Approach to equilibrium via Tsallis distributions in a realistic ionic–crystal model and in the FPU model

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Abstract

We report results of dynamical simulations exhibiting the occurrence of Tsallis distributions, and their eventual approach to Maxwell–Boltzmann distributions, for the normal-mode energies of FPU–like systems. The first result is that Tsallis distributions occur in an ionic crystal model with long–range Coulomb forces, which is so realistic as to reproduce in an impressively good way the experimental infrared spectra. So, such distributions may be expected to represent actual physical features of crystals. The second result is that Tsallis distributions for the normal mode energies occur in the classical FPU model too. This is in agreement with previous results obtained in the latter model, namely: by Antonopoulos, Bountis and Basios for the distributions of local observables (particles' properties as energies or momenta), and by the first of the present authors for the statistical properties of return times. All such results thus confirm the thesis advanced by Tsallis himself, i.e., that the relevant property for a dynamical system to present Tsallis distributions is that its dynamics should be not fully chaotic, a property which is known to actually pertain, in particular, to systems with long–range interactions.

1 Introduction

In Statistical Mechanics, by Tsallis probability density (often referred to as *distribution*) one denotes a two-parameter family of densities, which includes as a limit case the one–parameter Maxwell-Boltzmann family. Denoting by E the random variable under consideration (for us, indeed, energy), the

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Tsallis family with parameters $q \neq 1$ and $\beta > 0$ has the form (with a normalization factor C)

$$f_{q,\beta}(E) = C\left[1 + (q-1)\,\beta E\right]^{\frac{1}{1-q}} \ , \tag{1}$$

which reduces to the Maxwell–Boltzmann distribution $C\,e^{-\beta E}$ in the limit $q \to 1$. Distributions of such a type are often discussed in connection with the statistical mechanics of systems presenting long–range interactions. In fact, Tsallis distributions were actually observed in numerical simulations for models of FPU type presenting long–range interactions involving all particles, which should emulate Coulomb or gravitational interactions [1, 2, 3, 4, 5, 6]. Starting from peculiar non–equilibrium states, a transient state was observed, pretty well described by a Tsallis distribution with time–dependent parameters $q = q(t)$, $\beta = \beta(t)$, which for long enough times converges to $q(t) = 1$, i.e., to a Maxwell–Boltzmann distribution, and thus presumably to equilibrium (see however [7, 8]). On the other hand, in the paper [9] an analogous phenomenon was observed also for the classical, short–range, FPU model.

In the present paper we illustrate two results concerning Tsallis distributions for the normal mode energies of systems of FPU type. The first result is that Tsallis distributions converging to a Maxwell-Boltzmann one are met for the normal–mode energies of a realistic 3d FPU–like model. We are referring to an ionic crystal model (actually, a LiF model) containing Coulomb long–range interactions (see [10, 11, 12]), which has such a realistic character as to reproduce in an impressively good way (and indeed within a classical frame) the experimental infrared spectra. For example, an agreement between experimental data and theory over 9 orders of magnitude for the infrared spectra of LiF at room temperature, is exhibited in the first two figures of the paper [11]. The fact that Tsallis distributions show up in that model was briefly illustrated, through one figure and a few lines of comment, at the end of paper [12], and is here expounded in more detail. In our opinion these results indicate that Tsallis distributions represent actual physical features of crystals and, more in general, of atomic physics.

The second result originates within a more general frame, namely, the dynamical foundations of statistical mechanics, investigated in terms of the statistics of return times, with special attention to systems which are not fully chaotic [13]. In such a frame, already ten years ago it was pointed out by the first author [14] that, in the classical nearest–neighbor FPU model, the statistics of the return times is compatible with a Tsallis–type distribution in the full phase space. In particular such a phase–space distribution implies that the distribution of the normal–mode energies too be of Tsallis type (albeit with different parameters). With such a result for the return times in mind, we thus decided to investigate numerically the approach to equilibrium of the normal–mode energies in a classical FPU experiment (i.e., for a classical FPU model, and for initial data with only a few low–frequency modes excited). The result we found is that in such a case too the approach to equilibrium occurs through a Tsallis distribution with time–dependent parameters, albeit with some peculiarities with respect to the realistic long–range 3d model. Actually, a q–statistics in the classical FPU model was already reported for local observables in the paper [9], and so our result points out that this occurs also for the normal mode energies.

The common origin for the similar results (Tsallis distributions) in the two different cases (long–range or short–range interactions) can be caught at a dynamical level: namely, that in both cases one is dealing with not fully chaotic systems. This indeed was emphasized by Tsallis himself, by saying that "*every time we have a dynamics which is only weakly chaotic (typically at the frontier between regular motions and strong chaos), the need systematically emerges*" for a q–statistics (see [15], page 151).

The numerical results are illustrated in the next section 2, and some concluding remarks then follow.

2 The results

2.1 The models

We preliminarily add a few words about the models. The FPU model is just the standard $\alpha-\beta$ one, which is universally known, and is investigated here for $\alpha = 1$ and $\beta = 1$. We take fixed end condition, so that the Hamiltonian reads

$$H = \sum_{i=1}^{N} \frac{p_i^2}{2} + \sum_{i=0}^{N} V(x_{i+1} - x_i) \ , \quad x_0 = x_{N+1} = 0 \ ,$$

with $V(r) = \frac{1}{2}r^2 + \frac{\alpha}{3}r^3 + \frac{\beta}{4}r^4$.

The realistic ionic crystal model is the standard one of Solid State Physics, which was introduced long ago by the Born school. In the Born model (see for example [16]) one considers N ions in a working cell of side L with periodic boundary conditions, and one deals with the ions as if they were point particles, interacting through pure Coulomb forces (cared, as usual, through standard Ewald summations). The contribution of the

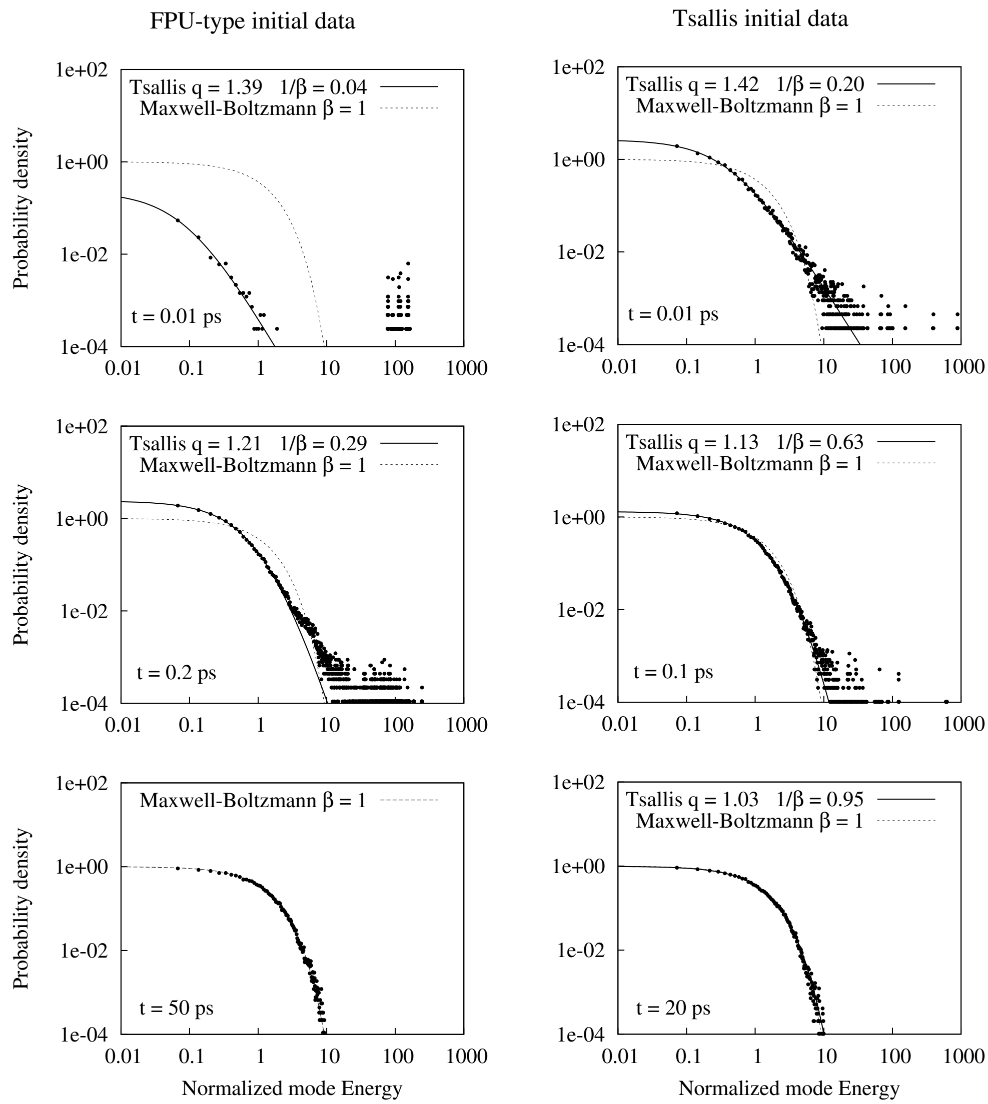

Figure 1: Histograms for the normalized normal–mode energies (i.e., their energies divided by the specific energy) at three different times (from top to bottom) for the realistic ionic crystal model. Left, initial condition of FPU type with a few low-frequency modes excited (see text); Right, initial condition of Tsallis type. Fit with a normalized Tsallis density (solid line), and comparison with a normalized Maxwell–Boltzmann density (dashed line). Number of particles $N = 4096$. Specific energy $\varepsilon = 537$ K (left) and $\varepsilon = 501$ K (right). The top panel of the left column shows that for FPU type initial data the energies of the low frequencies quickly attain a Tsallis distribution. The parameters of such a distribution are chosen in generating the initial data for the run of the right column. As in the left column only a small fraction of the modes is involved in the Tsallis distribution, the energy normalization factor produces for $1/\beta$ a value smaller than at the right, where all modes are involved.

electrons, which don't show up in the model but are known to produce polarization forces on the ions, is taken into account in a phenomenological way by introducing a short–range potential V^{phen} acting among the ions, with suitable "effective" charges substituted for the real ones. In our first paper [10] the phenomenological potential was just that originally proposed by Born, namely, $V^{phen}(r) = C/r^6$, whereas a more complex potential, depending on the pair of ions, was used in the subsequent papers [11, 12]. In the end, the Hamiltonian reads

$$H = \sum_{i=1}^{N} \frac{p_i^2}{2m_i} + \sum_{\mathbf{k}\in\mathbb{Z}^3} \sum_{i\neq j} V_{ij}(\mathbf{x}_{\mathbf{k}}^{ij}) \ ,$$

where we have defined $x_{\mathbf{k}}^{ij} = |\mathbf{x}^i - \mathbf{x}^j - L\mathbf{k}|$, while $V_{ij}(\mathbf{x}) = e_i e_j/|\mathbf{x}| + V_{ij}^{phen}(\mathbf{x})$. Here L is the side of the working cell, $\mathbf{k}$ a vector with integer components. More details can be found in the papers cited above.

2.2 The results for the realistic ionic–crystal model

We start with the results for the realistic model, which are collected in Figure 1, for two different initial conditions: classical FPU type (left) and Tsallis type (right), in the sense described a few lines below. The figures report the histograms of the normalized mode energies (i.e., their energies divided by the specific energy) at three different times, increasing from top to bottom, and exhibit how a Maxwell–Boltzmann distribution is attained for sufficiently long times. In the left column the initial condition is of the classical FPU type, i.e. with only a few low–frequency modes equally excited and random phases, and vanishing energy to the remaining modes (actually, the exited modes were all the ones having a frequency less than 100 cm^{-1}, in number of 94 out of the total number 12288 of modes). In the right column, instead, the initial data are generated according to a Tsallis distribution (with $q = 1.4$ and $1/\beta = 100$ K) for the energies, with random phases (the reason for such a choice of the parameters will be explained below). In both cases one has $N = 4096$, while the specific energy is $k_B T$ with $T = 537$ K (left) and $T = 501$ K (right).

In the left column (FPU–type initial data) a rather impressive result is already exhibited in the top panel. Indeed the panel corresponds to a time of just five integration steps (each of 2 fs), and it shows that, at such a very short time, the high energies remain essentially gathered at the right side, whereas the small energies constitute a separate group, and are already distributed pretty well according to a Tsallis law. Such an early occurring of a

Tsallis distribution seems to be an interesting nonequilibrium phenomenon, which was unknown to us. The central panel shows how at a subsequent time of 0.2 ps the two groups of energies (the small energies and the large ones) start merging, so that the Tsallis fit, which is based just on the low energies, now (at $q = 1.21$) fails in the tail. Eventually, at time 50 ps, the histogram is very well fitted by the Maxwell–Boltzmann distribution. So, the small discrepancy of the Tsallis fit at the intermediate time is just a peculiarity of the particular nonequilibrium initial condition chosen.

It is thus quite natural to ask what occurs when the initial energies are selected according to a Tsallis distribution. This is exhibited in the right column, where the parameters of the initial Tsallis distributions were taken equal to those of the early Tsallis distribution found for FPU-type initial data (upper panel of left column). The results reported in the right column show that in such a case there exists a time–invariance property, because the distribution actually evolves within the Tsallis two–parameter family. Notice that a very good fit with a Maxwell–Boltzmann distribution is already attained at $t = 20$ ps. This is at variance with the case of initial conditions of FPU type (left), which requires a longer time (50 ps). The reason is that the Tsallis initial conditions do not involve two different groups of energies. An evolution within the Tsallis family is in agreement with results available in the literature, and seems to be here exhibited in a particularly neat way.

2.3 The results for the classical nearest–neighbor FPU model

We report now, summarized in Figure 2, the results for the classical nearest–neighbor FPU model. We consider a system of $N = 32768$ particles with fixed ends, and we initially excite a packet of low frequency modes, which contains the 512 lowest ones, with equal energies and random phases. The specific energy was fixed at $\varepsilon = 0.0316$, a value for which the equipartition time, according to the paper [17], is of order of $5 \cdot 10^2$. We will consider here larger times because, obviously, the occurrence of a single distribution for the energies of any frequency, implies equal mean energy for all frequencies, i.e., equipartition.

In Figure 2 we give, in the different panels corresponding to increasing times, the distributions of the normalized energies of the modes which were not initially excited. The upper panel refers to the distribution after $1.25 \cdot 10^5$ integration steps (which, with our choice of the integration step, amounts to $t \simeq 10^3$), the central panel refers to a time of 10^6 integration steps ($t \simeq 8 \cdot 10^3$), and the lowest one to $8 \cdot 10^6$ integration steps ($t \simeq 6.4 \cdot 10^4$).

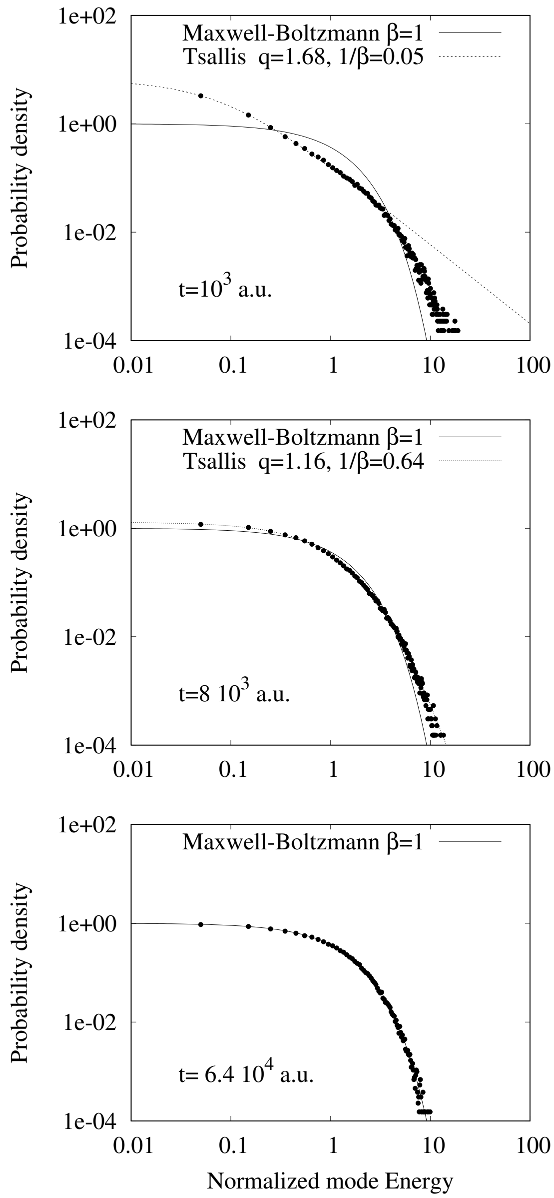

Figure 2: Same as Figure 1 for the classical nearest–neighbor FPU model. Initial condition with a few low–frequency modes excited. The histogram refers only to the energies of the modes that were not initially excited. The results are similar to those of the long–range realistic model, apart from some details, discussed in the text. Number of particles $N = 32768$. Number of initially excited modes: 512. Specific energy $\varepsilon = 0.0316$.

Each histogram was obtained using the data of four different trajectories, corresponding to different random choices of the phases of the excited modes.

The upper panel shows that at a short time the energy distribution is well fitted by a Tsallis one, apart from the high–energy tail, namely apart from energies larger than 3 times the specific energy, which appear to be exponentially distributed. As time increases, the crossover energy increases, and at a certain time (central panel) a Tsallis distribution fits well the histogram over the whole energy range. Such a distribution eventually becomes a Maxwell–Boltzmann one, as shown in the bottom panel.

The results are thus essentially similar to those of the realistic long–range case, apart from the fact that the occurrence of a Tsallis distribution requires a larger time scale. This is due to a fact that was observed since the first works on the FPU model. Namely, that for standard FPU–type initial conditions the dynamics builds up a rather stable low–frequency packet, in which the energies of the modes decay exponentially for increasing frequencies (see for example Table I of the paper [18]), so that the energy distributions too present an exponential tail persisting for rather long times. This fact seems to explain the crossover between the Tsallis distribution for the low energies and the exponential tail of the high energies, a crossover that shifts towards the large energies as time increases. Thus, at variance with the realistic long–range case, at very short times the Tsallis distribution should occur here too, but only for a very small range of low energies.

3 Conclusions

In the present paper two points were addressed. The fist one, which complements a result briefly sketched in [12], is that Tsallis distributions relative to mode energies occur in an extremely realistic model of a ionic crystal (entailing long range Coulomb interactions). Thus Tsallis distributions should be considered to represent actual features of atomic physics.

The second point concerns mode energy distributions for the classical FPU system. Motivated by previous studies on the statistics of the return times [14], we found Tsallis distributions for the latter model too, although presenting some peculiarities related to the 1d character of the classical model. In fact, the occurrence of Tsallis distributions for local observables in the classical FPU model had already been reported about ten years ago [9]. In any case, all these results confirm the thesis already proposed by Tsallis himself [15], namely, that the relevant dynamical feature for the occurring of Tsallis distributions should be lack of full chaoticity. In particular, they are thus expected to occur in systems presenting long–range interactions.

Acknowledgments

Funding: research carried out with the support of resources of Big&Open Data Innovation Laboratory (BODaI-Lab), University of Brescia, granted by Fondazione Cariplo and Regione Lombardia.

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