Centro Brasileiro de Pesquisas Físicas – CBPF
Coordenação de Física Teórica – COTEO

ENTROPIC EXTENSIVITY AND LARGE DEVIATIONS IN THE PRESENCE OF STRONG CORRELATIONS

Ugur Tirnaklia[a], Mauricio Marques[b], Constantino Tsallis[b,c,d]

PHYSICA D 431 (2022) 133132

INTRODUCTION

It is fair to consider the Maxwellian distribution of velocities and the exponential distribution of energies as the most important fingerprints of Boltzmann–Gibbs (BG) statistical mechanics. These facts mirror the Central Limit Theorem (CLT) which leads, when the number N of involved random variables increases indefinitely, to convergence towards Gaussian distributions, and the Large Deviation Theory (LDT) which characterizes the speed at which Gaussians are approached while N increases. To be more precise, the BG distribution p_{BG} associated with a many-body Hamiltonian $\mathcal{H}_N$ at thermal equilibrium is given by $p_{BG} \propto e^{-\beta\mathcal{H}_N}$ whenever $\mathcal{H}_N$ includes short-range interactions or no interactions at all. We may then write that $p_{BG} \propto e^{-[\beta\mathcal{H}_N/N]N}$, where, consistently with thermodynamics, $[\beta\mathcal{H}_N/N]$ is an intensive quantity. The corresponding LDT statement for a binary stochastic system with N random variables yielding n times say 0, and $(N-n)$ times say 1 concerns the probability $P_N(n/N > z) \in [0,1]$ of the random variable n/N taking values larger than a fixed value $z \in \mathbb{R}$ for increasingly large values of N. Under the hypothesis of probabilistic independence, or similar settings, we expect $P_N(n/N > z) \approx e^{-r_1(z)N}$, where the rate function $r_1$equals a BG relative entropy per particle. Therefore $r_1(z)N$ plays the role of a thermodynamic total entropy which, consistently with the Legendre structure of classical thermodynamics, is extensive.

Within nonextensive statistical mechanics (q-statistics for short), we typically tackle with long-range-interacting Hamiltonian systems, among other strongly correlated ones. The associated distributions of velocities appear to be Q-Gaussians with $Q > 1$, with Q approaching unity when the range of the interactions approaches the short-range regime. These facts are to be associated with a Q-Central Limit Theorem (Q-CLT) which leads, when $N \to \infty$, to a convergence on a Q-gaussian distribution. Sufficient conditions for the Q-CLT to hold are already available but the necessary conditions for a Q-CLT still remain as a challenge. The desirable mathematical counterpart for such systems would of course be to have a q-Large Deviation Theory (q-LDT) with a probability corresponding to $n/N - 1/2 \geq z$ given by $P(N,z) \approx e^{-r_q(z)N}$, where the rate function $r_q(z)$ would once again equal some relative nonadditive entropy per particle. The quantity $r_q(z)N$ is expected to play a role similar to that of a total system thermodynamic entropy which, as mentioned above, should always be extensive, i.e., $\propto N$ $(N \gg 1)$. Naturally, in order to unify all the above situations, we expect $q = f(Q)$, $f(Q)$ being a smooth function which satisfies $f(1) = 1$, thus recovering the usual LDT.

MODEL AND RESULTS

We focus on a scale-invariant probabilistic model based on the Laplace-de Finetti theorem for exchangeable stochastic processes. The random variables are binary (Ising-like) and can be either uncorrelated $(Q = 1)$ or strongly correlated $(Q > 1)$; each of them takes the values 0 and 1. A specific micro-state with n values 0 and $(N-n)$ values 1 corresponds to $r_n^N = 1/2^N$ for $Q = 1$ and to

$$r_n^N = \frac{B(\frac{3-Q}{2Q-2}+n, \frac{3-Q}{2Q-2}+N-n)}{B(\frac{3-Q}{2Q-2}, \frac{3-Q}{2Q-2})}$$

for long-tailed distributions $(1 < Q < 3)$, where $B(x,y) = \Gamma(x)\Gamma(y)/\Gamma(x+y)$ is the Euler Beta function. In this model, $(Q-1)$ measures the strength of the global correlations, and varies from 0 to 2. The $N \to \infty$ attractor of this model for fixed Q turns out to precisely be a Q-Gaussian, which makes it an interesting case for checking its LDT behavior.

We define $u_n^N \equiv \frac{(\frac{n}{N}-\frac{1}{2})}{\sqrt{(Q-1)(n/N)(1-n/N)}}$ e $\tilde{u}_n^N \equiv \frac{u_n^N}{2\max_{1,2,\dots,N-1}\{u_n^N\}}$ where $\max_{1,2,\dots,N-1}\{u_n^N\} = \frac{\frac{1}{2}-\frac{1}{N}}{\sqrt{(Q-1)(N-1)/N^2}}$. We also define the discrete width $du_n^N \equiv \frac{[(n/N)(1-n/N)]^{-3/2}}{4(N+1)\sqrt{Q-1}}$ from which it follows the (un-normalized) distribution $F_n^N = (du_n^N)^{-1}\frac{N!}{n!(N-n)!}r_n^N$, and, after normalization, we have $\tilde{F}_n^N \equiv \frac{F_n^N}{\sum_{n=1}^{N-1} F_n^N}$.

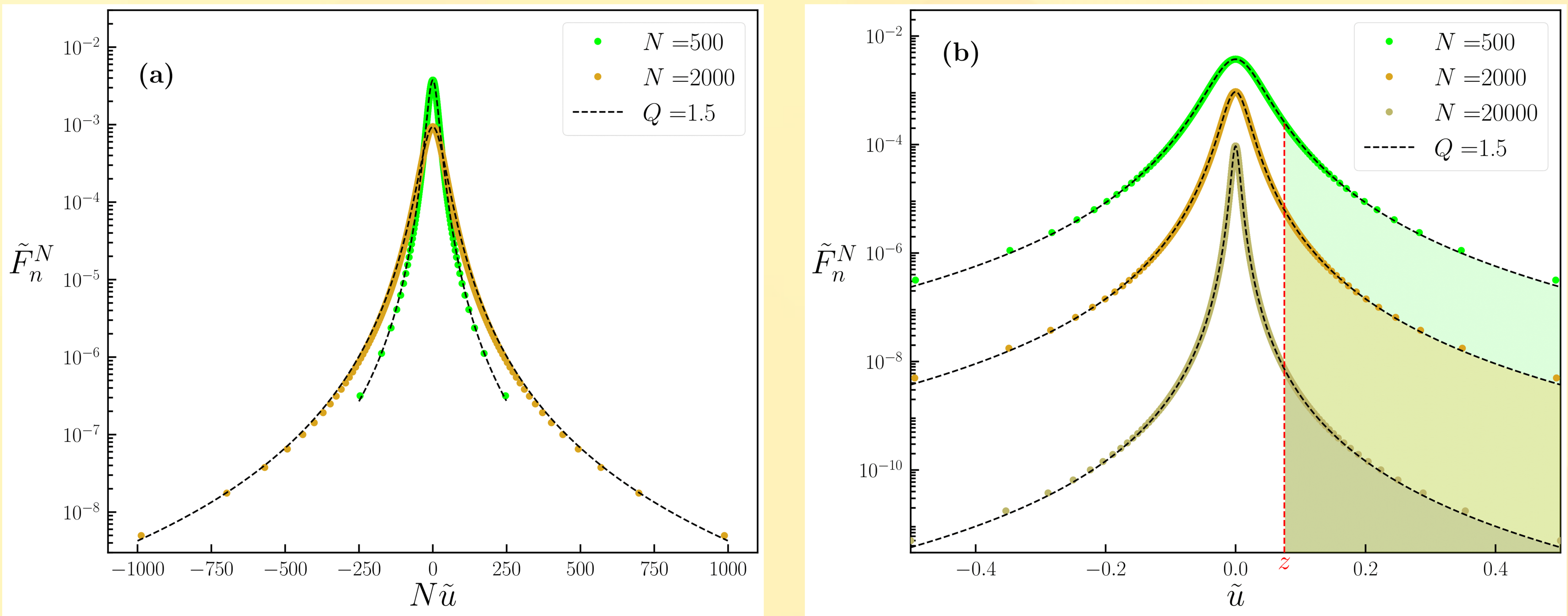

Fig 1: $\tilde{F}_n^N$ distributions are given for some representative values of N.

Now, in the LDT realm, we focus on the probability $P(N,z) \in [0,1]$ which is defined as that whose values of $\tilde{F}_n^N$correspond to $n/N > 1/2 + z$. We expect to numerically verify that $P(N,z) = P_0(Q,z)e_q^{-r_q(Q,z)N}$, with $P_0(Q,0) = 1/2$, $P_0\left(Q,\frac{1}{2}\right) = 0$, and $r_q(Q,0) = 0$.

By optimally fitting of $P(N,z)$ with respect to (q, r_q, P_0), we have heuristically found

$$q = 2 - \frac{1}{Q}, \qquad (1 \leq Q < 3).$$

For strongly correlated binary variables, we have from the literature

$$r_q(z) = \frac{1}{q_r - 1}\left\{\frac{1}{2}[(1+2z)^{q_r} + (1-2z)^{q_r}] - 1\right\} \sim 2q_r z^2 + \frac{2}{3}(3-q_r)(2-q_r)q_r z^4, \qquad (z \to 0).$$

Through the optimized fitting, we heuristically found the following relations

$$q_r = \frac{7}{10} + \frac{6}{10}\frac{1}{Q-1}, \qquad (1 < Q < 3).$$

$$P_0(Q,z) = \frac{1}{4} - \frac{2^u}{4}z^u + \frac{2^u}{4}\left(\frac{1}{2} - z\right)^u, \qquad (0 \leq z \leq 1/2).$$

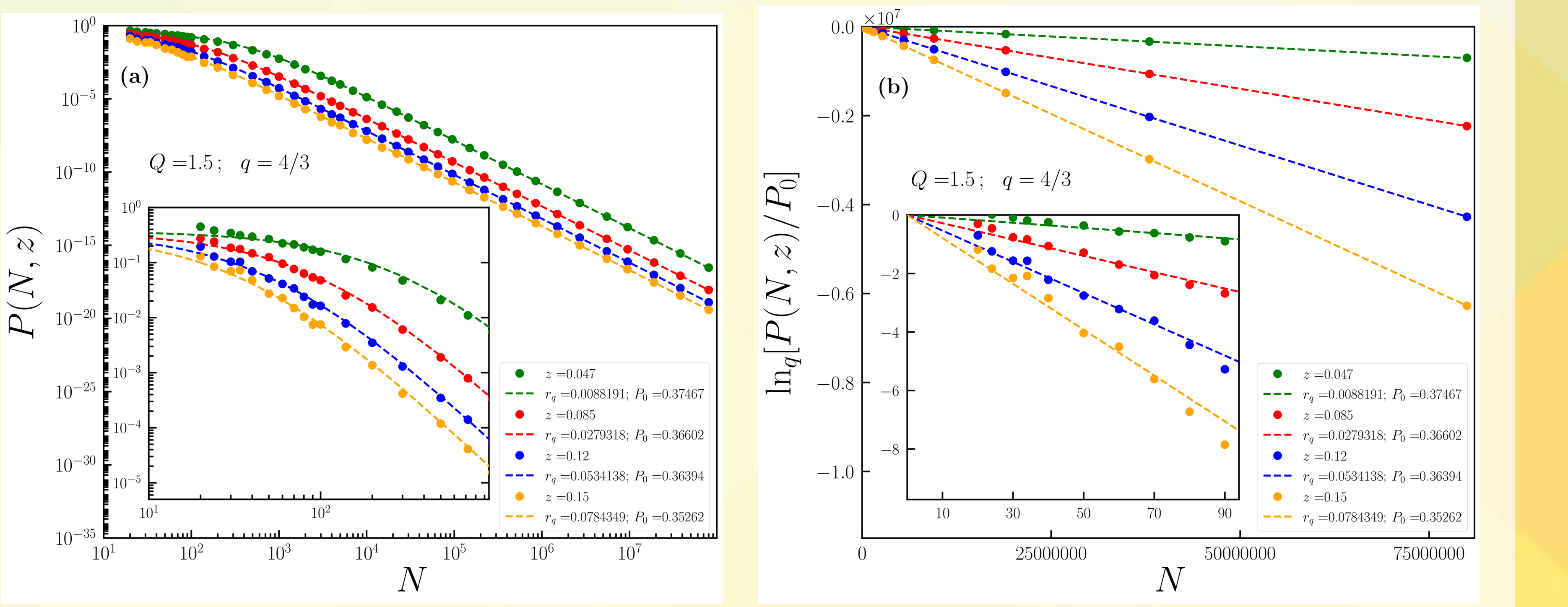

Fig 2: $P(N,z)$ representations.

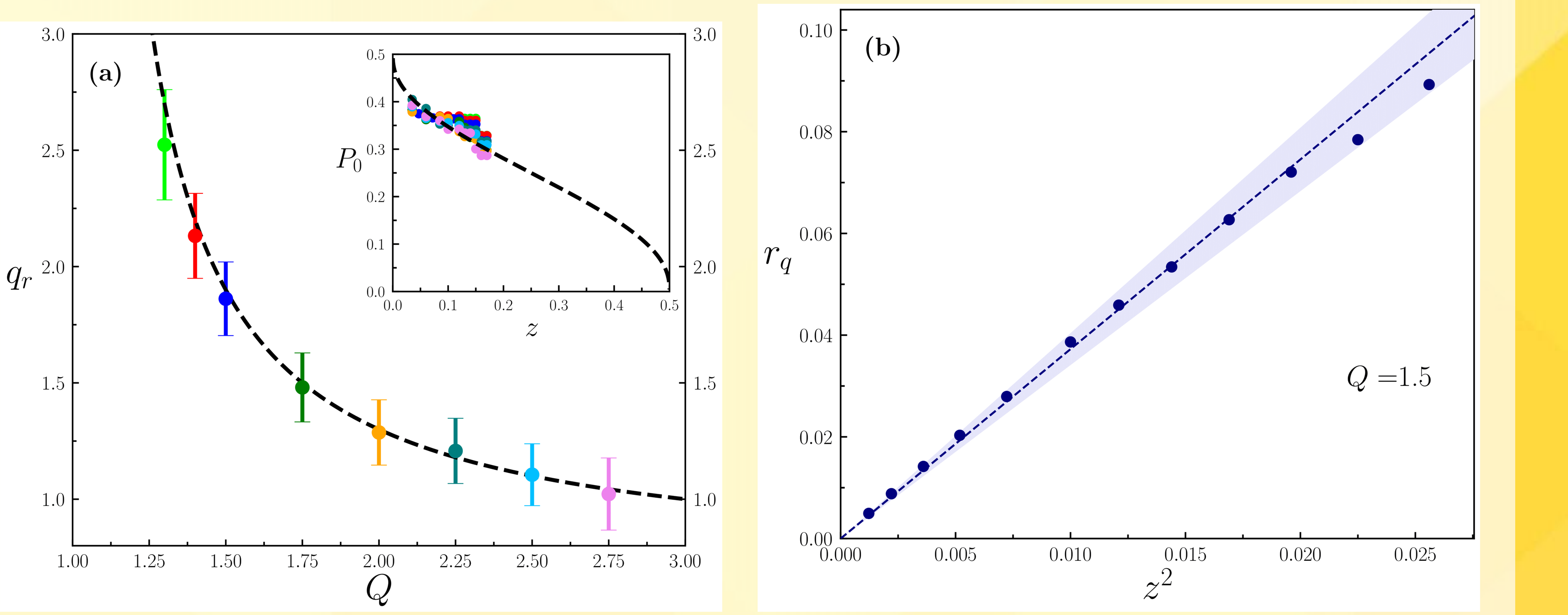

Fig 3: Fittings.

FINAL REMARKS

We conclude by reminding that our aim is to approach, within a more general context, the fingerprints of Boltzmann–Gibbs statistical mechanics, namely the Maxwellian distribution of velocities and the BG exponential weight for the energies. Indeed, in the realm of q-statistics based on nonadditive entropies, a Q-Gaussian distribution emerges for the velocities and a q-exponential weight emerges for the energies, with $Q \geq q \geq 1$, the equalities holding precisely for the BG theory. These generalizations should respectively mirror corresponding generalizations of the classical Central Limit Theorem and the Large Deviation Theory. This scenario has been successfully verified for a purely probabilistic model, as well as for some simple physical models in the literature.

In our paper, it has been possible to numerically discuss (with satisfactory precision in some cases) (i) The (Q,z)-dependence of the pre-factor $P_0(Q,z)$ (this is the first time such a pre-factor is focused on in the literature of complex systems); (ii) The possible identification of the rate function $r_q(z)$ with a nonadditive relative entropy whose index is q_r, definitively different from the index q (a possibility that has never been handled before); (iii) The Q-dependence q_r(Q), which includes an unexpected singularity at $Q = 1$ (a feature coming from the specificity of the model). This q_r(Q) dependence only became accessible due to the mathematical fact that all the necessary information is already available in the first asymptotic term, namely in the quadratic term of $r_q(z)$ as a function of z. To the best of our knowledge, the above three points have never before been simultaneously attained for any nontrivial model. Last but not least, in all models focused in the literature consulted, the values of (Q,q) are numerical ones, whereas in the present paper we have obtained analytical expressions for arbitrary real $Q > 1$.

The present results were generalized in a paper by Zamora and Tsallis [3].

REFERENCES

[1] TIRNAKLI, U.; MARQUES, M.; TSALLIS, C. Entropic extensivity and large deviations in the presence of strong correlations. *Physica D*, v. 431, p. 133132, 2022.
[2] TSALLIS, C. *Introduction to Nonextensive Statistical Mechanics: Approaching a Complex World*. New York: Springer, 2023.
[3] ZAMORA, D. J.; TSALLIS, C. Probabilistic models with nonlocal correlations: Numerical evidence of q-large deviation theory. *Physica A: Statistical Mechanics and its Applications*, v. 608, n. 1, p. 128275, 2022.

All additional references can be found in the original paper.

a Department of Physics, Faculty of Science, Ege University, Izmir, 35100, Turkey
b Centro Brasileiro de Pesquisas Fisicas and National Institute of Science and Technology for Complex Systems, Rua Xavier Sigaud 150, Rio de Janeiro, 22290-180, Brazil
c Santa Fe Institute, 1399 Hyde Park Road, Santa Fe, 87501, NM, USA
d Complexity Science Hub Vienna, Josefstädter Strasse 39, Vienna, 1080, Austria

mauriciomarx@gmail.com