Equilibrium statistics applied to "Small" systems, Phase transitions in nuclei in particular

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Abstract

Equilibrium statistics of finite Hamiltonian systems is fundamentally described by the microcanonical ensemble ($M\!E$). Canonical, or grand canonical partition functions are deduced by Laplace transform. Only in the thermodynamic limit they are equivalent to $M\!E$ for homogeneous systems. Therefore $M\!E$ is the only ensemble for non-extensive/inhomogeneous systems like nuclei or stars where the $\lim_{N\to\infty,\rho=N/V=const}$ does not exist. Phase transitions of first order are signaled by convexities of $S(E, N, Z, \cdots)$ [1]. Consequences of this general and basic peculiarity for nuclear statistics as well for the understanding of Statistical Mechanics in general are discussed.

Key words: Thermo-statistics for non-extensive systems like nuclei, atomic clusters and astro-objects [1] .

1 Introduction

In 1981 Randrup and Koonin [2] proposed the statistical (grand-canonical) decay of an excited nucleus into several light fragments. As the grand-canonical ensemble fixes the mean mass but has no information of the total mass M_t of the decaying nucleus, this works only for fragment masses $M_i \ll M_t$. This touches already the central point of the discussion to follow.

The statistical *multifragmentation* of a hot nucleus simultaneously into larger fragments was introduced by [3, 4]. Of course the finiteness of the total mass and charge is then crucial. Meanwhile statistical multifragmentation developed

[1] Proposed as major topic for the "World Consensus Initiative, WCI III in Texas A& M".

to a powerful and successful description see also [5, 6, 7, 8]. A presentation of its far-reaching implications for Statistical Mechanics in general is now demanding. The "World Consensus Initiative, WCI 2004" aims to present the exemplary significance of nuclear multifragmentation for broader physics.

2 Basic concepts of statistical mechanics of finite systems

Equilibrium statistics of finite Hamiltonian systems is fundamentally described by the microcanonical ensemble (*ME*) c.f. standard textbooks like Landau-Lifshitz[9] or Guggenheim [10].

The key quantity of all statistics, the entropy $S(E, N, Z, \cdots)$, is simply the logarithm of the size (area in $6N$-phase space in resolution of $2\pi\hbar$) of the microcanonical ensemble. It measures the microscopic redundancy of our information, or ignorance, about the system when only the dynamically conserved control-parameters $(E, N, Z, \cdots)$ (eventually also the volume V) are known. All equilibrium thermo-statics follows from the dependence of S on these conserved control parameters, sometimes called "extensive" parameters [1, 11]. Without any further dynamically conserved control parameters, besides the ones listed as arguments of $S(E, N, Z, \cdots)$, a mixing of the dynamics over the remaining microcanonical submanifold of the $6N$-dimensional phase space is usually assumed (ergodicity). This, however, may not be needed in the case of nuclear collision experiments where the collision is repeated some million times and various averages are taken.

Canonical, or grand canonical partition functions are deduced from the *ME* by Laplace transform [9, 10]. They are equivalent to the *ME* under asymptotic approximation (thermodynamic limit, $\lim_{N\to\infty,\rho=N/V=const}$). This means the system must be extensive, i.e. homogeneous and scaling with N. Non-extensive systems, e.g. nuclei, stars or galaxies, however, are inhomogeneous and do not allow to go to the thermodynamic limit. Therefore the *ME* is the only ensemble for non-extensive systems like nuclei or stars. It is interesting that the "schizophrenic" attitude of the statistical physics community to ignore this fact starts slowly to be realized [12].

3 Phase separation, the original motivation of thermodynamics

Phase transitions of first order are signaled by convexities of $S(E, N, Z, \cdots)$ [1, 13].

At such transitions large homogeneous systems become inhomogeneous and establish internal phase-boundaries. The surface-tension of these boundaries is one of the reasons for the convexities. Due to the convexity of e.g. $S(E)$ the kernel of the Laplace transform $E \to T$ becomes bimodal and signals the breaking of the system into two different phases [1, 13]. The convexities imply negative susceptibilities like a negative heat capacity, compressibility, etc.. These, however, are forbidden in any canonical theory.

4 Excursion to the treatment of phase transitions of first order by Chemical Thermodynamics

Systems studied in chemical thermodynamics consist of several *homogeneous macroscopic* phases $\alpha_1, \alpha_2, \cdots$ cf.[10]. Their mutual equilibrium must be explicitly constructed from outside.

Each of these phases are assumed to be macroscopic (in the "thermodynamic limit" $(N_\alpha \to \infty|_{\rho_\alpha = const})$). There is no common canonical ensemble for the entire system of the coexisting phases. Only the canonical ensemble of *each* phase separately becomes equivalent in the limit to its microcanonical counterpart.

The canonical partition sum of *each* phase α is defined as the Laplace transform of the underlying microcanonical sum of states $W(E)_\alpha = e^{S_\alpha(E)}$ [14, 15]

$$Z_\alpha(T) = \int_0^\infty e^{S_\alpha(E) - E/T_\alpha} dE. \tag{1}$$

The mean canonical energy is

$$< E_\alpha(T_\alpha) > = - \partial \ln Z_\alpha(T_\alpha)/\partial\beta_\alpha. \tag{2}$$
$$\beta_\alpha = \frac{1}{T_\alpha}.$$

In chemical situations proper the assumption of macroscopic individual phases is of course acceptable. In the thermodynamic limit $(N_\alpha \to \infty|_{\rho_\alpha = const})$ of a *homogeneous* phase α, the canonical energy $< E_\alpha(T_\alpha) >$ becomes identical to the microcanonical energy E_α when the temperature is determined by

$$T_\alpha^{-1} = \beta_\alpha = \left.\frac{\partial S_\alpha(E, V_\alpha)}{\partial E}\right|_{E_\alpha}. \tag{3}$$

The relative width of the canonical energy is

$$\Delta E_\alpha = \frac{\sqrt{< E_\alpha^2 > - < E_\alpha >^2}}{< E_\alpha >} \propto \frac{1}{\sqrt{N_\alpha}}. \tag{4}$$

The heat capacity at constant volume is (care must be taken about the constraints (!))

$$C_\alpha|_{V_\alpha} = \frac{\partial < E_\alpha(T_\alpha, V_\alpha) >}{\partial T_\alpha} \tag{5}$$

$$= \frac{< E_\alpha^2 > - < E_\alpha >^2}{T_\alpha^2} \geq 0. \tag{6}$$

Only in the thermodynamic limit ($N_\alpha \to \infty|_{\rho_\alpha = const}$) does the energy uncertainty $\Delta E_\alpha \to 0$, and the canonical and the microcanonical ensembles become equivalent. I do not know of any microscopic foundation of the canonical ensemble apart from the limit.

The positiveness of any canonical $C_V(T)$ or $C_P(T)$ is of course the reason why the inhomogeneous system of several coexisting phases ($\alpha_1 \& \alpha_2$) with an overall *negative* heat capacity cannot be described by a *single common* canonical distribution [16, 1].

5 Application to nuclear fragmentation

Now, certainly neither the phase of the whole multi-fragmented nucleus nor the individual fragments themselves can be considered as macroscopic homogeneous phases in the sense of chemical thermodynamics (CTh). Consequently, (CTh) cannot and should not be applied to fragmenting nuclei and the microcanonical description is ultimately demanded. This becomes explicitly clear by the fact that the configurations of a multi-fragmented nucleus have a *negative* heat capacity at constant volume C_V and also at constant pressure C_P (if at all a pressure can be associated to nuclear fragmentation [1]).

Not by accident are they intimately linked to the positive (wrong) curvature of $S(E, N, Z, \cdots)$. Consequently, several familiar analyses borrowed from ordinary solid-state physics of *homogeneous* systems must be questioned per se, e.g. finite-size scaling to derive transition parameters of an imaginative "nuclear matter" with fixed N/Z ratio. This is illusory in view of the then infinite Coulomb energy. Perhaps, under sufficient awareness of this problematic, there may be some sense in such a procedure.

However, this view of the statistics of non-extensive systems is still rather unfamiliar and out of the main stream of Statistical Mechanics. Many basic axioms of Statistical Mechanics have to be reviewed like the ones recently introduced by Lieb and Yngvason [17], or even Clausius' "heat can only flow from hot to cold". On the other hand just *nuclear* experiments are especially suited to explore the many details and specialities of non-extensive equilibrium statistics, like negative heat capacities, or even constrained multiple correlations, see e.g. the contribution to the WCI by Michela d'Agostino, or the beautiful calculations by Al.H. Raduta within his "sharp microcanonical model" [18]. Therefore, I believe we should especially emphasize this aspect at the WCI. Just this is a message we shall deliver to the general physics community. We should *not press* all our results into conventional homogeneous macroscopic and scaling physics of, or to, a fictitious, non existing "nuclear matter" with $Z \sim N$. This would be only approximate anyhow and moreover would hide the special aspects of non-extensivity and the crucial constraint by finiteness, which make the statistics in nuclear physics (as also in astro-physics) so different from ordinary homogeneous macroscopic thermodynamics. *This new insight is fundamentally significant for general statistical mechanics and for the understanding how* finite *many-body systems (among them the largest, astro-physical, ones) arrange themselves under the constraint of their size.* Phase transitions of scaling systems are better seen and investigated in ordinary solid state systems. A more detailed discussion within the general frame of thermo-statistics was given at the "Next2003" [19].

6 Outlook

There is a deep and fascinating aspect of *nuclear* fragmentation: First, in nuclear fragmentation we can measure the whole statistical *distribution* of the ensemble event by event. Not only their mean values are of physical interest. Statistical Mechanics can be explored from its first microscopic principles in any detail well away from the thermodynamic limit. Second, and this may be more important: For the first time phase transitions to non-homogeneous phases can be studied where these phases are within themselves composed out of several nuclei. This situation is very much analogous to multi star systems like rotating double stars during intermediate times, where nuclear burning prevents their final implosion. The occurrence of negative heat capacities is an old well known peculiarity of the statistics of self-gravitating systems [20]. Also these cannot be described by a canonical ensemble. It was shown in [21, 19] how the *microcanonical* phase space of these self-gravitating systems has all the realistic configurations which are observed. Of course, the question whether these systems are interim equilibrized or not is not proven by this observation though it is rather unlikely.

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