscopic description of a many-body system within a few \( (M \sim 3) \) macroscopic control parameters and where \((6N - M \gg M)\) dof’s remain uncontrolled. Therefore, Thermodynamics describes all systems with the same \( M \) simultaneously. All systems under the same macroscopic constraints are simultaneously addressed by the theory. Statistical mechanics describes the whole \( 6N - M \) dimensional manifold, i.e. all points in then \( N \)-body phase-space with same energy \( E \), the microcanonical ensemble \( \mathcal{E} \). Consequently, it gives only probabilistic predictions how the average of the systems in the ensemble behave [19].

\(^1\) We denote manifolds in phase-space by calligraphic letters like \( \mathcal{E} \).
A large extensive system in a pure phase is self-averaging. In the thermodynamic limit a sharp peak of the probability distribution guarantees the identity of the average with the most likely configuration.

But what if the thermodynamic limit does not exist like for a non-extensive system? For a small system like a nucleus or an atomic cluster the same measurement must be performed very often and the average be taken before its thermodynamic behavior can be seen.

2.4 Boltzmann’s principle, the microcanonical ensemble

The key quantity of statistics and thermodynamics is the entropy $S$. Its most fundamental definition is as the logarithm of the area $W(E)$ of the manifold $E$ in the N-body phase-space by Boltzmann’s principle [20]:

$$W(E, N, V) = \epsilon_0 \text{tr}\delta(E - H_N)$$

$$\text{tr}\delta(E - H_N) = \int \frac{d^3 p}{N!(2\pi\hbar)^3} \frac{d^3 q}{N!(2\pi\hbar)^3} \delta(E - H_N). \quad (2)$$

$$S = k \cdot \ln W \quad (3)$$

Boltzmann’s principle is the only axiom necessary for thermo-statistics. With it Statistical Mechanics and also Thermodynamics become geometric theories. For instance all kinds of phase-transitions are entirely determined by topological peculiarities of $E(E, N, \cdots)$ and thus of $S(E, N, \cdots)$ see below.

Local or global constraints?

In microcanonical statistics the “extensive”, better conserved, control parameters as energy, volume, particle number etc. can be determined macroscopically sharp. There may well be small, microscopic violations of some microscopic conservation laws due to the non-ideal nature of the container. Therefore, we allow small fluctuations in these microscopically conserved quantities. Evidently, it does not matter whether the entropy $S(E, N, V)$ has an extremum or not. Its local value is significant. It is uniquely defined by eqs. (2,3) as a high-dimensional integral. It is thus everywhere multiply differentiable, – certainly the most important difference to canonical statistics. This is especially important at phase-separations where the curvature of $S(E, N, V)$ is positive c.f. section 3.1.

Why not canonical?

In the canonical statistics, also in Tsallis “non-extensive statistics” e.g. the energy is fixed in the mean by Lagrange parameters like $\beta = 1/T$. This works only if the microcanonical ensemble is self-averaging. Now for non-extensive situations like at phase-separations e.g. the energy $E(T)$ as function of the Lagrange
parameter like $T$ is multi-valued c.f. section 3.1(ambiguity · · ·). This leads to
the (in view of standard Thermodynamics) surprising negative heat-capacity c.f.
section 3.1(negative heat capacity · · ·), which is well documented even experimentally c.f.[11,21–33].

At points of negative curvature of $S(E, N, · · ·)$ the canonical ensemble
is not an orthode

In chapter 1.5 of his book[4] Gallavotti presented an axiomatic deduction
of thermo-statistics starting from the definition of an orthode.

Following Boltzmann’s heat theorem [34] he defines an ensemble to be an
orthode when an infinitesimal change of the energy $dE$ and volume $dV$ makes

$$\frac{dE}{T} + \frac{P dV}{T}$$

an exact differential, at least in the thermodynamic limit. Here $T$ the “temper-
ature” is the average kinetic energy per particle and $P$ the “pressure” is defined
as the average momentum transfer per unit time and unit surface area of the
container.

Clearly this definition is of little help for a non-extensive system and/or
when the thermodynamic limit does not exist, where a given $T$ or $P$ does not
fix the energy or volume. It fails in situations where the canonical ensemble is
not equivalent to the microcanonical one, i.e. also at phase-transitions.

3 Equilibrium Thermodynamics

3.1 Phase transitions

Relation to Yang-Lee theory

In conventional extensive thermodynamics phase transitions are indicated by
the Yang-Lee zeros of the grand-canonical partition sum $Z$ in the thermody-
namic limit. In order to generalize the definition of phase transitions also to
non-extensive systems I start for the moment with the Laplace transform from
the microcanonical density of states $e^S$ to the grand-canonical one (here the

\[2\] In fact the paper [24] pointed explicitely to the fundamental failure of the canonical
ensembles near first order phase transitions in general and its non-equivalence to
the fundamental micro-ensemble which shows a negative heat capacity there. It was
rejected by Gary S. Grest, the Divisional Associate Editor of statistical mechanics of
PRL, June 3 1997, with the argument: “I am not convinced that the microcanonical
ensemble is more physical than the canonical ensemble. After all, phase transitions
in the experimental world are at constant temperature and not at constant energy.”
If this would be true, a ship would not have been able to sail on the surface of the
ocean, America would never have been discovered and PRL would not even exist.
discreteness of \( N \) does not matter): 

\[
Z(T, \mu, V) = \int_0^\infty \frac{dE}{\epsilon_0} \int dN \ e^{-[E-\mu N-TS(E)]/T}
\]

(5) 

\[
= \frac{V^2}{\epsilon_0} \int_0^\infty \ e^{-V[e-\mu n-Ts(e,n)]/T}
\]

(6) 

\[
\approx e \ cons.+lin.+quadr.
\]

The linear term is explicitly put to 0 by solving 

\[
\frac{1}{T} = \frac{\partial S}{\partial E} \bigg|_{e_s,n_s}
\]

(7) 

\[
\frac{\mu}{T} = -\frac{\partial S}{\partial N} \bigg|_{e_s,n_s}
\]

(8) 

\[
\left( \frac{P}{T} = \frac{\partial S}{\partial V} \bigg|_{e_s,n_s} \right)
\]

(9) 

If \( s(e,n) \) is concave (has negative principal curvatures), and there is a single solution \( e_s,n_s \) of eqs. (7) and (8), the stationary point, where integral (6) is a double Gaussian integral along the two principal curvatures \( v_1, v_2 \) and the free-energy density is:

\[
\frac{F(T,\mu,V)}{V} = \frac{-T \ln(Z) + \mu N_s}{V} \rightarrow e_s - Ts_s + T \ln \left( \frac{\sqrt{-\lambda_1}}{\sqrt{-\lambda_2}} \right) + o \left( \frac{\ln V}{V} \right)
\]

The curvature matrix \( c(e, n) \) of \( s(e, n) \)

\[
c(e,n) = \begin{pmatrix}
\frac{\partial^2 s}{\partial e^2} & \frac{\partial^2 s}{\partial e \partial n} \\
\frac{\partial^2 s}{\partial e \partial n} & \frac{\partial^2 s}{\partial n^2}
\end{pmatrix}
\]

(10) 

has the eigenvalues : \( \lambda_1 \geq \lambda_2 \rightarrow \) eigenvectors : \( v_1, v_2 \)  

Hessian \( d(e, n) \)

\[
\|c(e, n)\| = \lambda_1 \lambda_2
\]

(11) 

(12) 

In general \( \lambda_1 \) can have either sign. This leads to a new, deeper definition of thermodynamic phases:

**Classification by the local topology of curvature**

- A single stable phase is defined by \( \lambda_1 < 0 \). Here \( s(e, n) \) is concave (downwards bended) in both directions, fig. (1). There is only a single solution of:

\[
\frac{1}{T} = \frac{\partial S}{\partial E} \bigg|_{e_s,n_s}
\]

(13) 

\[
\frac{\mu}{T} = -\frac{\partial S}{\partial N} \bigg|_{e_s,n_s}
\]

(14)
Here is a one to one mapping of the (grand)-canonical ↔ the micro-ensemble. The (grand)-canonical has in the thermodynamic limit the same analytical properties as the micro-ensemble. It is everywhere smooth, multiply differentiable. There are no discontinuities neither in ln \( Z \) nor its derivatives.

![Diagram](image)

**Fig. 1.** Mono-phase. The order parameter \( o \) is defined in subsection “order parameter”.

- A transition of first order with phase-separation and surface tension is indicated by the maximum curvature \( \lambda_1(e, n) > 0 \). \( s(e, n) \) has a convex intruder (upwards bended with Pseudo-Riemannian geometry) in the direction \( v_1 \) of the largest curvature (order parameter). There are at least three solutions \((e_s, n_s)\): \( o_1, o_2, o_3 \) see figure (2) of

\[
\beta = \frac{1}{T} = \frac{\partial S}{\partial E}\bigg|_{e_s, n_s} \quad (15)
\]

\[
\nu = -\frac{\mu}{T} = \frac{\partial S}{\partial N}\bigg|_{e_s, n_s} \quad (16)
\]

The whole region \( \{o_1, o_3\} \) is mapped by eq. (6) into a single point \((T_{fr}, \nu_{fr})\) in the canonical ensemble which is consequently non-local in \( o \) and bimodal. This is the origin of the Yang-Lee singularities. I.e. if the largest curvature of \( s(e, n) \) is \( \lambda_1 \geq 0 \) both ensembles are not equivalent as already pointed out by us in 1993[35,36,24,37] see also Barré et al [38]. The possibility of positive curvatures (Pseudo Riemannian geometry) is the main difference to the Riemannian geometry proposed by G. Ruppeiner[1,39]. Ruppeiner discusses shortly phase transitions of first order and points out that there is no divergence of the correlation length \( \xi \) like at second-order transitions and \( \xi \) remains of the order of the interface thickness, i.e. finite. He does not mention (or is not interested in) the positivity of the curvature of \( s(e, n) \), which encodes important information about the surface tension, see below.
and which is also the essential reason why the canonical formalism does not apply to non-extensive systems.

• A continuous ("second order") transition with vanishing surface tension, where two neighboring phases become indistinguishable. I.e. where the three stationary solutions \( o_1, o_2, o_3 \) move into one-another. This is at the extremum of \( \lambda_1 \) in the direction of order parameter \( \mathbf{v}_{\lambda=0} \cdot \nabla \lambda_1 = 0 \). These are the catastrophes of the Laplace transform eq.(6) \( E \rightarrow T \) and the critical points of the transition. If it is also on the border line \( \lambda_1 = 0 \) of the first order transition (where \( \lambda_1 < 0 \)), it is the critical end-point of the transition. It is an open question whether a line of second-order transition is also the locus of the critical end-point of a first-order transition in a hidden parameter [37].

**Physical origin of positive curvature, the surface tension**
For short-range forces it is linked to the interphase surface tension. This is demonstrated for a system of 1000 Na-clusters by figure (3).
Fig. 3. MMMC [37] simulation of the entropy \( s(e) \) per atom (\( e \) in eV per atom) of a system of \( N_0 = 1000 \) sodium atoms at an external pressure of 1 atm. At the energy \( e \leq e_1 \) the system is in the pure liquid phase and at \( e \geq e_3 \) in the pure gas phase, of course with fluctuations. The latent heat per atom is \( q_{lat} = e_3 - e_1 \). Attention: the curve \( s(e) \) is artificially sheared by subtracting a linear function \( 25 + e \times 11.5 \) in order to make the convex intruder visible. \( s(e) \) is always a steeply monotonic rising function. We clearly see the global concave (downwards bending) nature of \( s(e) \) and its convex intruder. Its depth is the entropy loss due to additional correlations by the interfaces. It scales \( \propto N^{-1/3} \). From this one can calculate the surface tension per surface atom \( \sigma_{surf}/T_{tr} = \Delta s_{surf} * N_0/N_{surf} \). The double tangent (Gibbs construction) is the concave hull of \( s(e) \). Its derivative gives the Maxwell line in the caloric curve \( T(e) \) at \( T_{tr} \), fig. (4). In the thermodynamic limit the intruder would disappear and \( s(e) \) would approach the double tangent from below. Nevertheless, even there, the probability of configurations with phase-separations are suppressed by the (infinitesimal small) factor \( e^{-N^{2/3}} \) relative to the pure phases and the distribution remains strictly bimodal in the canonical ensemble. The region \( e_1 < e < e_3 \) of phase separation gets lost.

**Negative heat capacity as signal for a phase transition of first order**
As explained in figure (4) for the example of the \( q = 10 \) Potts-model, a positive curvature (convex intruder) of \( S(E) \) in the energy direction corresponds to a characteristic *backbending* of the caloric curve \( T(E) \) or \( \beta(E) \), and to a negative heat-capacity \( c \), the general signal for a phase transition of first order as proposed by us more than 15 years ago [41,21,35,25,37,42]:

\[
c = \frac{\partial E}{\partial T} = -\left( \frac{\partial S}{\partial E} \right)^2 \frac{\partial^2 S}{\partial^2 E}
\]
Table 1. Parameters of the liquid–gas transition of small sodium clusters (MMMC-calculation [37]) in comparison with the bulk for a rising number $N_0$ of atoms. $N_{surf}$ is the average number of surface atoms (estimated here as $\sum N_{cluster}^2/3$) of all clusters with $N_i \geq 2$ together. $\sigma/T_{ir} = \Delta s_{surf}^* N_0/N_{surf}$ corresponds to the surface tension. Its bulk value is adjusted to agree with the experimental values of the $a_s$ parameter which we used in the liquid-drop formula for the binding energies of small clusters, c.f. Brechignac et al. [40], and which are used in this calculation [37] for the individual clusters.

|      | $N_0$ | 200  | 1000 | 3000 | bulk |
|------|-------|------|------|------|------|
| Na   | $T_{ir}$ [K] | 940  | 990  | 1095 | 1156 |
|      | $q_{lat}$ [eV] | 0.82 | 0.91 | 0.94 | 0.923 |
|      | $s_{boil}$      | 10.1 | 10.7 | 9.9  | 9.267 |
|      | $\Delta s_{surf}$ | 0.55 | 0.56 | 0.44 |      |
|      | $N_{surf}$      | 39.94 | 98.53 | 186.6 | $\infty$ |
|      | $\sigma/T_{ir}$ | 2.75 | 5.68 | 7.07 | 7.41 |

This was later-on further elaborated by Chomaz and Gulminelly [28,43–46] and experimentally verified [30,31].

Connecting such a system at $e_1 + \delta E, T_1$ with another one at $e_3 - \delta E > e_1 + \delta E, T_3$ and $T_1 > T_3$ then the latter one heats up to $T_{combined} = T_3 + \Delta T$ by loosing energy, whereas the former one cools down to $T_{combined} = T_1 - \Delta T$ by gaining energy. Here one of the Clausius formulation of the Second Law gets invalidated: “Heat flows always from the hotter to the cooler body.” Or with other words in the region of negative heat capacity a system acts in equilibrium as a refrigerator. This is well within ordinary classical thermodynamics! However, here Ruppeiner’s Riemannian geometry [1] must be extended to a Pseudo-Riemannian geometry.
The topology of the curvature $c(e, n)$ de-covers the global phase-diagram

Figure (5) shows the example of a micocanonical global phase diagram of the Potts ($q = 3$) lattice-gas as function of the energy $e = E/L^2$ per lattice-point and the relative occupancy $n = N/L^2$ [47]. $L \times L$ is the size of the lattice taken to be $L = 50$, and $0 \leq N \leq L^2$ is the number of occupied sites.
The Hamiltonian of the lattice gas is:

\[ H = - \sum_{i,j} o_i o_j \delta_{\sigma_i, \sigma_j} \]  

(18)

\[ n = L^{-2} N = L^{-2} \sum_i o_i. \]

with the occupancy \( o_i = \begin{cases} 1, & \text{spin particle in site } i \\ 0, & \text{vacancy in site } i \end{cases} \).

![Fig. 5. Global phase diagram or contour plot of the curvature determinant (Hessian), eqn. (12), of the 2-dim Potts-3 lattice gas with 50 * 50 lattice points. \( n \) is the number of particles per lattice point, \( e \) is the total energy per lattice point. The line (-2,1) to (0,0) is the ground-state of the lattice-gas eq. (18) as function of \( n \). The most right curve is the locus of configurations with completely random spin-orientations (maximum entropy). The whole physics of the model is between these two boundaries. At the green lines the Hessian is \( \det = 0 \), this is the boundary of the region of phase separation (the triangle \( AP_mB \)) with a negative Hessian. The region of Pseudo-Riemannian geometry; At the blue lines is a minimum of \( \det(e, n) \) in the direction of the largest curvature \( (\mathbf{v}_{\lambda_{\text{max}}} \cdot \nabla \det = 0) \), these are lines of second order transition; In the triangle \( AP_mC \) is the pure ordered (solid) phase (\( \det > 0 \)); Above and right of the line \( CP_mB \) is the pure disordered (gas) phase (\( \det > 0 \)); The crossing \( P_m \) of the boundary lines is a multi-critical point. It is also the critical end-point of the region of phase separation (\( \det < 0 \)). The red region around the multi-critical point \( P_m \) corresponds to a flat (cylindric) region of \( \det(e, n) \sim 0 \) and \( \nabla \lambda_{\text{1}} \sim 0 \), details see [47]; \( C \) is the analytically known position of the critical point which the ordinary \( q = 3 \) Potts model (without vacancies) would have in the thermodynamic limit \( N \rightarrow \infty \), from [47].
Order parameters
Definition: In the geometric theory, the order parameter $o$ of a phase-transition is defined as the length of the trajectory along the direction of maximum curvature in the global phase-diagram see fig (6). Progressing in that direction one experiences the transition from one phase to the other. In the thermodynamic limit (when it exists) the region of positive maximum curvature is jumped over by the canonical ensemble and the order parameter jumps here also (traditional definition of the order parameter). It is important to notice that the order parameter is not a simple linear function of the control parameters like $E, N$ c.f. fig. (6).

If there are more control parameters ($e, n, \cdots$) there might be a situation where because of some underlying symmetry the eigenvalue of largest curvature $\lambda_1$ is degenerate. In those cases the order parameter is multi-dimensional. All these features, convex regions, curvatures of $s(e, n, \cdots)$ are topological properties of the entropy surface $s(e, n, \cdots)$ determined by the area of the manifold of constant energy etc. within the N-body phase space.

![Fig. 6. Various trajectories of maximum curvature $\lambda_1$, $v_1 =$order parameter, for the global phase-diagram of fig. (5). Left and below the multi-critical point $P_m$, in the region of phase-separation (positive maximum curvature $\lambda_1$) we see an approximately linear behavior. Here $\beta(e, n) =$const. is approximately parallel to $\nu(e, n) =$const. and parallel to $v_1(e, n)$.](image)

Ambiguity of intensive parameters and the canonical ensemble
Fig. (7) explains what happens if one plots the entropy $s(e, n)$ vs. the “intensive” quantities $\beta = \partial S/\partial E$ and $\nu = \partial S/\partial N$ as one would do for the grand-canonical
Fig. 7. Plot of the entropy $s(e, n)$ as function $s_{\text{micro}}(\beta, \nu)$ of the “intensive” variables ($\nu = \partial s/\partial n = -\beta \mu$) in the figure labeled as “nu” and $\beta = \partial s/\partial e$ is called “beta”. The lines which build the surface are lines for $\beta$-cons. The positions of the points $A, D, B, C$ defined in fig. (5) are only roughly indicated. The convex intruder between the lines $\hat{AP}_{m}B$ and the ground-state line $\hat{AD}B$ of fig. (5), where $s_{\text{micro}}(\beta, \nu)$ becomes multi-valued as function of $\nu > \nu_{P_{m}}$ and $\beta > \beta_{P_{m}}$, here seen from the side, is indicated by shadowing. This corresponds to phase-separation at a first order transition.

At the bottom the projection of the entropy surface onto the $\{\beta, \nu\}$ plane is shown as contour plot (lines of equal $S(\beta, \nu)$). The convex part (region of phase-separation) is hidden behind the dark “critical” line in the $(\beta, \nu)$-plane.

ensemble: As there are several points $e_{i}, n_{i}$ with identical $\beta, \nu$, $s_{\text{micro}}(\beta, \nu)$ is a multi-valued function of $\beta, \nu$. The entropy surface $s_{\text{micro}}(e, n)$ is folded onto itself. In the projection in fig. (7) on the $\beta, \nu$-plane, these points show up as a black critical line (dense region). This black line continues over the multi-critical point $P_{m}$ towards $C$ indicating the direction towards the critical point of the ordinary $q = 3$ Potts model at $n = 1$ (zero vacancies). Between $P_{m}$ and $C$ the slopes

$$\frac{\partial s}{\partial \beta}|_{\nu} = \frac{1}{d}[\beta s_{nn} - \nu s_{ne}]$$ (19)

or

$$-\frac{\partial s}{\partial \nu}|_{\beta} = \frac{1}{d}[\beta s_{en} - \nu s_{ee}]$$ (20)
are negative large but finite.

The information given by the projection would be all information which can be obtained from the conventional grand-canonical entropy $s(T, \mu, V)$, if we would have calculated it from the Laplace transform, eq.(6).

The back folded branches, the convex intruder of $s(e, n)$, the region of phase-separation, is jumped over in the Laplace transform eq. (6) and gets consequently lost in $Z(T, \mu)$. Here $s(T, \mu)$ becomes non-analytical $\leftrightarrow$ Yang-Lee singularity. This demonstrates the far more detailed insight into phase transitions and critical phenomena obtainable by the geometrical interpretation of microcanonical thermo-statistics [17] but which is not accessible by the canonical treatment, c.f. the similar arguments of Gibbs [48].

### 3.2 Rotating self-gravitating systems

**Stars and multi-star clusters**

The most interesting and important non-extensive systems are self-gravitating ones. I.e. systems with the Hamiltonian

$$H_N \equiv H_N(\{r_i\}, \{p_i\}) = \frac{1}{2m} \sum_{i=1}^{N} p_i^2 + \Phi(\{r_i\})$$

with the gravitation $\Phi(\{r_i\}) = -Gm^2 \sum_{i<j} |r_i - r_j|^{-1}$. $r_i$, $p_i$ and $m$ denote, respectively, the position, momentum and mass of the $i$-th particle. Because of the long range of the gravitation the total potential energy is $\propto N^2$ and consequently non-extensive.

The statistical equilibrium of self-gravitating systems without angular-momentum was first considered by Thirring [11] who pointed out that microcanonically these systems have a negative heat capacity and therefore the microcanonical and canonical ensembles are not equivalent.

Here, we overcome the simple Thirring model and investigate the equilibrium of rotating, self-gravitating systems in a spherical symmetric box under various energies $E$ and angular-momenta $L$. These calculations are done by E.V. Votyakov [12].

The following approximations are used:

a) Mean-field approximation: We approximate any $N$-body spatial density $\rho_N = \rho(r_1, \ldots, r_N)$ by the non-correlated product of single-particle densities [12] and work henceforth in the single-particle $\mu$-space.

$$\rho_N(r_1, \ldots, r_N) \approx \prod_{i=1}^{N} \rho(r_i)$$

and the gravitation interaction:

$$\Phi[\rho_N] \approx -Gm^2 \sum_{i<k} \int \frac{\rho(r_i)\rho(r_k)}{|r_i - r_k|} d\mathbf{r}_i d\mathbf{r}_k$$
The aim is now to find those density profiles $\rho(r)$ that maximize the (mean-field) entropy ($k = 1$)

$$S^m_N(E, L) = \ln W^m_N(E, L)$$

$W^m_N$ being the mean-field approximation to the microcanonical “partition sum”, i.e. the sum of all uncorrelated many-body states ($W^m_N \leq W_N$). After integrating over the $N$-momenta:

$$W^m_N(E, L) = \frac{A}{N!} \int \left[ E - \frac{1}{2} L T^{-1} L - \Phi[\rho] \right]^{\frac{3N-5}{2}} P[\rho] d\rho(r)$$

where $P[\rho]$ is the probability to observe a density profile $\rho \equiv \rho(r)$.

We use the same trick as Lynden-Bell [49] and avoid configurations with high densities where other physical processes like nuclear reactions become more important than gravity. To achieve this, we subdivide the spherical volume $V$ into $K$ identical cells labeled by the positions of their centers. The idea is to replace the integral over $V$ with a sum over the cells. In order to avoid overlapping and to cure the short-distance singularity of the Newtonian potential we assume that each cell may host up to $n_0$ particles ($1 \ll n_0 \ll N$ but $Kn_0 > N$). This condition is essentially equivalent to consider hard spheres instead of point particles. The probability $P[\rho]$ to find a given density profile $\rho(r)$ is now proportional to the number of ways in which our $N$ particles can be distributed inside the $K$ cells with maximal capacity $n_0$ and individual occupancies $n(r_k)$ or $\rho(r_k) = n(r_k)K/V$. A simple combinatorial reasoning leads to

$$P(\rho) = \prod_{\text{cells } k, \sum n(r_k) = N} \left( \frac{n_0}{n(r_k)} \right)^{n(r_k)}.$$  \hspace{1cm} (27)

This looks analogous to a Fermi-Dirac statistics, however, here only in coordinate space. This guarantees the strict non-overlapping condition. $\rho$ can nowhere be larger than $\rho_0 = n_0K/V$. In contrast, in a recent paper Chavanis and Ispolatov [50] use Fermi-Dirac statistics in phase-space.

We express $S^m_N$ as a functional of the density profile $\rho(r)$, such that

$$\int_V \rho(r) dr = N$$ \hspace{1cm} (28)

and subsequently find the $\rho(r)$’s that maximize $S^m_N$. This leads to the self-consistent integral equation:

$$\log \frac{\rho(x)}{\rho_0 - \rho(x)} = -\frac{\beta}{\Theta} U(x) + \frac{1}{2} \beta (\omega \times x)^2 - \mu$$ \hspace{1cm} (29)

or, equivalently,

$$\rho(x) = \frac{\rho_0}{1 + e^{\frac{\beta}{\Theta} U(x) - \frac{1}{2} \beta (\omega \times x)^2 + \mu}}$$ \hspace{1cm} (30)
where $\omega[\rho]$ is the angular velocity (related to the total angular momentum by the relation $L = I[\rho] \omega[\rho]$), and $\beta[\rho]$ and $U(x)$ are respectively defined as

$$\beta = \frac{3/2}{E - \frac{1}{2}L^T (I[\rho])^{-1} L - \Phi[\rho]}$$  \hspace{1cm} (31)$$

$$U(x) = -\int \frac{\rho(x')}{|x - x'|} \, dx'$$  \hspace{1cm} (32)$$

$$\Phi[\rho] = \frac{1}{2} \int U(x) \rho(x) \, dx$$  \hspace{1cm} (33)$$

b) To solve eq.(30), Votyakov [12] expands $\rho(r_i)$ into spherical harmonics:

$$\rho(r_i) = \sum_{l,m} b_{l,m}(|r_i|) \, Y_{lm}(\Theta_i, \phi_i)$$  \hspace{1cm} (34)$$

and ignores for simplicity reasons all odd $l, m$ as well also all $l > 16$. I.e. he allows only for parity even, upside – down symmetric configurations (this is later overcome). The expansion into spherical harmonics has the advantage that the original non-linear self-consistent three-dimensional integral equation (30) becomes now a finite self-consistent set of coupled one-dimensional and two-dimensional integral equations. As function of energy and total angular-momentum the microcanonical global phase-diagram defined by the topology of the curvature (Hessian) of $S(E, N)$ shows an astonishing rich picture see fig.(8).

This example proves the superiority of the geometrical, topological, interpretation of thermo-statistics. It reproduces realistically many different configurations of even gravitating systems. No canonical description nor Tsallis non-extensive statistics had achieved this.
Fig. 8. Global phase diagram of a self-gravitating system as function of energy $E$ and angular-momentum $L$ in dimension-less units. Systematic calculations were done only in the dotted region. There are 3 different mono-phases (regions of negative maximum curvature $\lambda_1 < 0$): A single star plus some gas at small $E$ and $L$; at high energy and moderate $L$, a gas phase; and at large $L$ configurations of broken spherical symmetries with double-star systems. The mixed phase is the region with positive maximum curvature $\lambda_1 > 0$ where at least two different phases (single star and gas (low $L$), single star and double star systems, eventually rings, at intermediate $L$ are in competition, finally double-stars and gas compete with one-another at large $L$ and $E$.

4 Approach to equilibrium, Second Law

4.1 Zermelo’s paradox

When Zermelo [16] argued against Boltzmann, that following Poncarré any many-body system must return after the Poincarré recurrence time $t_{rec}$ and consequently its entropy cannot grow indefinitely, Boltzmann [34] answered that for any macroscopic system $t_{rec}$ is of several orders of magnitude larger than the age of the universe, c.f. Gallavotti [4]. Still today, this is the answer given when the Second Law is to be proven microscopically, c.f. [51]. Then, Zermelo’s paradox becomes blunted.

Here, I argue, even a small system approaches equilibrium with a rise of its entropy $\Delta S \geq 0$ under quite general conditions. Thus, Zermelo’s objection must be considered much more seriously.

However, care must be taken, Boltzmann’s definition of entropy eq.(3) is only for systems at equilibrium. To be precise: in the following I will consider the equilibrium manifold $\mathcal{E}(E,V_a)$ at $t \leq t_0$. At $t_0$ the macroscopic constraint $V_a$
is quickly removed e.g. a piston pulled quickly out to \( V_a + V_b \), and the ensemble is followed in phase-space how it approaches the new equilibrium manifold \( \mathcal{E}(E, V_a + V_b) \) see fig.(9).

### 4.2 The solution

Entropy does not refer to a single point in \( N \)-body phase space but to the whole ensemble \( \mathcal{E} \) of points. It is the \( \ln(W) \) of the geometrical size \( W \) of the ensemble. Every trajectory starting at different points in the initial manifold \( \mathcal{M}(t = t_0) = \mathcal{E}(E, V_a) \in \mathcal{E}(E, V_a + V_b) \) spreads in a non-crossing manner over the available phase-space \( \mathcal{E}(E, V_a + V_b) \) but returns after \( t_{rec} \). Different points of the manifold, or trajectories, have different \( t_{rec} \) which are normally incommensurable. I.e. the manifold \( \mathcal{M}(t) \) spreads irreversibly over \( \mathcal{E}(E, V_a + V_b) \).

**Mixing**

When the system is dynamically mixing then the manifold \( \mathcal{M}(t) \) will “fill” the new ensemble \( \mathcal{E}(E, V_a + V_b) \). Though at finite times the manifold remains compact due to Liouville and keeps the volume \( W(E, V_a) \), but as already argued by Gibbs \[52,53\] \( \mathcal{M}(t) \) will be filamented like ink in water and will approach any point of \( \mathcal{E}(E, V_a + V_b) \) arbitrarily close. Then, \( \lim_{t \to \infty} \mathcal{M}(t) \) becomes dense in the new, larger \( \mathcal{E}(E, V_a + V_b) \). The closure \( \mathcal{M}(t = \infty) \) becomes equal to \( \mathcal{E}(E, V_a + V_b) \). I.e. the entropy \( S(t = \infty) > S(t_0) \). This is the Second Law for a finite system.

**Macroscopic resolution, fractal distributions and closure [19]**

We calculate the closure of the ensemble by box counting \[54\]. Here the phase-space is divided in \( N_\delta \) equal boxes of volume \( \delta^{6N} \). The number of boxes which overlap with \( \mathcal{M}(t) \) is \( N_\delta \) and the box-counting volume is then:

\[
\Omega_d(\delta) = N_\delta \delta^d, \quad \text{here with } d = 6N - 1 \tag{35}
\]

\[
\Omega_d = \lim_{\delta \to 0} \Omega_d(\delta). \tag{36}
\]

The box-counting method is illustrated in fig.(9). The important aspect of the box-counting volume of a manifold is that it is equal to the volume of its closure.

At finite times \( \mathcal{M}(t) \) is compact. Its volume \( W(t) \) equals that of its closure \( \equiv W(t_0) \). However, calculated with finite resolution \( \delta > 0 \), \( W_\delta(t) \) becomes \( \geq W(t) \) for \( t \) larger than some \( t_\delta \), where

\[
W_\delta(t) = \int d^3p d^3q \frac{d^{3N} p d^{3N} q}{(2\pi\hbar)^{3N}} \delta (E - H_N \{ q(t), p(t); [q(t_0), p(t_0) \in \mathcal{E}(V_a)] \}) \tag{37}
\]

\[
\int d^3q f(q)d^3q = \Omega(\delta)\overline{f(q)}. \tag{38}
\]

A natural finite resolution would be

\[
\delta = \sqrt{2\pi\hbar}. \tag{38}
\]
Of course the actual problem will often allow a much coarser resolution because of the insensitivity of the usual macroscopic observables. Then the equilibration time $t_\delta$ will also be much shorter.

Thus the new definition of Boltzmann’s principle eqs. (2) is:

$$S = \ln(W_\delta),$$

or mathematically correct, though unphysical, at infinite times:

$$S = \lim_{\delta \to 0} \lim_{t \to \infty} \ln(W_\delta(t)) = N \ln\left(\frac{V_a + V_b}{V_a}\right) + S(t_0).$$

$$V_a \quad V_b \quad V_a + V_b$$

$t < t_0$ $t > t_0$

**Fig. 9.** The compact set $E(t_0)$, left side, develops into an increasingly folded but non-crossing “spaghetti”-like distribution $E(t, t_0)$ in the phase-space with rising time $t$ after opening the volume $V_b$. The right figure shows only the early form of the distribution. At much later times it will become more and more fractal and finally dense in the new larger phase space. The grid illustrates the boxes of the box-counting method. All boxes which overlap with $M(t, t_0)$ contribute to the box-counting volume and are shaded gray. Their number is $N_\delta$.

### 5 Conclusion

The geometric interpretation of classical equilibrium Statistical Mechanics by Boltzmann’s principle offers an extension also to the equilibrium of non-extensive systems.

Because microcanonical Thermodynamics as a macroscopic theory controls the system by a few, usually conserved, macroscopic parameters like energy, particle number, etc. it is an intrinsically probabilistic theory. It describes all systems...
with the same control-parameters simultaneously. If we take this seriously and avoid the so called thermodynamic limit \( \lim_{V \to \infty, N/V = \rho} \), the theory can be applied to the really large, usually inhomogeneous, self-gravitating systems. In chapter (3.2) it is shown how this new approach enables to view many realistic astro-physical configurations as equilibrium configurations under the control of total energy and angular-momentum, c.f.[12].

Within the new, extended, formalism several principles of traditional Statistical Mechanics turn out to be violated and obsolete. E.g. we saw that at phase-separation heat (energy) can flow from cold to hot. Or phase-transitions can be classified unambiguously in astonishingly small systems. These are by no way exotic and wrong conclusions. On the contrary, many experiments have shown their validity. I believe this approach gives a much deeper insight into the way how many-body systems organize themselves than any canonical statistics is able to. The thermodynamic limit clouds the most interesting region of Thermodynamics, the region of inhomogeneous phase-separation.

Because of the only one underlying axiom, Boltzmann’s principle eq.(3), the geometric interpretation keeps statistics most close to Mechanics and, therefore, is most transparent. The Second Law \( \Delta S \geq 0 \) is shown to be valid in closed, small systems under quite general dynamical conditions.

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