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

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Abstract

In Statistical Mechanics, Tsallis distributions were apparently conceived in connection with systems presenting long–range interactions. In fact, they were observed in numerical computations for models of such a type, as occurring in the approach to equilibrium, i.e., to a Maxwell–Boltzmann distribution. Here we exhibit two apparently new results. The first one is that Tsallis distributions occur also 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. Thus such distributions may be expected to be actual physical features of crystals. The second result is that Tsallis distributions occur in the standard short–range FPU model too, so that the presence of long–range interactions is not a necessary condition for Tsallis distributions to occur. In fact, this is in agreement with a previous result of the first author in connection with the statistics of return times for the classical FPU model. We thus confirm the thesis advanced by Tsallis himself, 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 to long–range systems.

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

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

which reduces to the Maxwell–Boltzmann distribution $Ce^{-\beta E}$ in the limit $q \to 1$. Distributions of such a type were apparently conceived as being suited for 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 very 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, namely, to equilibrium.

In the present paper we illustrate two apparently new results concerning Tsallis distribution for systems of FPU type. At variance with the mentioned works, our results concern distributions of the normal–mode energies rather than distributions of the particle energies (or momenta). Curiously enough it seems that, apparently, investigations for distributions of normal–mode energies in FPU–type systems were never performed in the more than seventy years elapsed since the original FPU work.

The first result is that Tsallis distributions converging to a Maxwell-Boltzmann one are met also for the normal–mode energies of a realistic 3–d FPU–like model. We are referring to an ionic crystal model (actually, a LiF model) with Coulomb long–range interactions (see [7, 8, 9]), which has such a realistic character as to reproduce in an impressively good way (and indeed within a classical frame) the experimental infrared spectra. An agreement between experimental data and theory over 9 orders of magnitude for the infrared spectra of LiF, is exhibited in the first two figures of the paper [8]. So the present result seems to
indicate that Tsallis distributions may be actual physical features of crystals.

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 \cite{10}. In such a frame, already ten years ago it was pointed out by the first author \cite{11} 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 model.

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. The thesis is thus that Tsallis distributions show up in dynamical systems which are not fully chaotic. In particular such a class is well known to contain long–range systems in the thermodynamic limit. So the present work seems to support the thesis advanced by Tsallis himself, namely, 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 \cite{12}, page 151). In other words, the original idea that Tsallis distributions show up in long–range systems is correct, but it is the much more general property of presenting only partially chaotic motions, that plays the relevant role.

The new numerical results are illustrated in the next section and some concluding remarks then follow.
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: initial condition of FPU type (left) and of Tsallis type (right). 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).
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 [13]) 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 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 [7] 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 [8, 9]. In the end, the Hamiltonian reads

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

where we have defined $x_{ik}^{ij} = |x^i - x^j - Lk|$, while $V_{ij}(x) = e_ie_j/|x| + V_{phen}(x)$. Here $L$ is the side of the working cell, $k$ 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). The figures report the histograms of
the normalized mode energies (i.e., their energies divided by the spe-
cific 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, with only a few low–frequency modes equally
excited with random phases, and vanishing energy to the remaining
modes (actually, all the modes 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 condition is of Tsallis type (with $q = 1.4$
and $1/\beta = 100$ K). 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 impressi-
result is already exhibited in the top panel. Indeed the panel corre-
sponds 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 gath-
ered 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 immediate 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 ener-
gies, 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
themselves are extracted according to a Tsallis distribution. This is
exhibited in the right column, which shows 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, which is at variance with the case of initial conditions
of FPU type (left), that 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.
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 $\varepsilon = 0.0316$. 
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 [14], 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 the figure we report, 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 ($t \simeq 6.4 \cdot 10^4$). 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 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 [15]), 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. In conclusion, at variance with the long–range case, at very short times the Tsallis distribution should occur here too, but only for a very small range of low energies.

Anyhow, long–range interactions seem not to be necessary for the occurring of Tsallis distributions evolving towards a Maxwell–Boltzmann distribution. Moreover, another interesting fact is that the attainment of equipartition does not guarantee the attainment of equilibrium (see also [16][17]).

3 Conclusions

The main result of the present paper seems to be that Tsallis distributions are observed during the approach to equilibrium for the normal–mode energies of FPU–like systems, not only in the case of long–range interactions for which they were apparently conceived, but also in the case of short–range interactions, albeit with some peculiar features in the latter case. Such a result might have been expected, on the basis of previous results for the statistics of return times in dynamical systems, obtained in the frame of the dynamical foundations of statistical mechanics. From such results it is confirmed that the relevant dynamical feature for the occurring of Tsallis distributions should be lack of full chaoticity, which is the thesis advanced by Tsallis himself, for example in [12].

A final comment concerns a metastability phenomenon for which indications were given in previous works in the long–range case (see for example ref. [2]). Namely, the function $q = q(t)$ would present a plateau, and moreover the length of the plateau would strongly increase for increasing $N$. This is a very interesting perspective, but the results available to us in the realistic model are not yet sufficiently clear in this connection.

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