

Nuclear multifragmentation, Its relation to general physics

A rich test-ground of the fundamentals of statistical mechanics.*

D.H.E. Gross

¹ Hahn-Meitner Institute Glienickerstr. 100

14109 Berlin, Germany

gross@hmi.de; <http://www.hmi.de/people/gross/>

² Freie Universität Berlin, Fachbereich Physik.

Received: date / Revised version: date

Abstract. Heat can flow from cold to hot at any phase separation, even in macroscopic systems. Therefore also Lynden-Bell's famous gravo-thermal catastrophe [1] must be reconsidered. In contrast to traditional canonical Boltzmann-Gibbs statistics this is correctly described only by microcanonical statistics. Systems studied in chemical thermodynamics (ChTh) by using canonical statistics consist of several *homogeneous macroscopic* phases cf. [2]. Evidently, macroscopic statistics as in Chemistry cannot and should not be applied to non-extensive or inhomogeneous systems like nuclei or galaxies. Nuclei are *small and inhomogeneous*. Multi-fragmented nuclei are even more inhomogeneous and the fragments even smaller. Taking this serious, fascinating perspectives open for statistical nuclear fragmentation as test ground for the basic principles of statistical mechanics, especially of phase transitions, and without the use of the thermodynamic limit. Moreover, there is a lot of similarity between the accessible phase space of fragmenting nuclei and inhomogeneous multi stellar systems.

PACS. 0 1.55.+b - 0 4.40.-b - 0 5.20.Gg - 2 5.70.Pq - 6 4.60.-i - 6 5.40.Gr - 9 7.80.-d

1 Introduction

In 1981 Randrup and Koonin [3] proposed the statistical (grand-canonical) decay of an excited nucleus into several light fragments. As the grand-canonical ensemble fixes the mean mass by an intensive control parameter, the chemical potential μ , but has no information about 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 difference between intensive parameters (fields) used in canonical statistics in contrast to the mechanical extensive control parameters used in microcanonical statistics.

The statistical *multifragmentation* of a hot nucleus simultaneously into larger fragments was introduced by [4, 5]. Of course the finiteness of the total mass and charge is then crucial. Meanwhile statistical multifragmentation developed to a powerful and successful description even of sophisticated correlations seen in nuclear multifragmentation, c.f. also [6–9]. A presentation of its far-reaching implications for the fundamental understanding of Statistical Mechanics in general is now demanding.

Here I will give mainly the motivation. In section [Fundamentals ...] I address the general basis of statistical mechanics without invoking the thermodynamic limit. Then I give the physical definition of entropy S , I show how phase-separation is necessarily linked to convexities of $S(E)$ and negative heat capacities. In section [Statistical Fragmentation] I present shortly the application to three characteristic phenomena: Nuclear multifragmentation, the frag-

mentation of small atomic clusters and finally the fragmentation of stellar objects under large angular-momentum.

In the subsection [Nuclear fragmentation] I only discuss the implications of the new formalism for statistical nuclear fragmentation. In this presentation of the “World Consensus Initiative” (WCI) there will be many contributions that compare detailed experimental data to the predictions of the different models for statistical multifragmentation of hot nuclei. Here I will put the new statistics of nuclear multifragmentation into a more general perspective: I show how, similar to nuclear fragmentation, also atomic clusters fragment with rising excitation into more and more medium sized fragments. In close similarity to nuclear multifragmentation also the accessible phase space of self-gravitating astro-physical systems splits under rising energy and/or angular momentum into various inhomogeneous phases of single stars, rotating multi-star systems, and sometimes even more exotic configurations as ring systems and others.

2 Fundamentals of thermo-statistics without thermodynamic limit

Since the beginning of Thermodynamics in the first half of the 19. century its original motivation was the description of steam engines and the liquid to gas transition of water. Here water becomes inhomogeneous and develops a separation of the gas phase from the liquid, i.e. water boils. Thus phase-separation were in the focus some 170 years ago. Every child realizes phase-separation by the

inter-phase surface. It is an irony of the history of statistical mechanics that phase transitions of first order are to be realized by the academic construct of a Lee-Yang singularity.

A little later statistical mechanics was proposed by Boltzmann[10] to explain the microscopic mechanical basis of Thermodynamics. Up to now it is generally believed that this is given by the Boltzmann-Gibbs canonical statistics. As traditional canonical statistics works only for homogeneous, infinite systems, phase separations remain outside of standard Boltzmann-Gibbs thermo-statistics, which, consequently, signal phase-transitions of first order by Yang-Lee singularities.

It is amusing that this fact that is essential for the original purpose of Thermodynamics to describe steam engines was never treated completely in the past 150 years. The system must be somewhat artificially split into (still macroscopic and homogeneous) pieces of each individual phase [2]. The most interesting configurations like two co-existing phases cannot be described by a single canonical ensemble. Important inter-phase fluctuations remain outside the picture, etc. This is all hidden due to the restriction to homogeneous systems in the thermodynamic limit.

Also the second law can rigorously be formulated only microcanonically. Already Clausius [11–13] distinguished between external and internal entropy generating mechanisms. The second law is only related to the latter mechanism [14], the internal entropy generation. Again, canon-

ical Boltzmann-Gibbs statistics is insensitive to this important difference.

For this purpose, and also to describe small systems like fragmenting nuclei or non-extensive ones like self-gravitating very large systems, we need a new and deeper definition of statistical mechanics and as the heart of it: of entropy.

2.1 What is entropy?

Entropy, S , is the characteristic entity of thermodynamics. Its use distinguishes thermodynamics from all other physics; therefore, its proper understanding is essential. The understanding of entropy is sometimes obscured by frequent use of the Boltzmann-Gibbs canonical ensemble, and the thermodynamic limit. Also its relationship to the second law is often beset with confusion between external transfers of entropy $d_e S$ and its internal production $d_i S$.

The main source of the confusion is of course the lack of a clear *microscopic and mechanical* understanding of the fundamental quantities of thermodynamics like heat, external vs. internal work, temperature, and last not least entropy, at the times of Clausius and possibly even today.

Clausius [11, 12] defined a quantity which he first called the “*value of metamorphosis*”, in German “*Wert der Verwandlung*” in [12]. Eleven years later he [13] gave it the name “entropy” S :

$$S_b - S_a = \int_a^b \frac{dE}{T}, \quad (1)$$

where T is the absolute temperature of the body when the momentary change is done, and dE is the increment

(positive resp. negative) of all different forms of energy (heat and potential) put into resp. taken out of the system. (Later, however, we will learn that care must be taken of additional constraints on other control parameters like e.g. the volume, see below).

From the observation that heat does not flow from cold to hot (see subsection Zeroth Law) he went on to enunciate the second law as:

$$\Delta S = \oint \frac{dE}{T} \geq 0, \quad (2)$$

which Clausius called the “*uncompensated metamorphosis*”. As will be worked out later the second law as presented by eq.(2) remains valid even in cases where heat (energy) flows during relaxation from low to higher temperatures.

Prigogine [14], c.f. [2], quite clearly stated that the variation of S with time is determined by two, crucially different, mechanisms of its changes: the flow of entropy $d_e S$ to or from the system under consideration; and its internal production $d_i S$. While the first type of entropy change $d_e S$ (that effected by exchange of heat $d_e Q$ with its surroundings) can be positive, negative or zero, the second type of entropy change $d_i S$ is fundamentally related to its spontaneous internal evolution (“*Verwandlungen*”, “*metamorphosis*” [11]) of the system, and states the universal irreversibility of spontaneous transitions. It can be only positive or zero in any spontaneous transformation.

Clausius gives an illuminating example in [12]: When an ideal gas suddenly streams under insulating conditions from a small vessel with volume V_1 into a larger one ($V_2 > V_1$), neither its internal energy U , nor its temperature

changes, nor external work done, but its internal (Boltzmann-)entropy S_i eq.(3) rises, by $\Delta S = N \ln(V_2/V_1)$. Only by compressing the gas (e.g. isentropically) and creating heat $\Delta E = E_1[(V_2/V_1)^{2/3} - 1]$ (which must be finally drained) it can be brought back into its initial state. Then, however, the entropy production in the cycle, as expressed by integral (2), is positive ($= N \ln(V_2/V_1)$). This is also a clear example for a microcanonical situation where the entropy change by an irreversible metamorphosis of the system is absolutely internal. It occurs during the first part of the cycle, the expansion, where there is no heat exchange with the environment and no work done, and consequently no contribution to the integral(2). The construction by eq.(2) is correct though artificial. After completing the cycle the Boltzmann-entropy of the gas is of course the same as initially. All this will become much more clear by Boltzmann’s microscopic definition of entropy, which will moreover clarify its real *statistical* nature:

Boltzmann[10] later defined the entropy of an isolated system (for which the energy exchange with the environment $d_e Q \equiv 0$) in terms of the sum of possible configurations, W , which the system can assume consistent with its constraints of given energy and volume:

$$\boxed{S = k^* \ln W} \quad (3)$$

as written on Boltzmann’s tomb-stone, with

$$W(E, N, V) = \int \frac{d^{3N} \vec{p} \, d^{3N} \vec{q}}{N!(2\pi\hbar)^{3N}} \epsilon_0 \delta(E - H\{\vec{q}, \vec{p}\}) \quad (4)$$

in semi-classical approximation. E is the total energy, N is the number of particles and V the volume. Or, more

appropriate for a finite quantum-mechanical system:

$$W(E, N, V) = Tr[\mathcal{P}_E] \quad (5)$$

$$= \sum_{\substack{\text{all eigenstates } n \text{ of } H \text{ with given } N, V, \\ \text{and } E < E_n \leq E + \epsilon_0}}$$

and $\epsilon_0 \approx$ the macroscopic energy resolution. This is still up to day the deepest, most fundamental, and most simple definition of entropy. There is no need of the thermodynamic limit, no need of concavity, extensivity and homogeneity. In its semi-classical approximation, eq.(4), $W(E, N, V, \dots)$ simply measures the area of the sub-manifold of points in the $6N$ -dimensional phase-space (Γ -space) with prescribed energy E , particle number N , volume V , and some other time invariant constraints which are here suppressed for simplicity. Because it was Planck who coined it in this mathematical form, I will call it the Boltzmann-Planck principle.

The Boltzmann-Planck formula has a simple but deep physical interpretation: W or S measure our ignorance about the complete set of initial values for all $6N$ microscopic degrees of freedom which are needed to specify the N -body system unambiguously[15]. To have complete knowledge of the system we would need to know (within its semiclassical approximation (4)) the initial positions and velocities of all N particles in the system, which means we would need to know a total of $6N$ values. Then W would be equal to one and the entropy, S , would be zero. However, we usually only know the value of a few parameters that change slowly with time, such as the energy, number of particles, volume and so on. We generally know very little about the positions and velocities of the particles.

The manifold of all these points in the $6N$ -dim. phase space, consistent with the given macroscopic constraints of E, N, V, \dots , is the microcanonical ensemble, which has a well-defined geometrical size W and, by equation (3), a non-vanishing entropy, $S(E, N, V, \dots)$. The dependence of $S(E, N, V, \dots)$ on its arguments determines completely thermostatics and equilibrium thermodynamics.

Clearly, Hamiltonian (Liouvillean) dynamics of the system cannot create the missing information about the initial values - i.e. the entropy $S(E, N, V, \dots)$ cannot decrease. As has been further worked out in [16] and more recently in [17] the inherent finite resolution of the macroscopic description implies an increase of W or S with time when an external constraint is relaxed. Such is a statement of the second law of thermodynamics, which requires that the *internal* production of entropy be positive or zero for every spontaneous process. Analysis of the consequences of the second law by the microcanonical ensemble is appropriate because, in an isolated system (which is the one relevant for the microcanonical ensemble), the changes in total entropy must represent the *internal* production of entropy, see above, and there are no additional uncontrolled fluctuating energy exchanges with the environment.

2.2 The Zero'th Law in conventional extensive Thermodynamics

In conventional (extensive) thermodynamics thermal equilibrium of two systems (1 & 2) is established by bringing them into thermal contact which allows free energy ex-

change. Equilibrium is established when the total entropy

$$S_{1+2}(E, E_1) = S_1(E_1) + S_2(E - E_1) \quad (6)$$

is maximal:

$$dS_{1+2}(E, E_1)|_E = dS_1(E_1) + dS_2(E - E_1) = 0. \quad (7)$$

Under an energy flux $\Delta E_{2 \rightarrow 1}$ from 2 \rightarrow 1 the total entropy changes to lowest order in ΔE by

$$\Delta S_{1+2}|_E = (\beta_1 - \beta_2)\Delta E_{2 \rightarrow 1} \quad (8)$$

$$\beta = dS/dE = \frac{1}{T}. \quad (9)$$

Consequently, a maximum of $S_{total}(E = E_1 + E_2, E_1)|_E \geq S_{1+2}$ will be approached when

$$\text{sign}(\Delta S_{total}) = \text{sign}(T_2 - T_1)\text{sign}(\Delta E_{2 \rightarrow 1}) > 0. \quad (10)$$

From here Clausius' first formulation of the Second Law follows: "Heat always flows from hot to cold". Essential for this conclusion is the *additivity* of S under the split (eq.6). There are no correlations, which are destroyed when an extensive system is split. Temperature is an appropriate control parameter for extensive systems.

It is further easy to see that the heat capacity of an extensive system with

$$S(E, N) = Ns(e = E/N) = 2S(E/2, N/2)$$

is necessarily non-negative

$$C_V(E) = \partial E / \partial T = - \frac{(\partial S / \partial E)^2}{\partial^2 S / \partial E^2} \geq 0 : \quad (11)$$

The combination two pieces of $N/2$ particles each, one at the specific energy $e_a = e_2 - \Delta e/2$ and a second at $e_b = e_2 + \Delta e/2$, must lead to $S(E_2, N) \geq S(E_a/2, N/2) + S(E_b/2, N/2)$, the simple algebraic sum of the individual

entropies because by combining the two pieces one normally loses information. This, however, is for extensive systems equal to $[S(E_a, N) + S(E_b, N)]/2$, thus $S(E_2, N) \geq [S(E_a, N) + S(E_b, N)]/2$. I.e. *the entropy $S(E, N)$ of an extensive system is necessarily non-convex, $\partial^2 S / \partial E^2 \leq 0$* and eq. 11 follows. In the next subsection we will see that therefore *extensive systems cannot have phase transitions of first order.*

2.3 No phase separation, no boiling water, without a convex, non-extensive $S(E)$

At phase separation the weight $e^{S(E)-E/T}$ of the configurations with energy E in the definition of the canonical partition sum

$$Z(T) = \int_0^\infty e^{S(E)-E/T} dE \quad (12)$$

becomes here *bimodal*, at the transition temperature it has two peaks, the liquid and the gas configurations which are separated in energy by the latent heat. Consequently $S(E)$ must be convex ($\partial^2 S / \partial E^2 > 0$, like $y = x^2$) and the weight in (12) has a minimum between the two pure phases. Of course, the minimum can only be seen in the microcanonical ensemble where the energy is controlled and its fluctuations forbidden. Otherwise, the system would fluctuate between the two pure phases by an, for macroscopic systems even macroscopic, energy $\Delta E \sim E_{lat} \propto N$ of the order of the latent heat. Canonically, phase separations are unstable, however, not microcanonically, and of course not in real nature. The heat capacity is

$$C_V(E) = \partial E / \partial T = - \frac{(\partial S / \partial E)^2}{\partial^2 S / \partial E^2} < 0. \quad (13)$$

I.e. *the convexity of $S(E)$ and the negative heat capacity are the generic and necessary signals of phase-separation*[18]. It is amusing that this fact that is essential for the original purpose of Thermodynamics to describe steam engines and boiling water seems never been really recognized in the past 150 years. However, such macroscopic energy fluctuations and the resulting negative specific heat are already early discussed in high-energy physics by Carlitz [19].

The existence of the negative heat capacity at phase separation has a surprising but fundamental consequence: Combining two systems with negative heat they will relax with a flow of energy from the lower to the higher temperature! This is consistent with the naive picture of an *energy equilibration*. Thus *Clausius' "energy flows always from hot to cold", i.e. the dominant control-role of the temperature in thermo-statistics as emphasized by Hertz [20] is violated*. Of course this shows quite clearly that *unlike to extensive thermodynamics the temperature is not the appropriate control parameter in non-extensive situations like e.g. at phase separations, nuclear fragmentation, or stellar systems.*[21]

By the same reason the well known paradox of Antonov in astro-physics due to the occurrence of negative heat capacities must be reconsidered: Lynden-Bell [1] uses standard arguments from extensive thermodynamics that a system a with negative heat capacity $C_a < 0$ in gravitational contact with another b with positive heat capacity $C_b > 0$ will be unstable: If initially $T_a > T_b$ the hotter system a transfers energy to the colder b and by this both

become even hotter! If $C_b > -C_a$, T_a rises faster than T_b and this will go for ever. This is wrong because just the opposite happens, the hotter a even *absorbs* energy from the colder b and both system come to equilibrium at the same intermediate temperature c.f. [22,21]. Negative heat can only occur in the microcanonical ensemble. Temperature is *not* controlling the direction of energy (heat) flow when the heat capacity is negative. This is controlled by *entropy* according to the second law. Isothermal self-gravitating systems appear somehow paradox. Moreover, one cannot argue as for extensive systems $S_{1+2} = S_1 + S_2$ and $E_{1+2} = E_1 + E_2$ as discussed above. There are far reaching correlations between the two systems due to long-ranged gravity.

In the thermodynamic limit $N \rightarrow \infty$ of a system with short-range coupling the depth of the convex intruder $\Delta S_{surf} \sim N^{2/3}$, i.e. $\Delta S_{surf}/N = \Delta s_{surf} \propto N^{-1/3}$ must go to 0 due to van Hove's theorem. Of course it is only the *specific* surface entropy $\Delta S_{surf}/N$ which disappears. As phase separation exists also in the thermodynamic limit, by the same arguments as above, *the curvature of $S(E)$ remains convex, $\partial^2 S/(\partial E)^2 > 0$. Consequently, the negative heat capacity should also be seen in ordinary macroscopic systems in chemistry!*

Searching for example in Guggenheims book [2] one finds some cryptic notes in §3 that the heat capacity of steam at saturation is negative. No notice that *this is the generic effect at any phase separation!* It is characteristic that nuclear chemists like L. Moretto opposed for long against the necessity of negative heat at first order phase

transitions in nuclei c.f. [23] and claimed artificial unphysical effects to be responsible. Therefore, let me recapitulate in the next subsection how chemists treat phase separation of macroscopic systems and then point out why this does not work in non-extensive systems like fragmenting nuclei, at phase separation in normal macroscopic systems, or large astronomical systems.

2.4 Macroscopic systems in Chemistry

Systems studied in chemical thermodynamics consist of several *homogeneous macroscopic* phases $\alpha_1, \alpha_2, \dots$ cf.[2]. Their mutual equilibrium must be explicitly constructed from outside.

Each of these phases are assumed to be homogeneous and macroscopic (in the “thermodynamic limit” ($N_\alpha \rightarrow \infty|_{\rho_\alpha=const}$)). 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 $W(E)_\alpha = e^{S_\alpha(E)}$ [24, 25]

$$Z_\alpha(T) = \int_0^\infty e^{S_\alpha(E) - E/T_\alpha} dE. \quad (14)$$

The mean canonical energy is

$$\begin{aligned} \langle E_\alpha(T_\alpha) \rangle &= -\partial \ln Z_\alpha(T_\alpha) / \partial \beta_\alpha. \\ \beta_\alpha &= \frac{1}{T_\alpha}. \end{aligned} \quad (15)$$

In chemical situations proper the assumption of homogeneous macroscopic individual phases is of course accept-

able. In the thermodynamic limit ($N_\alpha \rightarrow \infty|_{\rho_\alpha=const}$) of a *homogeneous* phase α , the canonical energy $\langle E_\alpha(T_\alpha) \rangle$ becomes identical to the microcanonical energy E_α when the temperature is determined by

$$T_\alpha^{-1} = \beta_\alpha = \left. \frac{\partial S_\alpha(E, V_\alpha)}{\partial E} \right|_{E_\alpha}. \quad (16)$$

The relative width of the canonical energy is

$$\Delta E(T)_\alpha = \frac{\sqrt{\langle E_\alpha^2 \rangle_T - \langle E_\alpha \rangle_T^2}}{\langle E_\alpha \rangle_T} \propto \frac{1}{\sqrt{N_\alpha}}. \quad (17)$$

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

$$C_{\alpha|V_\alpha} = \frac{\partial \langle E_\alpha(T_\alpha, V_\alpha) \rangle}{\partial T_\alpha} \quad (18)$$

$$= \frac{\langle E_\alpha^2 \rangle_{T_\alpha} - \langle E_\alpha \rangle_{T_\alpha}^2}{T_\alpha^2} \geq 0. \quad (19)$$

Only in the thermodynamic limit ($N_\alpha \rightarrow \infty|_{\rho_\alpha=const}$) does the relative energy uncertainty $\Delta E_\alpha \rightarrow 0$, and the canonical and the microcanonical ensembles for each homogeneous phase (α) become equivalent. This equivalence is the *only* justification of the canonical ensemble controlled by intensive temperature T , or chemical potential μ , or pressure P . I do not know of any microscopic foundation of the canonical ensemble and intensive control parameters apart from the limit. This is also the reason why e.g. the Clausius-Clapeyron equation as an equation between intensive variables is *not* applicable away from the thermodynamic limit e.g. in nuclei in clear contrast to opposite claims by [26].

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 (α_1 & α_2) with an overall *negative* heat capacity cannot be described by a *single common* canonical distribution [27, 18].

This new fundamental interpretation of thermo statistics was introduced to the chemistry community in [28, 21].

2.5 A remark on "non-equilibrium" thermodynamics of small systems

Prigogine quite clearly gives a short introduction into the logical foundations of non-equilibrium thermodynamics in the book [29]. The system is assumed to be composed by small subsystems internally in thermodynamic equilibrium. Each one is itself macroscopic and homogeneous that the conventional canonical Boltzmann-Gibbs statistics applies. However, the individual subsystems are not assumed to be in mutual thermodynamic equilibrium. There are temperature- and/or pressure-gradients, there may be a flow of the subsystems etc. Hydrodynamics or heat conductivity are examples. Clearly, this is certainly not possible in small systems like atomic nuclei or atomic clusters. Therefore, attempts to transfer macro-thermodynamic concepts like temperature or Gibbs-free energy $G(T, P)$ to nano-objects [30] like single biological molecules and the exploration of Jarzynski's equality [31] must be considered with reservation. Temperature, and pressure are ill defined in such small objects [32].

3 Statistical fragmentation

3.1 Nuclear fragmentation

The new lesson to be learned is that if one defines the phases by individual peaks in $e^{S(E)-E/T}$ in (12), then there exist also *inhomogeneous phases* like in fragmented nuclei or stellar systems. The general concept of thermo-statistics becomes enormously widened.

However, before applying the microcanonical thermo-statistics to nuclear collisions a clarification is necessary: Nuclear collisions are *transient* phenomena. Thus a theory of statistical nuclear fragmentation is an *approximation* to a *dynamical* process. This is well known and applies as well to the old Weisskopf-theory of the statistical decay of a compound nucleus. The scenario one has in mind is that the emissions of fragments over the barrier is so slow that all accessible exit channels are tested. This is the open phase space *at or on top of the exit barrier*. In the statistical fragmentation model *MMMC* [18] this is taken care of by sampling all fragments under non-overlapping conditions inside a "freeze-out" volume corresponding to $\sim 5 \times V_0$ the volume of the nucleus in its groundstate. The average distance between neighboring fragments is then about 2fm. Consequently, the asymptotic (Coulomb) energy of the fragments at infinite separation is irrelevant. It is not understandable how this could be forgotten in [33] and again in [26]. The new discovery of nuclear *multifragmentation* by [5] was the clear recognition that within a time of $\ll 10^{-21}$ sec *several* medium sized fragments can cross the decay barrier. This is much shorter than the time

the fragments need to come out of mutual Coulomb fields, a fact discussed in detail in chapter 5.2.1 of my book [18]. This crucial aspect is totally ignored in [33,23,26], but commented in [34](a comment rejected by PRC with the argument that this is all well known to the community, sic!).

Now, certainly neither the phase of the whole multifragmented nucleus nor the individual fragments themselves can be considered as macroscopic homogeneous phases in the sense of chemical thermodynamics (ChTh). Consequently, (ChTh) 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 [35] and also at constant pressure C_P (if at all a pressure can be associated to nuclear fragmentation [18]).

The existence of well defined and separated peaks (phases, *if distinguished by conserved control parameters*) in the event distribution of nuclear fragmentation data is demonstrated in [36] from various points of view. This signal is in a small system like a nucleus by far more sophisticated and detailed than the simple jumping from liquid to gas in traditional macroscopic systems in chemistry. A lot more physics about the mechanism of phase transitions can be learned from such studies. This will be the topic of the contributions by P. Chomaz, F. Gulminelli and B.Tamain to the WCI.

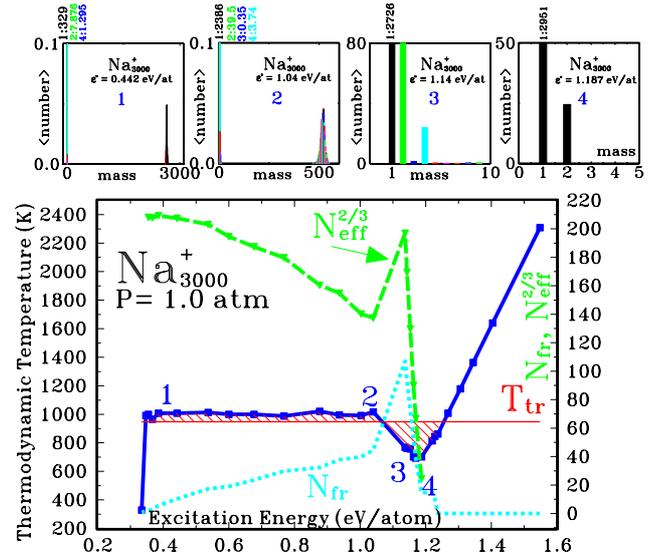


Fig. 1. Atomic cluster fragmentation, color online.

3.2 Atomic clusters

As there are several examples for nuclear multi-fragmentation in this report I will show the analogous development of the fragmentation of a single charged cluster of 3000 Na-atoms with rising excitation energy from the evaporation of a few Na-atoms over multifragmentation into monomers, dimers up to 10-mers towards finally the total vaporisation of the original cluster. Notice that this occurs all within the range of the backbending (i.e. the negative heat capacity) of the caloric curve.

To compare with usual macroscopic conditions, the calculations were done at each energy using a volume $V(E)$ such that the microcanonical pressure $P = \frac{\partial S}{\partial V} / \frac{\partial S}{\partial E} = 1 \text{ atm}$. The inserts above give the mass distribution at the various points. The label "4:1.295" means 1.295 quadrimers on average. This gives a detailed insight into what happens with rising excitation energy over the transition region: At the beginning ($e^* \sim 0.442 \text{ eV}$) the liquid sodium drop

evaporates 329 single atoms and 7.876 dimers and 1.295 quadrimers on average. At energies $e \gtrsim 1\text{eV}$ the drop starts to fragment into several small droplets (“intermediate mass fragments”) e.g. at point 3: 2726 monomers, 80 dimers, ~ 5 trimers, ~ 15 quadrimers and a few heavier ones up to 10-mers. The evaporation residue disappears. This multifragmentation finishes at point 4. It induces the strong backward swing of the caloric curve $T(E)$. Above point 4 one has a gas of free monomers and at the beginning a few dimers. This transition scenario has a lot similarity with nuclear multifragmentation. The total interphase surface area $\propto N_{eff}^{2/3} = \sum_i N_i^{2/3}$ with $N_i \geq 2$ (N_i the number of atoms in the i th cluster) stays roughly constant up to point 3 even though the number of fragments ($N_{fr} = \sum_i$) rises monotonically. Notice, the caloric curve between point 1 and 2 looks like Moretto’s “compound nucleus for ever” [37], though the temperature is higher than T_{tr} and the decay is not evaporation for ever. In contrast to claims in [37] there is considerable multifragmentation.

3.3 Fragmentation of astrophysical systems

The necessity of using “extensive” instead of “intensive” control parameter is explicit in astrophysical problems. E.g.: for the description of rotating stars one conventionally works at a given temperature and fixed angular velocity Ω c.f. [38]. Of course in reality there is neither a heat bath nor a rotating disk. Moreover, the latter scenario is fundamentally wrong as at the periphery of the disk the rotational velocity may even become larger than velocity of light. Non-extensive systems like astro-physical ones do

not allow a “field-theoretical” description controlled by intensive fields!

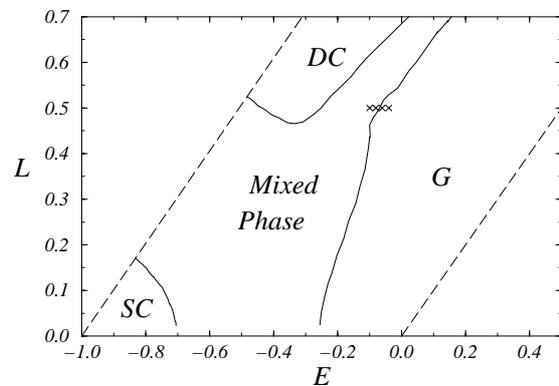


Fig. 2. Phase diagram of rotating self-gravitating systems in the energy-angular-momentum (E, L)-plane [39]. DC: region of double-stars, G: gas phase, SC: single stars. In the mixed region one finds various exotic configurations like ring-systems in coexistence with gas, double stars or single stars. In this region of phase-separation the heat capacity is negative and the entropy $S(E, L)$ is convex. The dashed lines $E - L = -1$ (left) and $E = L$ (right) delimit the region where calculations were carried out.

E.g. configurations with a maximum of random energy

$$E_{random} = E - \frac{\Theta \Omega^2}{2} - E_{pot} \quad (20)$$

and consequently with the largest entropy are the ones with smallest moment of inertia Θ , compact single stars. Just the opposite happens when the angular-momentum L and not the angular velocity Ω are fixed:

$$E_{random} = E - \frac{L^2}{2\Theta} - E_{pot}. \quad (21)$$

Then configurations with large moment of inertia are maximizing the phase space and the entropy. I.e. eventually double or multi stars are produced, as observed in reality.

In figure 2 one clearly sees the rich and realistic microcanonical phase-diagram of a rotating gravitating system controlled by the “extensive” parameters energy and angular-momentum. [39]

3.4 Outlook

It 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 including eventual inter-phase fluctuations. 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. By our studies of nuclear fragmentation we found [25,27] the very general appearance of a negative heat and the necessary convexity of the entropy $S(E)$ at any phase separation which seems to be little known in thermodynamics. *Clausius’ version of the second law “heat always flows from hot to cold” is in general violated at any phase separation even in macroscopic systems.*

In nuclear fragmentation there may be other conserved control parameters besides the energy: E.g. in the recent paper by Lopez et al. [40] a bimodality, may be phase separation, in the mass-symmetry of the fragments is demonstrated controlled by the transferred spin and not by excitation energy. This is an interesting, though still theoretical, example of the rich facets of the fragmentation phase transition in *finite* systems which goes beyond the liquid-gas transition and *does not exist in chemistry*. Angular

momentum is a very crucial control parameter in stellar systems.

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 of several nuclei. This situation is very much analogous to multi star systems like rotating double stars during intermediate times, when 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 [1,41]. Also these cannot be described by a canonical ensemble. It was shown in [17,22] 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 really fill uniformly this phase space, i.e. whether they are interim equilibrated or not is not proven by this observation though it is rather likely.

Microcanonical thermo-statistics is proven to give a realistic, objective picture of a broad scenario of real physical phenomena, much broader than conventional canonical thermodynamics.

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