Entropy Formula with Reservoir Fluctuations

How to get $q > 1$ Tsallis distribution?

T.S. Biró G.G. Barnaföldi P. Ván K. Ürmössy

Heavy Ion Research Group

MTA Wigner Research Centre for Physics, Budapest

April 27, 2014

Talk given by T. S. Biró at Eotvos University Statistical Physics Seminar, 2014.05.21.

J.Uffink, J.van Lith: Thermodynamic Uncertainty Relations; Found.Phys.29(1999)655

”Bohr and Heisenberg suggested that the thermodynamical fluctuation of temperature and energy are complementary in the same way as position and momenta in quantum mechanics.”

B.H.Lavenda: Comments on "Thermodynamic Uncertainty Relations" by J.Uffink and J.van Lith; Found.Phys.Lett.13(2000)487

”Finally, the question about whether or not the temperature really fluctuates should be addressed. ... If the energy fluctuates so too will any function of the energy, and that includes any estimate of the temperature.”

J.Uffink, J.van Lith: Thermodynamic Uncertainty Relations Again: A Reply to Lavenda; Found.Phys.Lett.14(2001)187

"In this interpretation, the uncertainty $\Delta\beta$ merely reflects one's lack of knowledge about the fixed temperature parameter β. Thus β does not fluctuate."

"Lavenda's book uses these ingredients to derive the uncertainty relation $\Delta\beta \cdot \Delta U \geq 1$. Our paper observes that, on the same basis, one actually obtains a result even stronger than this, namely $\Delta\beta \cdot \Delta U = 1$."

Outline

Outline

Variances of functions of distributed quantities

Let x be distributed with small variance and $\langle x \rangle = a$. Consider a Taylor expandable function

$$f(x) = f(a) + (x-a)f'(a) + \frac{1}{2}(x-a)^2 f''(a) + \dots$$

Up to second order the square of it is given by

$$f^2(x) = f^2 + 2(x-a)ff' + (x-a)^2 \left[f'f' + ff'' \right] + \dots$$

denoting $f(a)$ shortly by f. Expectation values as integrals deliver

$$\langle f \rangle = f + \frac{1}{2}\Delta x^2 f'' \qquad \langle f \rangle^2 = f^2 + \Delta x^2 ff'' \qquad \langle f^2 \rangle = f^2 + \Delta x^2 (f'f' + ff'')$$

Finally we obtain $\boxed{\Delta f = |f'|\, \Delta x}$

One Variable EoS: $S(E)$

Product of variances

$$\Delta E \cdot \Delta\beta = 1 \tag{1}$$

Connection to the (absolute) temperature:

$$|C|\Delta T \cdot \frac{\Delta T}{T^2} = 1 \tag{2}$$

Relative variance scales like 1/SQRT of heat capacity!

$$\frac{\Delta T}{T} = \frac{\Delta\beta}{\beta} = \frac{1}{\sqrt{|C|}} \tag{3}$$

C is proportional to the heat bath size (volume, number of degrees of freedom) in the thermodynamical limit.

Deficiences of the Gauss picture

1. $w(\beta) > 0$ for $\beta < 0$ (finite probability for negative temperature)
2. $\langle e^{-\beta\omega} \rangle$ is not integrable in ω (it cannot be a canonical one-particle spectrum)

Outline

1. Temperature and Energy Fluctuations
2. Finite Heat Bath Effects
   - Ideal Gas
   - Deformed Entropy Formulas
3. LHC spectra vs multiplicity

Ideal Gas: microcanonical statistical weight

The one-particle energy, ω, out of total energy, E, is distributed according to a statistical weight factor which depends on the number of particles in the reservoir, N:

$$P_1(\omega) = \text{phase space factor}(\omega) \cdot \left(1 - \frac{\omega}{E}\right)^N \tag{4}$$

Superstatistics: N itself has a distribution (based on the physical model of the reservoir and on the event by event detection of the spectra).

Ideal Reservoir: bosons or fermions

n particles among k cells: bosons $\binom{n+k}{n}$, fermions $\binom{k}{n}$ ways.

(Negative) binomial distribution: a subspace (n,k) out of (N,K) in the limit $K \to \infty$ and $N \to \infty$ while $f = N/K$ is fixed.

$$B_{n,k}(f) := \lim_{K\to\infty} \frac{\binom{n+k}{n}\binom{N-n+K-k}{N-n}}{\binom{N+K+1}{N}} = \binom{n+k}{n} f^n (1+f)^{-n-k-1}. \tag{5}$$

$$F_{n,k}(f) := \lim_{K\to\infty} \frac{\binom{k}{n}\binom{K-k}{N-n}}{\binom{K}{N}} = \binom{k}{n} f^n (1-f)^{k-n}. \tag{6}$$

Norm and Pascal triangle

Binomial expansion:

$$(a+b)^k = \sum_{n=0}^{\infty} \binom{k}{n} a^n b^{k-n} \tag{7}$$

Replace k by $-k-1$ and a by $-a$, noting that

$$\binom{-k-1}{n} = \frac{(-k-1)(-k-2)\dots(-k-n)}{n!} = (-1)^n \frac{(k+1)(k+2)\dots(k+n)}{n!} = (-1)^n \binom{n+k}{n}.$$

we arrive at

$$(b-a)^{-k-1} = \sum_{n=0}^{\infty} \binom{n+k}{n} a^n b^{-n-k-1} \tag{8}$$

Bosonic reservoir

Reservoir in hep: E is fixed, N fluctuates according to NBD.

$$\sum_{N=0}^{\infty}\left(1-\frac{\omega}{E}\right)^{N} B_{N,K}(f)=\left(1+f\frac{\omega}{E}\right)^{-K-1} \tag{9}$$

Note that $\langle N\rangle = (K+1)f$ for NBD. Then with $T = E/\langle N\rangle$ and $q-1=\frac{1}{K+1}$ we get

$$\left(1+(q-1)\frac{\omega}{T}\right)^{-\frac{1}{q-1}}$$

This is **exactly** a $q>1$ Tsallis-Pareto distribution.

Fermionic reservoir

E is fixed, N is distributed according to BD:

$$\sum_{N=0}^{\infty} \left(1 - \frac{\omega}{E}\right)^N F_{N,K}(f) = \left(1 - f\frac{\omega}{E}\right)^K \tag{10}$$

Note that $\langle N \rangle = Kf$ for BD. Then with $T = E/\langle N \rangle$ and $q - 1 = -\frac{1}{K}$ we get

$$\left(1 + (q-1)\frac{\omega}{T}\right)^{-\frac{1}{q-1}}$$

This is **exactly** a $q < 1$ Tsallis-Pareto distribution.

Boltzmann limit

In the $K \gg N$ limit (low occupancy in phase space)

$$\binom{N+K}{N} f^N (1+f)^{-N-K-1} \longrightarrow \frac{K^N}{N!}\left(\frac{f}{1+f}\right)^N \dots$$
$$\binom{K}{N} f^N (1-f)^{K-N} \longrightarrow \frac{K^N}{N!}\left(\frac{f}{1-f}\right)^N \dots \quad (11)$$

After normalization this is the **Poisson** distribution:

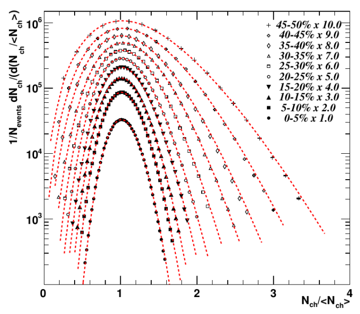
$$\Pi_n(x) = \frac{\langle N \rangle^N}{N!} e^{-\langle N \rangle} \quad \text{with} \quad \langle N \rangle = K \frac{f}{1 \pm f} \quad (12)$$

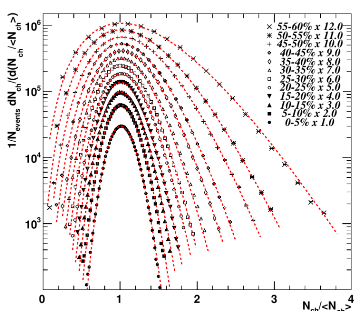
The result is **exactly** the Boltzmann-Gibbs weight factor:

$$\sum_{N=0}^{\infty} \left(1 - \frac{\omega}{E}\right)^N \Pi_N(\langle N \rangle) = e^{-\omega/T}. \quad (13)$$

Experimental NBD distributions PHENIX PRC 78 (2008) 044902

Au + Au collisons at $\sqrt{s_{NN}} = 62$ (left) and 200 GeV (right). Total charged multiplicities.





$$K \approx 10 \to 20.$$

Summary of ideal reservoir fluctuations

In all the three above cases

$$T = \frac{E}{\langle N \rangle}, \quad \text{and} \quad q = \frac{\langle N(N-1) \rangle}{\langle N \rangle^2} \tag{14}$$

Ideal gas with general reservoir fluctuations

Canonical approach: expansion for small $\omega \ll E$.
Tsallis-Pareto distribution as an approximation:

$$\left(1+(q-1)\frac{\omega}{T}\right)^{-\frac{1}{q-1}} = 1 - \frac{\omega}{T} + q\frac{\omega^2}{2T^2} - \dots \tag{15}$$

Ideal reservoir phase space up to the subleading canonical limit:

$$\left\langle \left(1-\frac{\omega}{E}\right)^N \right\rangle = 1 - \langle N \rangle \frac{\omega}{E} + \langle N(N-1) \rangle \frac{\omega^2}{2E^2} - \dots \tag{16}$$

To subleading in $\omega \ll E$

$$\mathbf{T} = \frac{\mathbf{E}}{\langle \mathbf{N} \rangle}, \qquad \mathbf{q} = \frac{\langle \mathbf{N}(\mathbf{N}-1) \rangle}{\langle \mathbf{N} \rangle^2} = 1 - \frac{1}{\langle N \rangle} + \frac{\Delta N^2}{\langle N \rangle^2}. \tag{17}$$

General system with general reservoir fluctuations

Canonical approach: expansion for small $\omega \ll E$.

$$\langle e^{S(E-\omega)-S(E)} \rangle_{\omega \ll E} = \langle e^{-\omega S'(E)+\omega^2 S''(E)/2-\ldots} \rangle \tag{18}$$

$$= 1 - \omega \langle S'(E) \rangle + \frac{\omega^2}{2} \langle S'(E)^2 + S''(E) \rangle - \ldots \tag{19}$$

Compare with expansion of Tsallis

$$\left(1 + (q-1)\frac{\omega}{T}\right)^{-\frac{1}{q-1}} = 1 - \frac{\omega}{T} + q\frac{\omega^2}{2T^2} - \ldots \tag{20}$$

Interpret the parameters

$$\frac{1}{T} = \langle S'(E) \rangle, \qquad q = 1 - \frac{1}{C} + \frac{\Delta T^2}{T^2} \tag{21}$$

with $\langle S''(E) \rangle = -1/CT^2$ expressed via the heat capacity of the reservoir, $1/C = dT/dE$.

Understanding the parameter q

in terms fluctuations

Opposite sign contributions from $\langle S'^2 \rangle - \langle S' \rangle^2$ and from $\langle S'' \rangle$.

In all cases approximately

$$q = 1 - \frac{1}{C} + \frac{\Delta T^2}{T^2}.$$

- $q > 1$ and $q < 1$ are both possible
- for Gaussian temperature fluctuations $q = 1$
- for any relative variance $\Delta T / T = 1/\sqrt{C}$ it is exactly $q = 1$
- for ideal gas and C distributed as NBD or BD, the Tsallis form is exact

Deformed entropy $K(S)$

Use $K(S)$ instead of S to gain more flexibility for handling the subleading term in ω!

$$\langle e^{K(S(E-\omega))-K(S(E))}\rangle = 1-\omega\frac{d}{dE}K(S(E)) + \frac{\omega^2}{2}\left(\frac{d^2}{dE^2}K(S(E))+\left(\frac{d}{dE}K(S(E))\right)^2\right) \quad (22)$$

Note that

$$\frac{d}{dE}K(S(E)) = K'S', \qquad \frac{d^2}{dE^2}K(S(E)) = K''S'^2 + K'S'' \quad (23)$$

Compare this with the Tsallis power-law!

Tsallis parameters for deformed entropy

Using previous average notations and assuming that $K(S)$ is independent of the reservoir fluctuations (*universality*):

$$\begin{aligned} \frac{1}{T_K} &= K' \frac{1}{T}, \\ \frac{q_K}{T_K^2} &= \left(K'' + K'^2\right) \frac{1}{T^2} \left(1 + \frac{\Delta T^2}{T^2}\right) - K' \frac{1}{CT^2}. \end{aligned} \tag{24}$$

By choosing a particular $K(S)$ we can manipulate q_k.

Best handling of subleading terms: UTI principle

Applying our previous general result we obtain

$$q_K = 1 + \frac{\Delta T^2}{T^2} + \frac{(Cq+1)K'' - K'}{C\,K'^2} \qquad (25)$$

Not considering reservoir fluctuations $\Delta T/T = 0$ and $q = 1 - 1/C$.

One arrives at the original Universal Thermostat Independence (UTI) equation by demanding $q_K = 1$:

$$\frac{K''}{K'} = \frac{1}{C}. \qquad (26)$$

Deformed entropy formula

T.S.Biró, P.Ván, G.G.Barnaföldi, EPJA 49: 110, 2013

For ideal gas C is constant, without reservoir fluctuations $C = 1/(1-q)$.

The solution of eq.(26) delivers

$$K(S) = C\left(e^{S/C} - 1\right) \tag{27}$$

and one arrives upon using $K(S) = \sum_i p_i K(-\ln p_i)$ at the statistical entropy formulas of Tsallis and Rényi:

$$K(S) = \frac{1}{1-q}\sum_i \left(p_i^q - p_i\right), \qquad S = \frac{1}{1-q}\ln\sum_i p_i^q \tag{28}$$

Deformed formula with reservoir fluctuations

Demanding $q_K = 1$ one obtains the diff.eq.

$$\frac{\Delta T^2}{T^2} K'^2 - \frac{1}{C} K' + \left(1 + \frac{\Delta T^2}{T^2} \right) K'' = 0. \tag{29}$$

First integral (with constant λ and C_Δ)

$$K'(S) = \frac{1}{(1-\lambda)e^{-S/C_\Delta} + \lambda} \tag{30}$$

with $\lambda = C\Delta T^2/T^2$ and $C_\Delta = C + \lambda$.

Second integral

$$K(S) = \frac{C_\Delta}{\lambda} \ln\left(1 - \lambda + \lambda e^{S/C_\Delta} \right). \tag{31}$$

Generalized Tsallis formula

$$K(S) = \frac{C_\Delta}{\lambda} \sum_i p_i \ln\left(1 - \lambda + \lambda p_i^{-1/C_\Delta}\right). \tag{32}$$

For $\lambda = 1$ (Gaussian fluctuations) it is exactly the Boltzmann entropy!

For $\lambda = 0$ (no fluctuations in reservoir) it is exactly Tsallis entropy with $q = 1 - 1/C$.

For $\lambda \to \infty$ (very wide fluctuations) it is

$$K(S) = \sum_i p_i \ln\left(1 - \ln p_i\right). \tag{33}$$

The canonical p_i distribution is LambertW, it shows tails like the Gompertz distribution

Canonical distribution for $\lambda \to \infty$

$$\frac{\partial K(S)}{\partial p_i} = \ln\left(1 - \ln p_i\right) + p_i \frac{(-1/p_i)}{1 - \ln p_i} \tag{34}$$

Denote $x = -\ln p_i > 0$; then we have

$$\frac{\partial K}{\partial p_i} = \ln(1+x) - \frac{1}{1+x} = \alpha + \beta\omega_i. \tag{35}$$

It is worth to plot and study

$$F(x) = \ln(1+x) + 1 - \tfrac{1}{1+x} = 1 + \alpha + \beta\omega_i.$$

High probability (small $x = -\ln p_i$)

From

$$F(x) = 2x - \frac{3}{2}x^2 + \dots \tag{36}$$

it follows

$$p_i \approx e^{-\frac{1}{2}(1+\alpha+\beta\omega_i)} \tag{37}$$

This is a **Botzmann-Gibbs** statistical factor, just the Lagrange multiplier $\beta = 2/T$ looks different.

Low probability (large $x = -\ln p_i$)

From

$$F(x) = \ln x + \frac{1}{2x^2} + \dots \tag{38}$$

it follows that

$$p_i = e^{-e^{\alpha+\beta\omega_i}} \tag{39}$$

The **1-CDF of the Gompertz distribution** arises as

$$\frac{p(\omega_i)}{p(0)} = e^{e^{\alpha}\left(1-e^{\beta\omega_i}\right)} \tag{40}$$

Gompertz distribution: a wiki

About the Gompertz distribution: PDF $f(t)$, CDF $F(x) = \int_0^x f(t)dt = e^{\eta(1-e^{bt})}$, mean, mode, variance , MGF $\langle e^{-sx} \rangle$, etc.

Applications

- Demography: life-expectation shortens at high age
- Oncology: tumor growth rate is exponential
- Geophysics: scaling violation for earthquakes with large magnitudes
- Statistics: extreme value distribution (1-CDF)

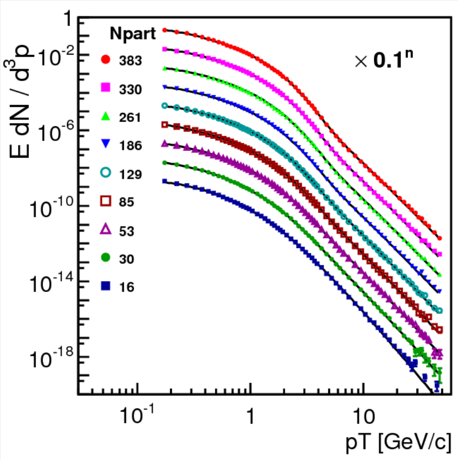
Outline

Statistical vs QCD power-law

- QCD power-law: constant power $(K+1) > 4$ (conformal limit)
- statistical power: $(K+1) = \langle N \rangle / f \propto$ reservoir size
- data fits: ALICE LHC $K+1$ powers vs N_{part}
- soft and hard power-laws differ for large N_{part}

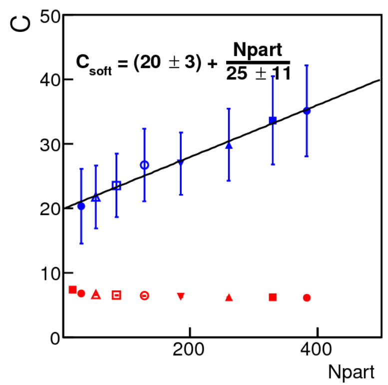
Soft and Hard Tsallis fits:

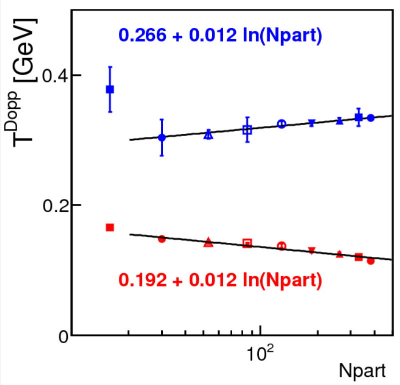
ALICE PLB 720 (2013) 52



change at $p_T = 4$ GeV.

Trends with N_{part}





Summary

- There are $S'(E)$-temperature fluctuations due to finite reservoirs; they cannot be Gaussian.
- Ideal gas reservoirs with NBD or BD number fluctuations lead to exact Tsallis distributions: $q = \frac{1}{k+1}$ and $q = 1 - \frac{1}{k}$.
- Tsallis distribution is the approximate canonical weight with fluctuating reservoirs: $q = 1 - 1/C + \Delta T^2/T^2$.
- New entropy formula; for infinite temperature fluctuations at finite heat capacity it is *parameter – free.*

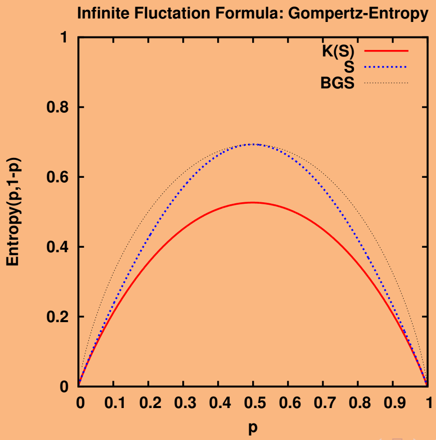
$$K(S) = \sum_i p_i \ln\left(1 - \ln p_i\right) .$$

Outlook

- Need for realistic modelling of the finite heat bath in heph.
- Adiabatically expanding systems have C_S not C_V.
- Non-extensivity must mean a finite $q-1$ even for infinite V or N.
- We have a procedure for general deformed entropy formulas.

BACKUP SLIDES

Binary Entropy in the Gompertz limit



$K(S)$-additive composition rule

With the result (31) for $K(S)$ the composition rule becomes

$$h(S_{12}) = h(S_1) + h(S_2) + \frac{\lambda}{C_\Delta} h(S_1) h(S_2) \tag{41}$$

with

$$h(S) = C_\Delta \left(e^{S/C_\Delta} - 1 \right) . \tag{42}$$

This is a combination of the ideal gas entropy-deformation, $h(S)$ and an original Tsallis composition law with $q - 1 = \lambda / C_\Delta$.

Ideal Photon Gas: Basic Quantities

Thermodynamic quantities from parametric Equation of State

$$E = \sigma T^4 V, \qquad pV = \frac{1}{3}\sigma T^4 V$$

Gibbs equation

$$TS = E + pV = \frac{4}{3}\sigma T^4 V$$

Entropy and Photon Number

$$S = \frac{4}{3}\sigma T^3 V, \qquad N = \chi\sigma T^3 V.$$

Ideal Photon Gas: Differentials

$$dE = 4\sigma T^3 V dT + \sigma T^4 dV$$

$$dp = \frac{4}{3}\sigma T^3\, dT$$

$$dS = 4\sigma T^2 V dT + \frac{4}{3}\sigma T^3 dV$$

$$dN = 3\chi\sigma T^2 V dT + \chi\sigma T^3 dV$$

Ideal Photon Gas: Heat Capacities

BLACK BOX scenario (V=const.)

$$C_V = 4\sigma T^3 V = 3S = 4\chi N, \qquad \left.\frac{\Delta T}{T}\right|_V = \frac{1}{2\sqrt{\chi N}}$$

ADIABATIC EXPANSION scenario (S=const.)

$$C_S = \sigma T^3 V = \frac{1}{4} C_V, \qquad \left.\frac{\Delta T}{T}\right|_S = \frac{1}{\sqrt{\chi N}}$$

IMPOSSIBLE scenario (p=const.)

$$C_p = \infty, \qquad \left.\frac{\Delta T}{T}\right|_p = 0$$

Ideal Photon Gas: Relations between Variances

Always: $\frac{\Delta S}{S} = \frac{\Delta N}{N}$

BLACK BOX (V=const.): $\frac{\Delta V}{V} = 0 \qquad \frac{\Delta N}{N} = 3\,\frac{\Delta T}{T}$

ADIABATIC (S=const.): $\frac{\Delta V}{V} = 3\,\frac{\Delta T}{T} \qquad \frac{\Delta N}{N} = 0$

ENERGETIC (E=const.): $\frac{\Delta V}{V} = 4\,\frac{\Delta T}{T} \qquad \frac{\Delta N}{N} = 7\,\frac{\Delta T}{T}$

Volume or temperature fluctuations or both?
Gorenstein,Begun,Wilk,...

Several Variables: $S(E,V,N,\ldots) = S(X_i)$

Second derivative of S wrsp extensive variables X_i constitutes a metric tensor g^{ij}.

It describes the variance $\Delta Y^i \Delta Y^j$ with Y associated intensive variables.

Its inverse tensor g_{ij} comprises the variance squares and mixed products for the X_i-s.

How to measure all this ?

- Fit Euler-Gamma or cut power-law $\Longrightarrow T, C$
- Check whether $\Delta T/T = 1/\sqrt{C}$

- If two different C-s, imply "sub + res" splitting

- Check E and ΔE by multiparticle measurements
- Vary T by $\sqrt{s}$ and C by N_{part}