Abstract

The purpose of this short paper dedicated to the 60th anniversary of Prof. Constantin Tsallis is to show how the use of mathematical tools and physical concepts introduced by Burr, Lévy and Tsallis open a new line of analysis of the old problem of non-Debye decay and universality of relaxation. We also show how a finite characteristic time scale can be expressed in terms of a $q$-expectation using the concept of $q$-escort probability. The comparison with the Weron et al. probabilistic theory of relaxation leads to a better understanding of the stochastic properties underlying the Tsallis entropy concept.

Key words: Tsallis entropy, non-Debye relaxation, universality, Lévy distributions.

1 Maximum entropy principle and probability distributions

Most of the probability distributions used in natural, biological, social and economic sciences can be formally derived by maximizing the entropy with adequate constraints (maxS principle)[1].

According to the maxS principle, given some partial information about a random variable $i.e.$ the knowledge of related macroscopic measurable quantities (macroscopic observables), one should choose for it the probability distribution that is consistent with that information but has otherwise a maximum uncertainty. In usual thermodynamics, the temperature is a macroscopic observable and the distribution functions are exponentials.

Quite generally, one maximizes the Shannon-Boltzmann (S-B) entropy:

$$S = - \int_a^b f(x) \ln f(x) dx$$  \hspace{1cm} (1)
subject to the conditions

\[\int_{a}^{b} f(x)dx = 1, \quad \int_{a}^{b} g_i(x)f(x)dx = g_i(x), \quad i = 1, 2, \ldots \quad (2)\]

Both limits \(a\) and \(b\) may be finite or infinite. The functions \(g_i(x)\) whose expectation value have been usually considered \([1]\) as constraints to build probability distributions are of the type

\[x, x^2, x^n, (x - <x>)^2, |x|, |x - <x|, \ln x, (\ln x)^2, \ln(1 \pm x), \exp(-x)\ldots\quad (3)\]

The maximum entropy probability density function (mepdf) depends on the choice of the limits of integration \(a\) and \(b\) and the functions \(g_i(x)\) whose expectation values are prescribed.

One constructs the Lagrangian

\[L = -\int_{a}^{b} f(x) \ln(f(x))dx\]

\[-\lambda_0(\int_{a}^{b} f(x)dx - 1) - \sum_{i} \lambda_i(\int_{a}^{b} g_i(x)f(x)dx - g_i(x))\quad (4)\]

and differentiating with respect to \(f(x)\) the method of Lagrange multipliers leads to :

\[f(x) = C \exp[-\sum_{i} \lambda_i g_i(x)]\quad (5)\]

The factor \(C\) is a normalization constant and the Lagrange parameters \(\lambda_i\) are determined by using the constraints (3). When this cannot be achieved simply, the parameters \(\lambda_i\) are parameters defined by the constraints. Most distributions derived from the constraints given in (3) possess finite second moments and hence belong to the domain of attraction of the normal distributions. Those which belong to the domain of attraction of the Lévy (stable) distribution \(i.e.\) the Cauchy and the Pareto distributions are obtained with a characteristic Lévy tail parameter (not to be confused with the exponent \(\alpha\) used in the constraints) defined by \(Pr(\xi_i \geq xt) = x^{-\alpha_L}Pr(\xi_i \geq t)\), in the range \(1 < \alpha_L \leq 2\), \([1]\) indicating that only a finite expectation value (first moment) can be defined.

The following example is relevant for non-Debye relaxations. If we derive the mepdf \(f(x)\) of the random variable \(X\) defined in the range \((0, \infty)\) and if we maximize the S–B entropy subject to the two constraints

\[< x^\alpha > = \int_{0}^{\infty} x^\alpha f(x)dx \quad < \ln x > = \int_{0}^{\infty} (\ln x)f(x)dx \quad (6)\]
using the Lagrange variational method, it can be shown easily that the following pdf

\[
f(x) = \frac{\alpha x^{\alpha-1}}{\langle x^\alpha \rangle} \exp\left[-\left(\frac{x^\alpha}{\langle x^\alpha \rangle}\right)\right]
\]

maximizes the S-B-entropy \[1\] provided

\[-\lambda_2 \ln x = \ln x^{\alpha-1}\]

In that case, if we chose \(< x^\alpha > = 1\) as the natural scale of the problem the exponent \(\alpha\) is related to \(\ln x\) as

\[< \ln x > = -\gamma/\alpha\]

where \(\gamma = \Gamma'(1) = 0.577215...\) is the Euler constant.

The Weibull distribution function is given by

\[F(x) = \int_0^\infty f(x')dx' = 1 - \exp(-x^\alpha/\langle x^\alpha \rangle)\]

As it is well known the Weibull distribution which is used in many physical problems exhibits a power law behavior \(F(x) = x^\alpha\) for \(x \to 0\). For \(\alpha < 1\), the Williams-Watts formula (stretched exponential) used for decades to fit the non-Debye relaxation function in the time domain\[2\].

2 Maximization with Tsallis entropy

A generalization of the S-B entropy is appropriate when the phenomena (physical, biological, economical...) are described by distributions with a Lévy characteristic parameter \(\alpha_L < 1\). Here we will start from the Tsallis non-extensive entropy

\[S_q = -\int_a^b f_q^q(x) \ln_q f_q(x)dx\]

subject to the conditions

\[\int_a^b f_q(x)dx = 1, \int_a^b g_{q,i}(x)f_q(x)dx = < g_{q,i}(x) >_q, \ i = 1, 2, \ldots\]

\[\tilde{f}_q(x) = \frac{f_q^q(x)}{\int_a^b f_q^q(x)dx}, \ f_q(x) = \frac{\tilde{f}_q^{1/q}(x)}{\int_a^b \tilde{f}_q^{1/q}(x)dx}\]
The function \( \tilde{f}_q(x) \) is the so-called "escort" probability \([3][4]\). Both limits of integration \( a \) and \( b \) may be finite or infinite. To generalize what has been done with the standard S-B. entropy we can consider the constraints (3) using the generalized \( q \)-exponential and \( q \)-logarithm functions (\( q \)-constraints).

\[
\ln_q x \equiv \frac{x^{1-q} - 1}{1-q} \quad \exp_q(x) \equiv [1 + (1 - q)x]^{\frac{1}{1-q}} \quad \text{with} \quad \ln_q(\exp_q(x)) = x
\]

(13)

The \( mepdf \) depends on the choice of \( a \) and \( b \) and the functions whose expectation values are prescribed.

One constructs the Lagrangian

\[
L_q = - \int_0^\infty f_q^q(x) \ln f_q(x) dx - 
\]

\[
-\lambda_0(\int_0^\infty f_q(x) dx - 1) - \sum_i \lambda_{q,i} (\int_0^\infty g_{q,i}(x) \tilde{f}_q(x) dx - < g_{q,i}(x) >) \quad (14)
\]

and differentiating with respect to \( f_q(x) \) one finds

\[
f_q(x) = C_q \exp_q[- \sum_i \lambda_{q,i} g_{q,i}(x)] \quad (15)
\]

\[
\tilde{f}_q(x) = \bar{C}_q f_q(x)^q \quad (16)
\]

The factors \( C_q \) are normalization constants and the Lagrange parameters \( \lambda_{q,i} \) are determined by using the \( q \)-constraints (11). When this cannot be achieved simply, the parameters \( \lambda_i \) are parameters defined by these constraints.

Here we will derive the \( mepdf \) \( f_q(x) \) of the random variable \( X \) generalizing the two constraints (6) leading to the Weibull distribution

\[
< x^\alpha >_q = \bar{g}_1 \quad (17)
\]

\[
< \log_q x >_q = \bar{g}_2
\]

Using the properties of \( \ln_q(x) \) and \( \exp_q(x) \), we obtain easily the generalization of the Weibull distribution as a generalized Pareto law (Burr\( X \hspace{1mm} I I \hspace{1mm} I I II : B_{b,c}(x) = \hspace{1mm} \).
\[ f(x) = \frac{\alpha x^{\alpha-1}}{\langle x^\alpha \rangle_q} \left[ 1 + \left( \frac{q-1}{2-q} \right) \frac{x^\alpha}{\langle x^\alpha \rangle_q} \right]^{-\frac{1}{q-1}} \]  

(18)

\[ F(x) = 1 - \left[ 1 + \left( \frac{q-1}{2-q} \right) \frac{x^\alpha}{\langle x^\alpha \rangle_q} \right]^{-\frac{2}{q-1}} \]  

(19)

provided

\[-\lambda_2 \ln x = (1 + (1 - q)\lambda_1 x^\alpha) \ln \langle x^\alpha \rangle_q \]  

(20)

which tends to (8) for \( q \to 1 \). If the natural scale \( \langle x^\alpha \rangle_q = 1 \), one can obtain for that case the following result:

\[ < \ln \langle x^\alpha \rangle_q > = \frac{(1 - q)\Gamma(1/(q - 1)) + (\frac{q-1}{2-q})^q \Gamma(3 - q)\Gamma(\frac{2-q}{q-1}) + q}{(1 - q)(2 - q)\Gamma(\frac{2-q}{q-1})} \]  

(21)

If \( q \to 1, < \ln \langle x^\alpha \rangle_q > \to -\gamma \) which is the result (9) obtained for the Weibull distribution. For \( \frac{2\alpha+1}{\alpha+1} < q < 2 \) this distribution belongs to the domain of attraction of the one-sided Lévy-stable law since we have

\[ \lim_{t \to \infty} \frac{1 - F_q(xt)}{1 - F_q(t)} = x^{-\alpha_L} \]  

(22)

with the heavy tail index

\[ \alpha_L = \alpha \frac{2 - q}{q - 1} < 1 \]  

(23)

In the limit \( q \to 1 \), we recover the stretched exponential Williams-Watts formula.

### 3 Universality in non-Debye relaxation

This result can be used to represent non-Debye relaxation if we identify the random variable \( X \) with the macroscopic waiting time \( \tilde{\Theta} \) as defined by Weron et al.\[7\][8][9]. We have:

\[ F_{\tilde{\Theta}}(t) = \Pr(\tilde{\Theta} < t) = \int_0^t f(s) ds = 1 - \left[ 1 + \left( \frac{q-1}{2-q} \right) \frac{t^\alpha}{\langle t^\alpha \rangle_q} \right]^{-\frac{2}{q-1}} \]  

(24)

The relaxation function \( \phi(t) \) can be written as the survival probability of the non equilibrium initial state of the relaxing system. Its value is determined by
the probability that the system as a whole will not make transition out of its original state until time $t$

$$
\phi_{\alpha,q}(t) = \Pr(\tilde{\theta} \geq t) = [1 + (\frac{q-1}{2-q})\frac{t^\alpha}{\langle \theta^\alpha \rangle_q}]^{-\frac{2-q}{q-1}} \tag{25}
$$

This expression has the form of one of the universal relaxation functions proposed in [7][8] as result of an elaborate study of the stochastic mechanisms underlying relaxation dynamics in non Debye complex systems.

$$
\phi_W(t) = [1 + k (At)^\alpha]^{-1/k} \tag{26}
$$

with $0 < \alpha < 1$ and $k \geq \alpha$.

The equivalence of the two formulas allows us to relate the parameter $k$ with the non-extensive parameter $q$:

$$
k = \frac{q-1}{2-q} \tag{27}
$$

This relation was already derived in [10]. In the limit $q \to 1$, we recover the stretched exponential Williams-Watts formula used to fit the time-domain relaxation data [11] [2].

The $q$-dependent scale parameter $A$ which is related to the the peak frequency $\omega_p$ of the response function in the frequency domain is materials and $q$-dependent and is now simply related to the escort probability average

$$
A_q = \langle \tilde{\theta}^\alpha \rangle_q^{-1/\alpha} \tag{28}
$$

and becomes the natural finite time scale in a physical system (for example the dipolar relaxation) which "choose" [7] the regime where the usual average of the waiting time is infinite i.e. $\alpha/k \leq 1$.

We can write the response function

$$
f(t) = -\frac{d\phi}{dt} = \alpha t^{-1}(tA)^\alpha[1 + k(At)^\alpha]^{-\frac{1}{1-k}} \tag{29}
$$

which gives the two power-law asymptotic behavior

$$
f_{\alpha}(t, k_W) = \begin{cases}
\alpha A(At)^{\alpha-1} \text{ for } At << 1 \\
\alpha A k^{-1-1/k}(At)^{-\alpha/k-1} \text{ for } At >> 1
\end{cases} \tag{30}
$$
and in the frequency range, where

\[ \chi(\omega) = \int_0^\infty \exp[-i\omega t] f(t) dt = \chi'(\omega) + i\chi''(\omega) \] (31)

obeys the Jonscher universal laws \[12][13]\]

\[ \lim_{\omega \to \infty} \frac{\chi''(\omega)}{\chi'(\omega)} = \cot(n\pi/2) \quad \lim_{\omega \to 0} \frac{\chi''(\omega)}{\chi'(0) - \chi'(\omega)} = \tan(m\pi/2) \] (32)

with \( n = 1 - \alpha, \ m = \alpha/k \) and \( k = \frac{q-1}{2-q} \).

The \( h \)-moment of the BurrXII distribution diverges if \( m = \alpha/k < h \). Therefore the expectation value of the random variable \( \tilde{\theta} \) diverges if \( m < 1 \) or \( q > \frac{2\alpha+1}{1+\alpha} \).

In the case of dipolar systems, most of the empirical data for the power-law exponents \( n \) and \( m \) are in the range \([0,1]\) and can be accounted for using the heavy-tailed BurrXII waiting-time distribution with \( \alpha/k \leq 1 \) for which \( \langle \tilde{\theta} \rangle = \infty \).

This presentation which avoids the usual weighted average of a Debye response function over a relaxation time or relaxation rate distribution confirms the relation obtained between the empirical exponents \( n \) and \( m \) and the ”fractal” exponent \( \alpha \) and the nonextensive exponent \( q \) derived by two of us \[10\] using more phenomenological arguments. In that model the cluster volume distribution was obtained from the max \( S_q \) principle and a ”fractal” relation between the cluster volume and its relaxation time was assumed.

The BurrXII distribution can be obtained as a smooth mixture of Weibull distributions compounded with respect to a random scale parameter distributed with the gamma distribution \[6\]. Using this fact we can rewrite (25) as

\[ \phi_{\alpha,q}(t) = \int_0^\infty \exp(-\lambda^\alpha t^\alpha) d\Gamma_{1/k,k}(\lambda^\alpha/A^\alpha) \] (33)

where

\[ \Gamma_{1/k,k}(\lambda^\alpha/A^\alpha) = \frac{1}{\Gamma(1/k)} \int_0^{\lambda^\alpha/A^\alpha} \left(\frac{x}{k}\right)^{1/k-1} e^{-x/k} d\left(\frac{x}{k}\right) \] (34)

is the generalized gamma distribution with scale parameter \( k \) and form factor \( \sigma = 1/k \). \[7\]. It is however to be noticed that this procedure leads to a relaxation function with a \( A \) factor defined as a usual \((q = 1)\) expectation value. By contrast the max \( S_q \) principle allows to define \( A \) as a natural scale in a situation where the expectation value cannot be defined.
4 Stochastic theory and Tsallis entropy

The discussion of the equivalence of the two results obtained for the “universal” relaxation function (25) and (26) from the max $S_q$ method and the Weron et al. stochastic theory [7][8] can lead to a better understanding of the stochastic properties underlying the Tsallis entropy concept as well as its possible generalization for more complex spatio-temporal dynamical systems.

The starting point is the observation of the fact that the relaxation function for the whole system i.e. its survival probability is just the probability of its first passage

$$\phi(t) = \Pr(\bar{\theta} \geq t) = \Pr(\min(\theta_{1N}, \ldots, \theta_{\nu N}, N))$$ (35)

where

$$\Pr(\theta_{iN} \geq t) = \langle e^{-\beta_{iN}t} \rangle$$ (36)

$$\phi(t) = \Pi^\nu_{iN} \Pr(\theta_{iN} \geq t) = \Pi^\nu_{iN} \Pr(e^{-\beta_{iN}t} \geq t) = \langle \exp(-\bar{\beta}_{iN}t) \rangle$$ (37)

with

$$\bar{\beta}_{iN} = \frac{\sum_{i=1}^{\nu N} \beta_{iN}}{a_N}$$ (38)

The quantity $\bar{\beta}$ is a random relaxation rate corresponding to the whole (macroscopic) system. The random relaxation rates $\beta_{i,N}$ and random waiting times $\theta_{i,N}$ are related to the relaxations of the local individual entities. $N$ is the number of total entities (atoms, molecules, dynamical clusters) able to relax, $\nu_N$ is the number of relaxing entities participating effectively in the relaxing process. It is important to notice that $\nu_N$ can be a fixed number or a random quantity.

The distribution of (38) can be approximated by the weak limit

$$\bar{\beta} = \lim_{N \to \infty} (a_N)^{-1} \bar{\beta}_N$$ (39)

where $a_N$ is the sequence of relevant normalizing constants. On the basis of limit theorems of probability theory, it is possible to define the distribution of the limit (39) even if the distribution of the individual relaxation rates $\beta_{i,N}$ and the number of $\nu_N$ of entities participating effectively in the relaxation process are known to a relatively limited extend only.
The macroscopic relaxing properties are clearly related to the probability distribution of the summand \( \tilde{\beta} \) (39). In the case of a deterministic fixed number of relaxing entities, Weron et al. [7] [8] have demonstrated, using the extremal value theorem, that if the \( \tilde{\theta} \) are distributed with a stretched exponential distribution, the only possible distribution for \( \tilde{\beta} \) is a one-sided stable Lévy distribution with index \( 0 < \alpha < 1 \) and we have:

\[
\Pr(\tilde{\theta} \geq t) = \int_0^\infty e^{-bt} dL_{\tilde{\beta}}(b) = e^{-(At)^\alpha} \tag{40}
\]

Using an heuristic argument one can understand physically that if the smallest local waiting time determines the macroscopic relaxation, this should correspond to the largest relaxation rate. It is not therefore surprising that the distribution dominated by the highest terms in (38) is for \( N \to \infty \) the stable one-sided Lévy distributions which has the property to be dominated asymptotically by the highest term [15] [14].

If the number \( \nu_N \) is a random variable, the scale parameter is a random variable and the BurrXII distribution is obtained if the scale distribution is the generalized gamma distribution (34). It can be easily shown by randomizing the scale parameter in (33) that

\[
\Pr(\tilde{\theta} \geq t) = \int_0^\infty e^{-bt} dF_{\tilde{\beta}}(b) = 1 - B_{\alpha,1/k}(k^{1/\alpha}At) = [1 + k (At)^\alpha]^{-1/k} \tag{41}
\]

where \( F_{\tilde{\beta}}(b) \) is the Mittag-Leffler distribution. In that case \( \tilde{\beta} \) is a \( \nu \)–stable random variable and stochastic theory arguments show that this result is obtained if \( \nu_N \) is distributed with a generalized negative binomial distribution [7].

\[
\Pr(\nu_N = n) = \frac{\Gamma(1/(k + n - 1)) \left( \frac{1}{N} \right)^{1/k} (1 - \frac{1}{N})^{n-1}}{\Gamma(1/k)(n-1)!} \quad n = 1, 2, ... \tag{42}
\]

5 Conclusions

In the case of non-Debye relaxation, the short-range interactions, geometric and dynamic correlations can be accounted for by maximizing the S-B entropy with adequate constraints. The small clusters and short-time relaxation can be described by a stretched exponential relaxation function. The exponent \( \alpha \leq 1 \) introduced in the constraints is a measure of the "non-idealness" of the relaxation processes at this scale (fluctuations of the size and intra-cluster
interactions). The system is extensive in the fractal time domain $t^{\alpha}$ and the distribution of the relaxation rates $\beta$ is heavy-tailed with a Levy tail exponent equal to $\alpha$.

Larger clusters relaxation and long time power law relaxation can be obtained by the $\text{max} S_q$ principle and depends on the exponent $\alpha/k$ with $k = \frac{q-1}{2-q}$. The $q$ non-extensivity parameter and the heavy tail properties of the waiting-time ($\theta$) distribution are directly related to the random number of relaxing entities at the meso-or microscopic level which gives rise to fluctuations of the usual extensive (i.e., corresponding to exponential distributions) time scale. In that sense the Tsallis entropy can be viewed as a technique to define a finite macroscopic scale when the number of entities participating to the spatio-temporal dynamical process is statistically fluctuating due to natural geometric and dynamical constraints. That scale can be defined as a $q$-expectation value using the concept of escort probability. This situation is typical of "frustrated" systems like glasses, polymers and porous materials.

Although our discussion has been limited to dipolar relaxation, our conclusions are relevant to a great number of non-exponential decay phenomena observed in nature [16][17].

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