Influence of the interaction range on the thermostatistics of a classical many-body system

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We numerically study a one-dimensional system of N classical localized planar rotators coupled through interactions which decay with distance as $1/r^\alpha$ ($\alpha \geq 0$). The approach is a first principle one (i.e., based on Newton's law) which, through molecular dynamics, yields the probability distribution of angular momenta. For α large enough we observe, for longstanding states corresponding to $N \gg 1$ systems, the expected Maxwellian distribution. But, for α small or comparable to unity, we observe instead robust fat-tailed distributions that are quite well fitted with q-Gaussians. These distributions extremize, under appropriate simple constraints, the nonadditive entropy S_q upon which nonextensive statistical mechanics is based. The whole scenario appears to be consistent with nonergodicity and with the q-generalized Central Limit Theorem. It confirms the more-than-centennial prediction by J.W. Gibbs that standard statistical mechanics are not applicable for long-range interactions (i.e., for $0 \leq \alpha \leq 1$) due to the divergence of the canonical partition function.

PACS numbers: 05.20.-y, 05.45.-a, 65.40.gd, 89.75.Da

More than one century ago, in his historical book *Elementary Principles in Statistical Mechanics* [1], J. W. Gibbs remarked that systems involving long-range interactions will be intractable within his and Boltzmann theory, due to the divergence of the partition function. This is of course the reason why no standard temperature-dependent thermostatistical quantities (e.g., a specific heat) can possibly be calculated for the free hydrogen atom, for instance. Indeed, unless a box surrounds the atom, an infinite number of excited energy levels accumulate at the ionization value, which yields a divergent canonical partition function at any finite temperature.

To transparently extract the deep consequences of Gibbs' remark, in the present paper we focus on the influence of the range of the interactions within an illustrative isolated classical system, namely the α-XY model [2], whose Hamiltonian is given by

$$\mathcal{H} = \frac{1}{2}\sum_{i=1}^{N} p_i^2 + \frac{1}{2}\sum_{i\neq j}\frac{1-\cos(\theta_i-\theta_j)}{r_{ij}^{\alpha}} \quad (\alpha \geq 0)\,, \tag{1}$$

where the planar rotators are located at the sites of a d-dimensional hypercubic lattice with periodic boundary conditions. For $d=1$, r_{ij} takes the values 1, 2, 3...; for $d=2$, it takes the values 1, $\sqrt{2}$, 2, ...; for $d=3$, it takes the values 1, $\sqrt{2}$, $\sqrt{3}$, 2, ... The distance between any two rotators is taken to be the minimal one given the periodic boundary conditions. Without loss of generality we have considered unit moment of inertia, and unit first-neighbor coupling constant; p_i and θ_i are canonical conjugate pairs. At the fundamental state, all rotators are parallel, say $\theta_i = 0, \forall i$, which corresponds to the ferromagnetically fully ordered case. At high enough energies, the values of $\{\theta_i\}$ are randomly distributed, which corresponds to the paramagnetic phase. In between, a second order phase transition occurs. The potential energy *per particle* varies with N like $\widetilde{N} \equiv \sum_{j=2}^{N}\frac{1}{r_{1j}^{\alpha}}$. This quantity can be approximated, for $\alpha/d < \infty$, by $d\int_1^{N^{1/d}} dr\, r^{d-1} r^{-\alpha} = \frac{N^{1-\alpha/d}-1}{1-\alpha/d}$, which in turn behaves, when $N \to \infty$, like $N^{1-\alpha/d}/(1-\alpha/d)$ if $0 \leq \alpha/d < 1$, like $\ln N$ if $\alpha/d = 1$, and like $1/(\alpha/d-1)$ if $\alpha/d > 1$. In other words, the total potential energy is extensive (in the thermodynamical sense) for $\alpha/d > 1$, and nonextensive otherwise. In order to accommodate to a common practice, we might re-write the Hamiltonian $\mathcal{H}$ as follows:

$$\bar{\mathcal{H}} = \frac{1}{2}\sum_{i=1}^{N} p_i^2 + \frac{1}{2\widetilde{N}}\sum_{i\neq j}\frac{1-\cos(\theta_i-\theta_j)}{r_{ij}^{\alpha}}\,, \tag{2}$$

which can now be considered as "extensive" for all values of α/d. This corresponds in fact to a rescaling of time (hence of p_i), as shown in [2]. Also, this rewriting takes into account the fact that, for all values of α/d, the thermodynamic energies (internal, Helmholtz, Gibbs) grow like $N\widetilde{N}$, the entropy, volume, magnetization, number of particles, etc, grow like N (i.e., remain extensive for *both* regions above and below $\alpha/d = 1$), and the temperature, pressure, external magnetic field, chemical potential, etc, must be scaled with $\widetilde{N}$ in order to have *finite* equations of states [3]. The particular case $\alpha = 0$ recovers the HMF model ([4] and references therein); the $\alpha \to \infty$ model corresponds to first-neighbor interactions (whose $d = 1$ case has been analytically studied [5]).

In addition to the above, it has already been shown that the special value $\alpha/d = 1$ also emerges dynamically. Indeed, for $N \to \infty$ and energies corresponding to the paramagnetic region, the largest Lyapunov exponent of the many-body system remains finite and positive for $\alpha/d > 1$, whereas gradually vanishes for $0 \le \alpha/d \le 1$. It vanishes like $N^{-\kappa}$, where $\kappa(\alpha/d)$ decreases from a positive value (close to $1/3$) to zero when α/d increases from zero to 1, and remains zero for $\alpha/d \ge 1$. It is interesting to emphasize that κ does not independently depend on (α, d), but only on the ratio α/d [2, 6, 7]. Consistently with the fact that, for all values of the energy per particle u in the paramagnetic region, the Lyapunov exponents vanish in the limit $N \to \infty$, κ does not depend on u.

Let us briefly mention at this point that the breakdown of ergodicity which emerges for $\alpha/d \le 1$ [8] points towards the inadequacy of the Boltzmann-Gibbs (BG) theory. It is the aim of nonextensive statistical mechanics [3, 9] to provide a way out of this kind of difficulty. Within this generalized theory, the stationary state is expected to yield a probability distribution $p_q = e_q^{-\beta_q \tilde{\mathcal{H}}}/Z_q(\beta_q)$ with $Z_q(\beta_q) \equiv \int dp_1...dp_N d\theta_1...d\theta_N e_q^{-\beta_q \tilde{\mathcal{H}}}$, where $e_q^x \equiv [1 + (1-q)x]^{1/(1-q)}$ ($q \in \mathcal{R}$; $e_1^x = e^x$). The index q is expected to characterize universality classes, possibly a function $q(\alpha/d)$ to be different from 1 for $0 \le \alpha/d < 1$, and equal to 1 for $\alpha/d \ge 1$. If this is so, an interesting quantity would of course be the one-momentum marginal probability $P(p_1) = \int dp_2...dp_N d\theta_1...d\theta_N e_q^{-\beta_q \tilde{\mathcal{H}}}/Z_q$. The functional form of $P(p_1)$ is unknown. A possibility could however be that, in the $N \to \infty$ limit, we simply have $P(p_1) \propto e_{q_m}^{-\beta_{q_m} p_1^2/2}$, i.e., a q_m-Gaussian form, where m stands for *momentum*. Indeed, q-Gaussians emerge extremely frequently in nonextensive-like systems (see, e.g., [10–15]; see also [16]). The index q_m could depend not only on α/d, but also, in principle, on u (we remind that the $d = 1$ critical point for $0 \le \alpha < 1$ is known to be $u_c = 3/4$). Now that we have outlined a possible thermostatistical scenario, let us present the molecular-dynamical results that we have obtained for the $d = 1$ Hamiltonian (2) with fixed (N, u), the total energy being Nu. We have used the Yoshida $4th$-order symplectic algorithm, and we have checked also through the standard $4th$-order Runge-Kutta one. We present in Fig. 1 the "temperature" $T(t) \equiv 2K(t)/N$, where $K(t)$ is the time-dependent total kinetic energy of Hamiltonian $\tilde{\mathcal{H}}$. The class of initial conditions that we run are the so-called water-bag for the moments, with $\theta_i = 0, \forall i$. As verified many times in the literature, a quasi-stationary state (QSS) exists for $0 \le \alpha/d < 1$ and $u \simeq 0.69$, after which a crossover is observed to a state whose temperature coincides with that analytically obtained within

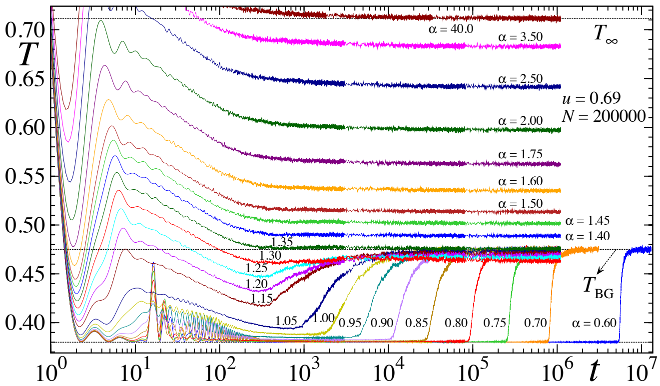

FIG. 1: Time dependence of $T(t) \equiv 2K(t)/N$ for a water bag typical *single* initial condition for $(u, N) = (0.69, 200000)$ and typical values of α. The upper horizontal line, at $T_\infty = 0.7114\ldots$, corresponds to the $(\alpha, N) \to (\infty, \infty)$ model at $u = 0.69$ [5]. The middle (lower) horizontal line, at $T \simeq 0.475$ ($T = 0.380$), indicates the BG thermal equilibrium temperature (the QSS base temperature, corresponding to zero magnetization), at $u = 0.69$ and $0 \le \alpha < 1$.

BG statistical mechanics [4]. The lifetime of this QSS appears to diverge with diverging N. It has been long thought that, after this crossover, the system consistently adopts a BG distribution in Gibbs Γ space, and therefore a Maxwellian distribution for $P(p_i)$. The facts that we now present reveal a much more complex situation, where robust q_n-Gaussians (or distributions numerically very close to them) emerge before the crossover (just before for most realizations of the initial conditions, but also quite before for not few of them) and remain so for huge times (practically for ever); n stands for *numerical*. This unexpected phenomenon occurs for u both below and above $u_c = 3/4$, and for α both below and above $\alpha = 1$ (up to $\alpha \simeq 2$). Let us emphasize that these q_n-Gaussians only develop their full shape if sufficient time has been run in order that the apparently stationary state has practically been attained. This time is extremely long for $0 < u \ll 3/4$ because the system is then almost integrable (indeed, the Hamiltonian can be straightforwardly checked to become very close to that of N coupled harmonic oscillators, by using $\cos(\theta_i - \theta_j) \sim 1 - \frac{1}{2}(\theta_i - \theta_j)^2$), and is also extremely long for $u \gg 3/4$ because once again the system is almost integrable (indeed, the Hamiltonian can be straightforwardly checked to become now very close to N independent localized rotators). Let us detail now how the single-initial-condition one-momentum distributions $P(p)$ are calculated within large time regions where T is sensibly constant: for each value of i, we register its p_i at very many (noted n) successive times separated by an interval τ, and then, following the recipe of the q-generalized Central Limit Theorem [17], calculate its arithmetic average $\bar{p}_i$ (thus corresponding to the interval $t \in [t_{min}, t_{max}]$ with $t_{max} - t_{min} = n\tau$). We

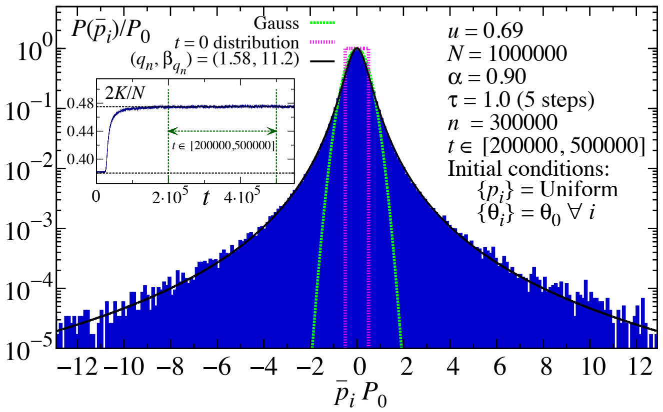

FIG. 2: A typical single-initial-condition one-momentum distribution $P(p)$ for $N = 10^6$, $u = 0.69$, $\alpha = 0.9$, $\tau = 1$ (corresponding to 5 molecular-dynamical algorithmic steps), calculated in the region $(t_{min}, t_{max}) = (200000, 500000)$ (see *Inset*), where the temperature coincides with that analytically calculated within BG statistical mechanics, namely $T(\infty) \equiv 2K(\infty)/N \simeq 0.475$. The total energy Nu is conserved within a relative precision of 10^{-5} or better. The continuous curve corresponds to $P(\bar{p})/P_0 = e_{q_n}^{-\beta_{q_n}^{(P_0)}[\bar{p}P_0]^2/2}$ with $(q_n, \beta_{q_n}^{(P_0)}) = (1.58, 11.2)$. The value of q_n corresponds to the red open circle in Fig. 3. Notice that here $1/\beta_{q_n}^{(P_0)} \neq T$. Each distribution has been rescaled with its own P_0.

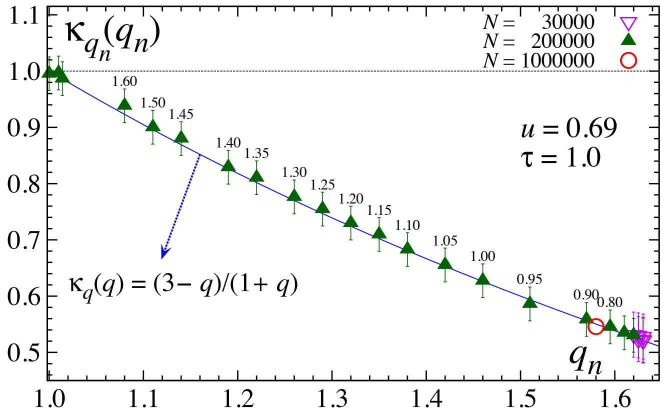

FIG. 3: q_n and q-kurtosis κ_{q_n} that have been obtained from the histograms corresponding to typical values of α (numbers indicated on top of the points). The red circle corresponds to Fig. 2. The continuous curve $\kappa_q = (3-q)/(1+q)$ is the analytical one obtained with q-Gaussians. Notice that κ_q is finite up to $q = 3$ (maximal admissible value for a q-Gaussian to be normalizable), and that it does not depend on β_{q_n}. The visible departure from the dotted line at $\kappa_q = 1$ corresponding to a Maxwellian distribution, neatly reflects the departure from BG thermostatistics.

then plot the histogram for the N arithmetic averages, as illustrated in Fig. 2. All the histograms that we have obtained for sufficiently large times t are well fitted with $e_{q_n}^{-\beta_{q_n} p^2/2}$, with (q_n, β_{q_n}) depending on (α, u, N, τ) as well as on (t_{min}, t_{max}). To check the quality of the fit we introduce (see Fig. 3) a conveniently q-generalized kurtosis (referred to as *q-kurtosis*), defined as follows:

$$\kappa_q = \frac{\int_{-\infty}^{\infty} dp\, p^4 [P(p)]^{2q-1} / \int_{-\infty}^{\infty} dp\, [P(p)]^{2q-1}}{3\left[\int_{-\infty}^{\infty} dp\, p^2 [P(p)]^q / \int_{-\infty}^{\infty} dp\, [P(p)]^q\right]^2}, \quad (3)$$

where we have used the escort distributions (see [18] and references therein). These distributions have the remarkable advantage of being finite up to $q = 3$, which is precisely the value below which q-Gaussians are normalizable, i.e. $\int_{-\infty}^{\infty} dp\, P_0 e_q^{-\beta_q p^2/2} = 1$ $(q < 3)$. The use of the standard kurtosis $\kappa_1 = \langle p^4 \rangle / 3 \langle p^2 \rangle^2$ has the considerable disadvantage that $\langle p^2 \rangle$ diverges for $q \geq 5/3$, and $\langle p^4 \rangle$ diverges for $q \geq 3/2$. Hence κ_1 becomes useless for $q \geq 3/2$, and it happens that some of the distributions that we observe do exhibit $q_n \geq 3/2$. If we use a q-Gaussian $P(p)$ within Eq. (3), we obtain, through a relatively easy calculation, $\kappa_q(q) = \frac{3-q}{1+q}$, as also shown in Fig. 3.

In Figs. 4 and 5 we illustrate (q_n, β_{q_n}) as functions of (α, u, τ) for large values of N. All the results for q_n have been also reported in Fig. 3. One of the interesting features that we can observe is that in all cases q_n approaches the BG value $q = 1$ when τ increases. However, this approach is nearly exponential for $(\alpha < 1,\ u < 0.75)$, $(\alpha > 1,\ u > 0.75)$, and $(\alpha > 1,\ u < 0.75)$, whereas it is extremely slow for $(\alpha < 1,\ u > 0.75)$ (notice that, in the latter case, q_n exhibits a zero slope with regard to τ at $\tau = 1$), precisely the region where the largest Lyapunov exponent approaches zero with increasing N. This suggests the following nonuniform convergence: $\lim_{N\to\infty} \lim_{\tau\to\infty} q_n(\alpha, u, N, \tau) = 1$ $(\forall \alpha)$, whereas $\lim_{\tau\to\infty} \lim_{N\to\infty} q_n(\alpha, u, N, \tau) > 1$ (for $0 \leq \alpha < 1$). Lack of computational strength has not allowed us to directly verify this conjecture. This leaves as an interesting open question whether $\lim_{\tau\to\infty} \lim_{N\to\infty} q_n(\alpha, u, N, \tau)$ recovers $\lim_{N\to\infty} q_m(\alpha, u, N)$, where the latter would correspond to successive approximations for increasingly large N.

Summarizing, it has been observed for at least one decade that, for $0 \leq \alpha < 1$, the longstanding QSSs of the present model exhibit anomalous distributions (Vlasov-like for some classes of initial conditions, and different, including q-Gaussian-shaped, ones for other classes) for the momenta of the rotators, whereas nothing particularly astonishing was expected to occur once the system had done the crossover to the (presumably stationary) state whose temperature coincides with that analytically obtained within the BG theory. The present results (obtained from first principles, i.e., using essentially nothing but Newton's law) neatly show that, if time is large enough so that the crossover has occurred (as illustrated in the Inset of Fig. 2), the situation is far more complex. Indeed, robust and longstanding q-Gaussian distributions are numerically observed under a wide variety

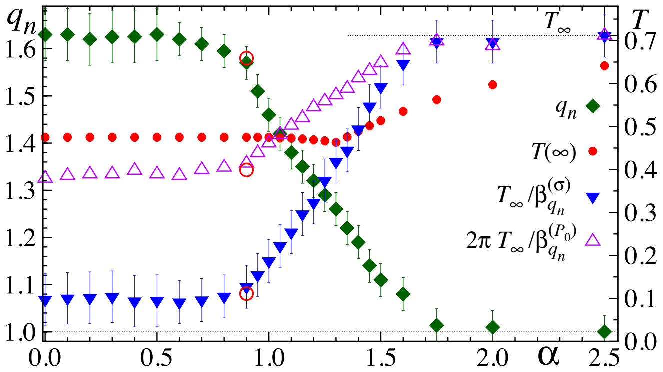

FIG. 4: α-dependences of (q_n, β_{q_n}) for $(u, \tau, N) = (0.69, 1.0, N)$, where $N = 200000$ ($N = 30000$) for $\alpha \geq 0.6$ ($\alpha \leq 0.5$), with n never smaller than 300000. We have verified the existence of finite-size effects, in particular, for α above and close to unity, q_n slowly decreases with increasing N. Notice that $T_\alpha(\infty) \equiv K(\infty)/2N \simeq 0.475$ up to $\alpha \simeq 1.35$, where it starts increasing (red full circles), and, for $\alpha \gg 1$, approaches the analytical value $T_\infty = 0.7114\ldots$[5] (by using the values that we have obtained up to $\alpha = 40$, we observe that approximatively $T_\infty - T_\alpha \simeq 0.4/\alpha^2$ for $\alpha \gg 1$). The red open circles correspond to the example in Fig. 2 (also indicated in Fig. 3). The dependence of T on (α, t) is noted $T_\alpha(t)$, hence confusion between $T(\infty)$ and T_∞ must be avoided. The full (open) triangles have been obtained from rescaled histograms where the momenta have been divided by the standard deviation σ (multiplied by P_0, as illustrated in Fig. 2). The error bars corresponding to the triangles are of the same order; the error bars of $T(\infty)$ are of the order of the full circles (red). Naturally, $P_0 \times \sigma$ is nearly constant; to take into account the numerical deviations (from a strict constant) due to parameters such as (N, n, τ), we have normalized both $\beta^{(\sigma)}_{q_n}$ and $\beta^{(P_0)}_{q_n}$ in such a way that the analytical value $T_\infty = 0.7114\ldots$ is recovered.

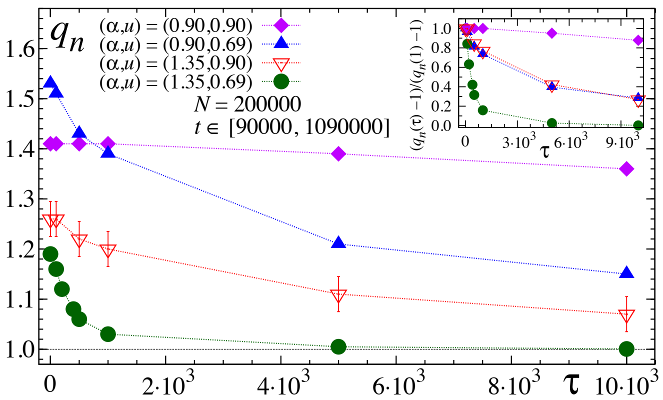

FIG. 5: τ-dependence of q_n for $N = 200000$, $(t_{min}, t_{max}) = (90000, 1090000)$ (hence $n = 1000000$ for $\tau = 1$), and typical values of u above and below the critical value $u_c = 0.75$, and of α above and below the special value $\alpha = 1$ (see [2]). All the errors bars are of the same order of those indicated on the red empty triangles. *Inset:* τ-dependence of $[q_n(\tau)-1]/[q_n(1)-1]$.

of situations. The fact that the temperature be the one predicted within the BG theory appears to be necessary but not sufficient for standard statistical mechanics to be applicable [19]. Indeed, the shape of the momenta distributions can considerably differ from Gaussians, and it is only when the correlations become negligible (i.e., when $\tau \gg 1$ and/or $\alpha \gg 1$) that the classical Maxwellian distribution (with $\beta_{q_n}^{-1} = T$) is to be (numerically) recovered. This example shows the great thermostatistical richness that a breakdown of ergodicity can cause. It also serves as an invitation for deeper analysis of the thermal statistics of all those very many models in the literature that are definitively nonergodic (e.g., glasses, spin-glasses, among others), and for which, nevertheless, the BG theory is used without further justification.

We acknowledge useful conversations with M. Jauregui, L.G. Moyano, F.D. Nobre, A. Pluchino, A. Rapisarda and L.A. Rios. We have benefited from partial financial support by CNPq, Faperj and Capes (Brazilian Agencies).

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"*In treating of the canonical distribution, we shall always suppose the multiple integral in equation (92)* [the partition function] *to have a finite value, as otherwise the coefficient of probability vanishes, and the law of distribution becomes illusory. This will exclude certain cases, but not such apparently, as will affect the value of our results with respect to their bearing on thermodynamics. It will exclude, for instance, cases in which the system or parts of it can be distributed in unlimited space [...]. It also excludes many cases in which the energy can decrease without limit, as when the system contains material points which attract one another inversely as the squares of their distances. [...]. For the purposes of a general discussion, it is sufficient to call attention to the assumption implicitly involved in the formula (92).*"

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[19] It is of course conceivable that, for $0 \leq \alpha/d \leq 1$ in the ordered limit $\lim_{N\to\infty} \lim_{t\to\infty}$ as well as for $\alpha/d > 1$ in any of the $(N,t) \to (\infty,\infty)$ limits, the Maxwellian distributions typical of thermal equilibrium are eventually recovered. However, the present work shows that, even for very large values of (N,t), this ultimate situation might be amazingly slow to be achieved (analogously to what occurs in systems such as those discussed in V. Schwammle, F.D. Nobre, and C. Tsallis, *Eur. Phys. J. B* **66**, 537 (2008)).