Tsallis Entropy and the transition to scaling in fragmentation

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Abstract

By using the maximum entropy principle with Tsallis entropy we obtain a fragment size distribution function which undergoes a transition to scaling. This distribution function reduces to those obtained by other authors using Shannon entropy. The treatment is easily generalisable to any process of fractioning with suitable constraints.

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As a result of developments in materials science, combustion technology, geology and many other fields of research, there has been an increase of interest in the problem of fragmentation of objects. Within this general field there is a collection of papers [1, 2, 3, 4] where a transition occurs from a "classical" distribution of fragments (*e.g.* log-normal or Rossin-Ramler- like) to a power law distribution. This transition has not been adequately explained in terms of any general principles, although in [1] the representation of the fragmentation process in terms of percolation on a Bethe lattice leads to a transition to a power law in the distribution of fragment sizes.
Some attempts have been made to derive the fragment size distribution function from the maximum entropy principle [5, 6], subject to some constraints which mainly came from physical considerations about the fragmentation phenomena. The resulting fragment distribution function describes the distribution of sizes of the fragments in a regime in which scaling is not present. As scaling invariably occurs when the energy of the fragmentation process is high, this suggests that the analysis is only applicable to low energies. However, the maximum entropy principle is completely universal and has an almost unlimited range of application. Consequently we would expect to be able to use it to describe the transition to scaling as the energy of the fracture grows.

The expression for the Boltzmann-Gibbs entropy S (*e.g.* Shannon's form) is given by

$$S = -k \sum_{i=1}^{W} p_i ln p_i, \tag{1}$$

where p_i is the probability of finding the system in the microscopic state i, k is Boltzmann's constant, and W is the total number of microstates.

This has been shown to be restricted to the domain of validity of Boltzmann-Gibbs (BG) statistics. These statistics seem to describe nature when the effective microscopic interactions and the microscopic memory are short ranged [7]. The process of violent fractioning, like that of droplet microexplosions in combustion chambers, blasting and shock fragmentation with high energies, etc, leads to the existence of long-range correlations between *all* parts of the object being fragmented.

Fractioning is a paradigm of non extensivity, since the fractioning object can be considered as a collection of parts which, after division, have an entropy larger than that of their union *i.e* if we denote by A_i the parts or fragments in which the object has been divided, its entropy S obeys $S(\bigcup A_i) < \sum_i S(A_i)$, defining a "superextensivity" [7] in this system . This suggests that it may be necessary to use non-extensive statistics, instead of the BG statistics. This kind of theory has already been proposed by Tsallis [8], who postulated a generalized form of entropy, given by

$$S_q = k \frac{1 - \int_0^\infty p^q(x) dx}{q - 1}. \tag{2}$$

The integral runs over all admissible values of the magnitude x and $p(x)dx$ is the probability of the system being in a state between x and $x + dx$. This entropy can also be expressed as

$$S_q = \int p^q(x) ln_q p(x) dx.$$

The generalized logarithm $ln_q(p)$ is defined in [7] as

$$ln_q(p) = \frac{p^{1-q} - 1}{1 - q}, \tag{3}$$

where q is a real number. It is straighforward to see that $S_q \to S$ when $q \to 1$, recovering BG statistics.

In this paper we use the entropy in eq.2 to consider the problem of atomization of liquid fuels.

The atomized drops in a low pressure regime follow a Nukiyama-Tanasawa-like distribution of sizes, a particular case of the Rossin-Ramler distribution [9]. As we already pointed out in [3], this distribution tends to a power-law, revealing scaling as the atomization pressure grows. Incidentally, this is essentially the same behavior as that reported in experiments on falling glass rods [2], mercury drops, [1] and on blasting oil drops [4]. So, let us maximise $\frac{S_q}{k}$ given by eq.2. If we denote the volume of a drop by V and some typical volume characteristic of the distribution by V_m, we can define a dimensionless volume $v = \frac{V}{V_m}$. Then, the constraints to impose are

$$\int_0^\infty p(v) dv = 1, \tag{4}$$

i.e., the normalization condition. The other condition to be imposed is mass conservation. But as the system is finite, this condition will lead to a very sharp decay in the asymptotic behavior of the droplet size distribution function (DSDF) for large sizes of the fragments. Consequently, we will impose a more general condition, like the "q-conservation" of the mass, in the form:

$$\int_0^\infty v p^q(v) dv = 1, \tag{5}$$

which reduces to the "classical" mass conservation when $q = 1$.

Equations 4 and 5 are the constraints to impose in order to derive the DSDF using the method of Lagrange multipliers by means of the construction of the function:

$$L(p_i; \alpha_1; \alpha_2) = S_q - \alpha_1 \int_0^\infty p(v) dv + \alpha_2 \int_0^\infty p^q(v) v dv \tag{6}$$

The Lagrange multipliers α_1 and α_2 are determined from eqs.4 and 5. The extremization of $L(p_i; \alpha_1; \alpha_2)$ leads to:

$$p(v)dv = C(1 + (q-1)\alpha_2 v)^{-\frac{1}{q-1}} dv \tag{7}$$

where the constant C is given by

$$C = \frac{q-1}{q} \alpha_1^{\frac{1}{q-1}}.$$

This is a DSDF expressed as a function of the volume of the droplets. It is convenient to formulate the problem in terms of a DSDF as a function of the dimensionless radius of the droplets $r = v^{1/3}$. Then the probability density is:

$$f_q(r) = 3Cr^2[1 + (q-1)\alpha_2 r^3)]^{-\frac{1}{q-1}}. \tag{8}$$

To obtain the DSDF the range of admissible values of q is $1 < q < 2$. This range of values of q also guarantees the adequate power law behavior of eq.8, since its asymptotic behavior for large r is

$$f_q(r) \sim \frac{1}{r^{\alpha+1}}, \tag{9}$$

where α is the generic power law exponent, $\alpha = 3\frac{2-q}{q-1}$. Also, if $q \to 1$, eq.8 leads to:

$$f(r) = 3r^2 exp(-r^3), \tag{10}$$

which is the a Nukiyama-Tanasawa DSDF, a particular case of the Rossin-Ramler distribution. This distribution has been previously obtained in [5]. Then, the DSDF that we have obtained reproduces the actual behavior of fragments in the process of breaking. It is easy to realise that the above viewpoint is applicable not only to atomization, but to any process of fractioning.

For a given regime of breakage, generally identified as that of the lowest energy of breakage, the fragment distribution function can be deduced through the maximum entropy principle using BG statistics. This low energy regime of breakage is such that the correlations between the different parts of the object are short-ranged. As the energy of breakage increases, long-range correlations become more and more important, which makes it necessary to introduce the Tsallis entropy as a generalization of the Shannon entropy.

Thus, we have confirmed that BG statistics cannot be applied to all fragmentation regimes and Tsallis entropy can be used to describe the transition into scaling. In this respect, the parameter q, which determines the "degree of nonextensivity" of the statistics, can be related to an effective temperature of breakage. As far as we know, this is the first formulation in terms of general

principles that leads to a DSDF which exhibits a transition to scaling.

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