Comment on: “Nonextensivity: from low-dimensional maps to Hamiltonian systems” by Tsallis et al.[1]

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The critique against using Boltzmann's *microcanonical* entropy, an "ensemble measure", as foundation of statistics is rebuffed. The confusion of the microcanonical distribution with the exponential Boltzmann-Gibbs (“BG”) distribution is pointed out. Boltzmann's principle is clearly superior over any Tsallis q-statistics in describing the equilibrium of small systems like nuclei and even self-gravitating systems as paradigm of non-extensive Hamiltonian systems.

Since 1981 thermo-statistics is addressed to highly excited (“hot”) nuclei [2, 3] and a little bit later to atomic clusters[4, 5, 6, 7, 8]. Not only the mass-dispersion, fragment-mass fluctuations, but most importantly the negative heat-capacity at fragmentation was predicted: Of course these systems cannot be treated in the thermodynamic limit (they are “non-extensive”) and many gospels of traditional canonical thermo-statistics have to be abolished. E.g. the canonical ensemble fails, it is not equivalent to the fundamental microcanonical ensemble, the specific heat can become *negative* and Clausius formulation of the Second Law is violated: “heat can only flow from hot to cold”, phase transitions are found unambiguously and sharply in all details in these small systems [8, 9]. This is the reason why this extension of statistics met severe resistance. Only recently after more than 20 years it becomes widely accepted in the nuclear physics community. There are meanwhile many experimental results, c.f. [10], earlier ones listed in [9], that confirm in great detail this new approach to the thermo-dynamics of these non-extensive systems including the “exotic” features mentioned above, see however [21]. Do we really need another 20 years to accept these ideas in the wider community of Statistical Physics? It seems so:

The conference held in Febr.2002 in Les Houches on "Dynamics and Thermodynamics of Systems with Long Range Interactions" addressed explicitely these non-extensive systems. In their contribution [1] to this conference Tsallis, Rapisarda, Latora and Baldovin illuminated the wide range of application of Tsallis q-statistics, again a *canonical* approach [11]. The main object of this formalism is the *dynamics* of many-body systems *out of equilibrium*. E.g. the change of the distance $\xi(t)$ of two initially neighboring points (the sensitivity to the initial conditions) under the logistic map $x_{t+1} = 1 - ax_t^2$ follows a q-exponential of t. q controls how strong the mixing of the dynamics is, which is a condition for equilibration.

The q-*entropy* addresses the distribution in phase-space: E.g. a narrow set of points develops under the logistic map with parameter $a > a_c = 1.4101\cdots$, with $S_{q=1}(t)$ rising linearly in time, whereas with $a = a_c$, i.e. at the edge of chaos $S_{q=0.2445\cdots}(t)$ is linear in time.

Now to Tsallis' “Sancta Sanctorum” of statistical mechanics[12], the statistical equilibrium of *Hamiltonian* systems. For a Hamiltonian system, the uniform population of the microcanonical manifold $\mathcal{E}$ is the definition of the *equilibrium* distribution. Its geometrical size $e^{S_B} = tr[\delta(E-H)]$ defines the equilibrium entropy, Boltzmann's entropy $S_B(E)$. Even the HMF-model discussed by Tsallis approaches it for a finite number of particles in the limit $t \to \infty$ [1]. There Tsallis' q-entropy has $q = 1$ and is identical to S_B. This finding agrees with my conclusion [13] and also in this book [9] that equilibrium Hamiltonian systems have S_B. Here it is essential to realize that Boltzmann's entropy refers to the *microcanonical* uniform population of the energy-manifold $\mathcal{E}$ and *not* to the canonical “Boltzmann-Gibbs” (BG) distribution as claimed by [1]. The difference is important at phase-separations. Here the canonical ensemble is not equivalent to the micro-ensemble not only for non-extensive systems (what is trivially the case in general) but also in the thermodynamic limit of ordinary extensive systems [8, 9]. Boltzmann's entropy $S_B(E)$ is well defined, multiply differentiable even at phase transitions, independently of whether it is extensive or not, i.e. $S_B(A+B)$ equals $S_B(A)+S_B(B)$ or not. I.e. the eventual non-extensivity of Hamiltonian systems does not demand any exotic entropy at equilibrium.

Before introducing Tsallis' non-extensive, canonical q-entropy one should better exploit the original *microcanonical* Boltzmann's statistics. Precisely, this is done by my geometric approach to statistical mechanics. Its success to predict the most sophisticated, and from the view of conventional canonical statistics exotic and surprising phenomena of phase transitions in small systems like hot nuclei was mentioned above. There is yet no alternative theory.

In this context a further remark: Tsallis et al. [1] quote Einstein's objection against the use of $S_B(E)$ in a lengthy discussion about the additivity (“extensivity”) of S for independent, non-interacting systems. Einsteins remark has nothing to do with the additivity of $S_B(E)$ for independent systems. It concerns the definition of equilibrium values of some macroscopic observables as time-averages $\overline{A}$ compared to Boltzmann's second definition as ensemble averages $<A>$. The advantage of the ensemble-probabilistic definition of $S_B(E)$ and of $<A>$ for non-extensive or small systems compared to time-averages $\overline{A}$ as favored by Einstein was in detail discussed already in [14] see also [15, 16].

Up to now the most realistic application of Boltzmann (not "BG"!)statistics to produce the microcanonical phase diagram of self-gravitating systems under various angular-momenta is given in [17]. Without any doubt this system is the paradigm of non-extensive Hamiltonian systems. Of course the singularity of the gravitation at high density must be shielded like in the Lynden-Bell statistics [18] which we use in [17]. At these densities the relevant physics is ruled by nuclear processes, like hydrogen burning, and has nothing to do with gravitation, has a completely different time scale and has also nothing to do with q-statistics [11]. In the whole Tsallis program there is by far nothing similarly realistic for non-extensive equilibrium systems. There is no alternative to the microcanonical Boltzmann statistics and to our geometrical foundation of equilibrium statistics applied to self-gravitating and rotating systems [17].

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[1] C. Tsallis, A. Rapisarda, V. Latora, and F. Baldovin. Nonextensivity: from low-dimensional maps to Hamiltonian systems. In T. Dauxois, S. Ruffo, E. Arimondo, and M. Wilkens Eds., editors, *Lecture Notes in Physics*, number 602, pages 148–171, Heidelberg, 2002. Springer.

[2] D.H.E. Gross and Meng Ta-chung. Production mechanism of large fragments in high energy nuclear reactions. In *4th Nordic Meeting on Intermediate and High Energy Physics*, page 29, Geilo Sportell, Norway, January 1981.

[3] D.H.E. Gross. Statistical decay of very hot nuclei, the production of large clusters. *Rep.Progr.Phys.*, 53:605–658, 1990.

[4] D.H.E. Gross, M.E. Madjet, and O. Schapiro. Fragmentation phase transition in atomic clusters I — microcanonical thermodynamics. *Z.Phys.D*, 39:75–83, 1997;http://xxx.lanl.gov/abs/cond-mat/9608103.

[5] M.E. Madjet, D.H.E. Gross, P.A. Hervieux, and O. Schapiro. Fragmentation phase transition in atomic clusters II — symmetry of Coulombic fission. *Z.Physik D*, 39:309–316, 1997;http://xxx.lanl.gov/abs/cond-mat/9610118.

[6] O. Schapiro, P.J. Kuntz, K. Möhring, P.A. Hervieux, D.H.E. Gross, and M.E. Madjet. Fragmentation phase transition in atomic clusters III — Coulomb explosion of metal clusters. *Z.Physik D*, 41:219–227, 1997;http://xxx.lanl.gov/abs/cond-mat/9702183.

[7] D.H.E. Gross and M.E. Madjet. Fragmentation phase transition in atomic clusters IV — the relation of the fragmentation phase transition to the bulk liquid-gas transition. *Z.Physik B*, 104:541–551, 1997; and http://xxx.lanl.gov/abs/cond-mat/9707100.

[8] D.H.E. Gross. *Microcanonical thermodynamics: Phase transitions in "Small" systems*, volume 66 of *Lecture Notes in Physics*. World Scientific, Singapore, 2001.

[9] D.H.E. Gross. Thermo-statistics or topology of the microcanonical entropy surface. In T.Dauxois, S.Ruffo, E.Arimondo, and M.Wilkens, editors, *Dynamics and Thermodynamics of Systems with Long Range Interactions*, Lecture Notes in Physics, pages 21–45,cond–mat/0206341, Heidelberg, 2002. Springer.

[10] B. Borderie. Dynamics and thermodynamics of the liquid-gas phase transition in hot nuclei studied with the Indra array. *J.Phys.G: Nucl.Part.Phys.*, 28:R212–R227, 2002.

[11] C. Tsallis. Nonextensive statistics: Theoretical, experimental and computational evidences and connections. *Braz.Journ.Physics*, 29:1, 1999.

[12] C. Tsallis. Entropic nonextensivity: a possible measure of complexity. *Chaos,Solitons,and Fractas*, page 13, 2002.

[13] D.H.E. Gross. Non-extensive Hamiltonian systems follow Boltzmann's principle not Tsallis statistics. – phase transitions, second law of thermodynamics. *Physica A*, 305:99–105, cond–mat/0106496, 2002.

[14] D.H.E. Gross. Ensemble probabilistic equilibrium and non-equilibrium thermodynamics without the thermodynamic limit. In Andrei Khrennikov, editor, *Foundations of Probability and Physics*, number XIII in PQ-QP: Quantum Probability, White Noise Analysis, pages 131–146, Boston, October 2001. ACM, World Scientific.

[15] D.H.E. Gross. Second law of thermodynamics, macroscopic observables within Boltzmann's principle but without thermodynamic limit. *submitted to Phys.Rev.E*, page 7, 2000; http://arXiv.org/abs/cond-mat/0101281.

[16] D.H.E. Gross. Geometric foundation of thermo-statistics, phase transitions, second law of thermodynamics, but without thermodynamic limit. *PCCP*, 4:863–872,http://arXiv.org/abs/cond–mat/0201235, (2002).

[17] E.V. Votyakov, H.I. Hidmi, A. De Martino, and D.H.E. Gross. Microcanonical mean-field thermodynamics of self-gravitating and rotating systems. *Phys.Rev.Lett.*, 89:031101–1–4; http://arXiv.org/abs/cond–mat/0202140, (2002).

[18] D. Lynden-Bell. Statistitcal mechanics of violent relaxation in stellar systems. *Mon. Not. R. astr. Soc.*, 136:101–121, 1967.

[19] M. Schmidt, R. Kusche, T. Hippler, J. Donges, W. Kornmüller, B. von Issendorff, and H. Haberland. Negative heat capacity for a cluster of 147 sodium stoms. *Phys.Rev.Lett.*, 86:1191–1194, 2001.

[20] C. Tsallis, B.J.C. Cabral, A. Rapisarda, and V. Latora. Comment on "negative specific heat for a cluster of 147 sodium atoms" by Schmidt et al. pages cond–mat/0112266, 2001.

[21] It is true that Tsallis et al. suggested in one case of an experimentally confirmed negative heat capacity (sodium clusters [19]) an alternative explanation [20]: In their 1-dim HMF-model they found a metastable state with most likely zero microcanonical measure, i.e. with no entropy. (It plays no role in the complete microcanonical ensemble, where is no sign of a backbending [8].) The average kinetic energy in this state shows a back-bending as function of the total energy. Now, the microcanonical temperature is $T = (\partial S_B(E)/\partial E)^{-1}$ and refers evidently to the whole microcanonical ensemble not to a single trajectory with zero measure. In view of this and the very qualitative nature and flatness of this "explanation" which is in contrast to the many other, very detailed and specific verifications of the prediction by the Boltzmann microcanonical ensemble listed above, one can safely ignore this alternative.