Strong correlations between the exponent α and the particle number for a Renyi-monoatomic gas in Gibbs' statistical mechanics

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Abstract

Appealing to the 1902 Gibbs' formalism for classical statistical mechanics (SM), the first SM axiomatic theory ever that successfully explained equilibrium thermodynamics, we will here show that already at the classical level there is a strong correlation between the Renyi's exponent α and the number of particles for very simple systems. No reference to heat baths is needed for such a purpose.

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1 Introduction

In his celebrated book of 2002, ELEMENTARY PRINCIPLES OF STATISTICAL MECHANICS [1], Gibbs put forward an axiomatic theory for statistical mechanics (SM) (the first one indeed of that kind) that was able to microscopically and successfully explain equilibrium thermodynamics. He invented the ensemble notion. All this happened 60 years *before the advent of MaxEnt*. One can certainly work on classical SM without appeal to MaxEnt, and this is what we are going to do here. Why? Because MaxEnt workings with q-generalized entropies have recently received serious questioning [2, 3], and we wish to disentangle our findings from MaxEnt.

Renyi's information measure S_R generalizes both Hartley's and Shannon's ones, quantifying our ignorance regarding a system's structural features. S_R is considered an important quantifier in variegated areas of science, for instance, ecology, quantum information, Heisenberg's XY spin chain model, theoretical computing, conformal field theory, quantum quenching, diffusion processes, etc. [4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15]. Also, the Renyi entropy is important in statistics as indicator of diversity. Here we tackle, using the classical statistical mechanics of Gibbs, the simplest conceivable systems, the ideal gas, and an ensemble of independent harmonic oscillators, showing that a strange phenomenology emerges even in these trivial scenarios. In particular a strong correlation between Renyi's exponent α and the particle number emerges, without appeal to the heat bath notion.

1.1 Gibbs postulates

They were advanced in 1902 and constituted the first ever axiomatics for classical statistical mechanics (SM) [1, 16]. Gibbs refers to a phase space location as the "phase" z of the system [16]. He also introduced the notion of ensemble. The following statements completely explain in microscopic fashion the corpus of classical equilibrium thermodynamics [16].

1) The probability that at time t the system will be found in the dynamical state characterized by z equals the probability $P(z)$ that a system randomly selected from the ensemble shall possess the phase z. 2) All phase-space neighborhoods (cells) have the same a priori probability. 3) The ensemble's probability $P(q_1, \dots, q_n, p_1, \dots, p_n, t)$ (self-explanatory notation) depends only upon the system's Hamiltonian $H(q_1, \dots, q_n, p_1, \dots, p_n, t)$ in an exponential (negative) fashion. 4) The time-average of a dynamical quantity F equals its average over the ensemble, evaluated using P.

The prevalent contemporary SM-axiomatics, suitable for quantum mechanics, is that of Jaynes [17], usually called MaxEnt, *which is not employed here.*

Now, it is well known that, for entropies like Renyi's, the second Gibbs' postulate has to be amended by replacing the exponential function by the so called q-exponential one e_q (for e_q's properties, see [18])

$$e_\alpha(-x) = [1-(1-\alpha)x]^{1/(1-\alpha)}, \;\; e_\alpha(-x) \to e^{-x} \;\; \text{for} \;\; \alpha \to 1, \tag{1.1}$$

and then, in the canonical ensemble,

$$P(H) \sim e_\alpha(-\beta H), \;\; \beta = 1/T, \tag{1.2}$$

with T the temperature.

1.2 Renyi's measure

Renyi's S_R is defined as [4]:

$$S_R = \frac{1}{1-\alpha} \ln \left(\int\limits_M P^\alpha d\mu \right), \tag{1.3}$$

and the accompanying (canonical ensemble) Gibbs' probability distribution P is given by 1.2. The general form of the partition function was derived by Gibbs in 1902 [see [1], Eq. (92)]. If Z stands for Renyi's partition function, one has

$$Z = \int\limits_M [1+(1-\alpha)\beta H]^{\frac{1}{\alpha-1}} \, d\mu, \tag{1.4}$$

$$P = \frac{1}{Z} [1+(1-\alpha)\beta H]^{\frac{1}{\alpha-1}} \, . \tag{1.5}$$

Herefrom we denote the classical energy by U and its mean value by $< U >$, and insist upon the fact that MaxEnt is NOT appealed to.

1.3 Renyi's and Tsallis' measures

It is well known [18] that S_R is intimately linked to Tsallis' entropy S_α [18, 19, 20]. In fact, one easily ascertains that, given

$$\mathcal{T}(\alpha) = \int P^\alpha d\mu, \tag{1.6}$$

$$S_\alpha = \frac{1}{1-\alpha}[\mathcal{T}(\alpha) - 1]d\mu, \tag{1.7}$$

then

$$S_R(\alpha) = \frac{1}{1-\alpha}\ln\left[(1-\alpha)S_\alpha + 1\right]. \tag{1.8}$$

Note that the Tsallis' canonical probabilities are also q-exponentials 1.5 [18, 19]. Accordingly, Tsallis results, within Gibbs' tenets, will necessarily coincide with those of Renyi's. Anything to be found below for the later will automatically be also valid in the Tsallis scenario as well.

2 Renyi's partition function for the monoatomic ideal gas

Using appropriate units, the partition function of $\nu-$dimensional monoatomic gas of n particles is ($[0 < \alpha \leq 1]$), after an adequate Gibbs' treatment is

$$Z = V^n \int\limits_{-\infty}^{\infty} \left[1 + \frac{\beta(1-\alpha)}{2m}(p_1^2 + p_2^2 + \cdots p_n^2)\right]^{\frac{1}{\alpha-1}} d^\nu p_1 d^\nu p_2 \cdots d^\nu p_n, \tag{2.1}$$

with V the volume. Using spherical coordinates in a space of νn dimensions, the above integral becomes

$$Z = \frac{2\pi^{\frac{\nu n}{2}} V^n}{\Gamma\left(\frac{\nu n}{2}\right)} \int\limits_0^\infty \left[1 + \frac{\beta(1-\alpha)}{2m}p^2\right]^{\frac{1}{\alpha-1}} p^{\nu n-1} dp. \tag{2.2}$$

We have integrated over the angles and taken $p^2 = p_1^2 + p_2^2 + \cdots p_n^2$. Changing variables in the fashion $x = p^2$, the last integral is

$$Z = \frac{\pi^{\frac{\nu n}{2}} V^n}{\Gamma\left(\frac{\nu n}{2}\right)} \int\limits_0^\infty \left[1 + \frac{\beta(1-\alpha)}{2m}x\right]^{\frac{1}{\alpha-1}} x^{\frac{\nu n-2}{2}} dx, \tag{2.3}$$

so that, appealing to ref.[21], we are led to

$$Z = V^n \left[\frac{2\pi m}{\beta(1-\alpha)}\right]^{\frac{\nu n}{2}} \frac{\Gamma\left(\frac{1}{1-\alpha} - \frac{\nu n}{2}\right)}{\Gamma\left(\frac{1}{1-\alpha}\right)}. \tag{2.4}$$

Note that the Γ's argument in the numerator can not vanish. Thus, $\frac{1}{1-\alpha}-\frac{\nu n}{2} > 0$ (strictly).

In similar fashion one evaluates the mean energy. One has

$$Z < U >= V^n \int_{-\infty}^{\infty} \left[1 + \frac{\beta(1-\alpha)}{2m}(p_1^2 + p_2^2 + \cdots p_n^2)\right]^{\frac{1}{\alpha-1}}$$

$$\frac{p_1^2 + p_2^2 + \cdots p_n^2}{2m} d^\nu p_1 d^\nu p_2 \cdots d^\nu p_n. \tag{2.5}$$

Integrating over the angles we find

$$Z < U >= \frac{\pi^{\frac{\nu n}{2}} V^n}{m\Gamma\left(\frac{\nu n}{2}\right)} \int_0^{\infty} \left[1 + \frac{\beta(1-\alpha)}{2m} p^2\right]^{\frac{1}{\alpha-1}} p^{\nu n+1} dp. \tag{2.6}$$

Now, using $x = p^2$ once more we are led to

$$Z < U >= \frac{\pi^{\frac{\nu n}{2}} V^n}{2m\Gamma\left(\frac{\nu n}{2}\right)} \int_0^{\infty} \left[1 + \frac{\beta(1-\alpha)}{2m} x\right]^{\frac{1}{\alpha-1}} x^{\frac{\nu n}{2}} dx. \tag{2.7}$$

At this point, we use again ref.[21] and get

$$< U >= \frac{V^n}{Z} \frac{\nu n}{2\beta(1-\alpha)} \left[\frac{2\pi m}{\beta(1-\alpha)}\right]^{\frac{\nu n}{2}} \frac{\Gamma\left(\frac{1}{1-\alpha} - \frac{\nu n}{2} - 1\right)}{\Gamma\left(\frac{1}{1-\alpha}\right)}. \tag{2.8}$$

One replaces now in this last result the value encountered above for Z and obtain

$$< U >= \frac{\nu n}{\beta[2\alpha - \nu n(1-\alpha)]}. \tag{2.9}$$

Finally, the derivative with respect to T yields for the specific heat at constant volume

$$C_V = \frac{\nu n k}{2\alpha - \nu n(1-\alpha)}. \tag{2.10}$$

3 Limits to the particle-number for Renyi's monoatomic gas

The original content of the present communication emerges from an analysis of the Gamma functions involved in evaluating Z and $< U >$. Remember that $[0 < \alpha \leq 1]$. According to (2.4), the integral (2.1) converges and becomes both positive and finite for

$$\frac{1}{1-\alpha} - \frac{\nu n}{2} > 0. \tag{3.1}$$

Analogously, according to (2.8), we need

$$\frac{1}{1-\alpha} - \frac{\nu n}{2} - 1 > 0. \tag{3.2}$$

These two conditions immediately set severe limitations on the particle-number n that read

$$1 \leq n < \frac{2\alpha}{\nu(1-\alpha)}. \tag{3.3}$$

There is a maximum permissible number of particles. For instance, if $\alpha = 1 - 10^{-2}, \nu = 3$, we have

$$1 \leq n < 66. \tag{3.4}$$

No more than 65 particles are allowed. Keeping the dimensionality 3, for $\alpha = 1/2$ only ONE particle is allowed! Even worse, for $\alpha = 1/4$, NO particles exist. Roughly, to have a number of particles of the order of 10^n, one needs α of the order of $1 - 10^{-n}$. Note that (3.3) implies $\alpha > \frac{\nu n}{2+\nu n}$. See Fig 1.

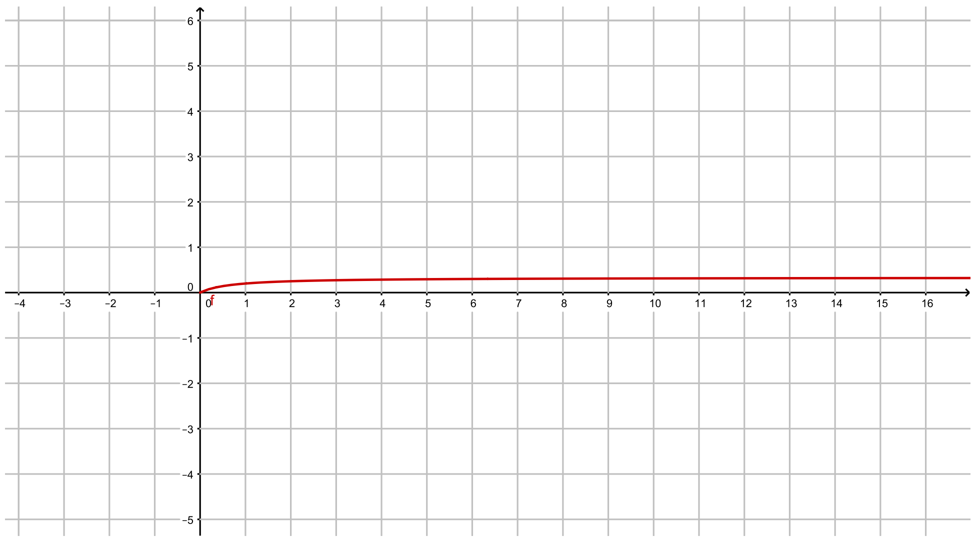

Figure 1: In the 3-dimensional case, we plot $\frac{n}{2+3n}$ vs n. The permitted values for α must lie above the represented curve.

4 Renyi's partition function for n independent harmonic oscillators

Using appropriate units, the partition function for n n−set of independent ν−dimensional Harmonic Oscillators is given by

$$Z = \int_{-\infty}^{\infty} \left[1 + \beta(1-\alpha)(p_1^2 + p_2^2 + \cdots p_n^2 + q_1^2 + q_2^2 + \cdots q_n^2)\right]^{\frac{1}{\alpha-1}}$$

$$d^\nu p_1 d^\nu p_2 \cdots d^\nu p_n d^\nu q_1 d^\nu q_2 \cdots d^\nu q_n. \tag{4.1}$$

We appeal again to spherical coordinates and integrate over the angles. One has

$$Z = \frac{2\pi^{\nu n}}{\Gamma(\nu n)} \int_0^{\infty} \left[1 + \beta(1-\alpha)p^2\right]^{\frac{1}{\alpha-1}} p^{2\nu n - 1} dp, \tag{4.2}$$

where $p^2 = p_1^2 + p_2^2 + \cdots p_n^2 + q_1^2 + q_2^2 + \cdots q_n^2$. We repeat the variables' change $x = p^2$ and are led to

$$Z=\frac{\pi^{\nu n}}{\Gamma(\nu n)}\int\limits_0^\infty [1+\beta(1-\alpha)x]^{\frac{1}{\alpha-1}}\, x^{\nu n-1}dx. \tag{4.3}$$

From ref.[21] we gather that

$$Z=\left[\frac{\pi}{\beta(1-\alpha)}\right]^{\nu n}\frac{\Gamma\left(\frac{1}{1-\alpha}-\nu n\right)}{\Gamma\left(\frac{1}{1-\alpha}\right)}, \tag{4.4}$$

and

$$Z<U>=\int\limits_{-\infty}^{\infty}\left[1+\beta(1-\alpha)(p_1^2+p_2^2+\cdots p_n^2+q_1^2+q_2^2+\cdots q_n^2)\right]^{\frac{1}{\alpha-1}}$$

$$(p_1^2+p_2^2+\cdots q_n^2)d^\nu p_1 d^\nu p_2\cdots d^\nu p_n d^\nu q_1 d^\nu q_2\cdots d^\nu q_n. \tag{4.5}$$

With spherical coordinates this becomes

$$Z<U>=\frac{2\pi^{\nu n}}{\Gamma(\nu n)}\int\limits_0^\infty \left[1+\beta(1-\alpha)p^2\right]^{\frac{1}{\alpha-1}}p^{2\nu n+1}dp, \tag{4.6}$$

and after setting $x=p^2$,

$$Z<U>=\frac{\pi^{\nu n}}{\Gamma(\nu n)}\int\limits_0^\infty [1+\beta(1-\alpha)x]^{\frac{1}{\alpha-1}}\, x^{\nu n}dx. \tag{4.7}$$

Recourse again to ref.[21] yields

$$<U>=\frac{1}{Z}\frac{\nu n}{\beta(1-\alpha)}\left[\frac{\pi}{\beta(1-\alpha)}\right]^{\nu n}\frac{\Gamma\left(\frac{1}{1-\alpha}-\nu n-1\right)}{\Gamma\left(\frac{1}{1-\alpha}\right)}. \tag{4.8}$$

Replacing Z above we reach, finally,

$$<U>=\frac{\nu n}{\beta[\alpha-\nu n(1-\alpha)]}, \tag{4.9}$$

and

$$C=\frac{\nu n k}{\alpha-\nu n(1-\alpha)}. \tag{4.10}$$

5 Limits to the number of independent harmonic oscillators

Finiteness of Z entails

$$\frac{1}{1-\alpha} - \nu n > 0, \tag{5.1}$$

and for $< U >$

$$\frac{1}{1-\alpha} - \nu n - 1 > 0. \tag{5.2}$$

Thus, a new maximum for n ensues

$$1 \leq n < \frac{\alpha}{\nu(1-\alpha)}, \tag{5.3}$$

and for $\alpha = 1 - 10^{-2}, \nu = 3$

$$1 \leq n < 33. \tag{5.4}$$

We see also that $1 > \alpha > 2/3$ for having a single-HO system. $1 > \alpha > 5/6$ is the condition for having a system of two oscillators, $1 > \alpha > 8/9$ the condition for having a system of three HO's, etc.

6 Discussion

We have been working within Gibbs' classical scheme for statistical mechanics. No appeal to MaxEnt was made. It was seen that demanding finiteness of the partition function and mean energy severely limits the number n of independent components of a system in a Renyi scenario (and also in a Tsallis nonadditive one). There are bounds for n. The most bizarre situation is encountered for some α-values that do not permit the system's existence because n can nor exceed zero.
These problem imply that there exists a strong correlation between α and the number of particles. This fact has been proposed in Refs. [22],-for instance. Although Renyi always considered α to be an independent parameter, one might argue that our present results do give additional impetus to the $\alpha - n$-correlation proposal, and thus deserve dissemination. Fig. 1 clearly illustrates this $\alpha - n$ correlation. α must lie above the curve drawn there.

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