Metastable states in the FPU system

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In this letter we report numerical results giving, as a function of time, the energy fluctuation of a Fermi–Pasta–Ulam system in dynamical contact with a heat bath, the initial data of the FPU system being extracted from a Gibbs distribution at the same temperature of the bath. The aim is to get information on the specific heat of the FPU system in the spirit of the fluctuation–dissipation theorem. While the standard equilibrium result is recovered at high temperatures, there exists a critical temperature below which the energy fluctuation as a function of time tends to an asymptotic value sensibly lower than the one expected at equilibrium. This fact appears to exhibit the existence of a metastable state for generic initial conditions. An analogous phenomenon of metastability was up to now observed in FPU systems only for exceptional initial data having vanishing Gibbs measure, namely excitations of a few low–frequency modes (as in the original FPU work).

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The Fermi–Pasta–Ulam system, i.e. a chain of particles interacting through (nearest–neighbour) weakly non–linear forces, was introduced (see [1]) with the aim of clarifying a fundamental problem in statistical mechanics, namely to understand how quickly is equilibrium attained (the so–called “rate of thermalization”). The state of the art can be summarized as follows. By numerical simulations with excitations of a few low–frequency modes, it was found that equipartition of the (time–averaged) mode energies, which is predicted by equilibrium statistical mechanics, is attained rather quickly if the initial energy is above a certain threshold. Below such a threshold one finds instead (see [2]), a quick relaxation to a state in which equipartition of energy obtains only within a packet of low–frequency modes, with an exponential tail towards the high–frequencies. The time needed for the formation of such a packet is found to increase as an inverse power of the specific energy as the latter is diminished. The subsequent evolution to the final equilibrium state (with full equipartition) is expected to occur on a much longer time scale, displaying a totally different dependence, possibly of exponential type, on inverse specific energy. Semi–analytical and numerical indications were first given in [3], and later confirmations were given for example in [4]. So, at low enough temperatures the system behaves as if it had attained a final equilibrium, although it is actually being in a kind of metaequilibrium state, somehow analogous to the familiar ones of glasses.

Now, the set of initial data with excitations of a few low–frequency modes, which are the ones dealt with in the above–mentioned results, is statistically irrelevant in the thermodynamic limit, being exceptional with respect to the Gibbs measure. So there naturally arises the question whether an analogous phenomenon of metaequilibrium occurs also for typical initial data, so as to be relevant for the foundations of Statistical Mechanics. On the other hand, typical initial data imply by definition equipartition of energy, so that it not clear which quantity should be observed in order to test whether a metaequilibrium state rather than an equilibrium one is being attained. In the present paper we propose a concrete quantity which is suitable to this end. Moreover, we report the results of some numerical computations, which appear to indicate that metaequilibrium states actually occur in a FPU system for typical initial data at low enough temperatures.

To this end, we make reference to the formula relating equilibrium specific heat and temporal energy fluctuations according to the fluctuation–dissipation theorem, namely

\[ \lim_{t \to +\infty} <(E(t) - E(0))^2>_T / (2NT^2) = C_V(T). \]  (1)
Here one considers a system in dynamical contact with a heat bath at a given temperature $T$, and $E(t)$ is the system’s energy at time $t$: furthermore, $< \cdot >_T$ denotes Gibbs average over the initial data at the same temperature $T$, while $C_V(T)$ is the corresponding equilibrium (canonical) specific heat (with the Boltzmann constant $k_B = 1$).

The quantity that we propose as a suitable observable is then nothing but the function $F(t, T) \equiv < E(t) - E(0) >_T / (2NT^2)$ itself. One should compute it for an FPU system in dynamical contact with a heat bath at temperature $T$, and plot it versus time. Indeed, on the one hand, such a quantity by definition makes reference to typical initial data. On the other hand, when plotted as a function of time, it starts up from zero and should attain, after a certain relaxation time, the equilibrium value $C_V(T)$. The relaxation time can then be concretely estimated as a function of temperature $T$. Now, one might agree that a metaequilibrium state has been exhibited if, for a given temperature $T$, the quantity $F(t, T)$ as a function of time is found to have relaxed to some definite value, sensibly lower than the equilibrium one. Indeed, in such a case, that value should legitimately be considered as estimating the specific heat which is observed in an actual measurement of time–length $t$.

The FPU system we consider is a chain of $N + 2$ particles of equal mass $m$ with fixed ends, interacting through a first neighbour quartic potential (the so called $\beta$–model); the Hamiltonian is thus (the lower index “f” standing for “free”, as opposed to “tot” used below for “total”)

$$H_f(p, q) = \sum_{i=1}^{N} \frac{p_i^2}{2m} + \sum_{i=0}^{N} \left[ \frac{\Omega^2}{2} (q_i - q_{i+1})^2 + \frac{\beta}{4} (q_i - q_{i+1})^4 \right],$$

with boundary conditions $q_0 = q_{N+1} = 0$, while $\Omega$ and $\beta$ are suitable parameters.

The interaction with a heat bath is modeled as follows. In principle, we think of the heat bath as a perfect gas constituted by a very large number of particles, each of which interacts, via a suitable rapidly decreasing potential, with the leftmost moving particle of the FPU system. Each collision then produces a certain exchange of energy between the body and the heat bath. However, it would be practically impossible to perform the numerical integrations for the resulting very large number of equations of motion. Thus, we choose as a model the related one in which the collisions with all the molecules of a large bath are replaced by the successive collisions with a single gas particle, the initial data of the particle before each collision being extracted from a Maxwellian distribution at temperature $T$; further details are given below. Denoting by $x, p_x$ the position and the momentum of the incoming gas particle, we thus consider the total system with Hamiltonian

$$H_{tot}(p_x, x, p, q) = \frac{p_x^2}{2m} + V(x - q_1) + H_f(p, q).$$

The interaction potential $V$ is taken of the form $V(r) = V_0 \cdot (L/r) \exp(-r/L)$, where $V_0$ and $L$ are the strength and the range respectively of the potential. The quantities $m, V_0$ and $L$ are chosen as units of mass, energy and length respectively, while the parameters $\Omega$ and $\beta$ are determined by a power expansion about the equilibrium point of a Lennard-Jones potential having $V_0$ as depth and $L$ as range. In this way, the unusual values $\Omega = 20$ and $\beta = 3600$ are obtained.

Concerning the initial data of the gas particle, for the position we take $x_o = 20 L$ (so that the initial interaction potential is negligible), while the momentum $p_{x_0}$ is extracted at random according to a Maxwellian distribution at a given temperature $T$. More precisely, it is well known that the constraint on the initial position requires a correction factor for the Maxwellian: in fact, the velocity has to be extracted from a distribution with density $\rho(p_x) = C p_x \exp(-p_x^2 / 2mT)$, with a normalization constant $C$. Concerning the initial data for the FPU system, they are extracted from a Gibbs distribution at temperature $T$, with reference to the full anharmonic Hamiltonian $H_f$ involving the quartic terms. The technical way in which this was implemented is described below.

Having thus chosen the initial data in the said way, the equations of motion corresponding to the total Hamiltonian $H_{tot}$ are integrated by the leap–frog method, and the collision is considered to have terminated when the position of the gas particle becomes again equal to $x_o$. At such a moment we read the value $E$ of the energy of the FPU system. We iterate the procedure by extracting each time a new random velocity for the incoming particle, while the data for the FPU system are left unchanged, i.e. the initial FPU data for the new collision are just equal to the final ones of the previous collision. Thus one obtains a sequence $\{E_n\}$ of energy values, and the exchanged energy up to “time” $n$ is then $(\Delta E)_n \equiv E_n - E_0$, where $E_0$ is the initial energy. In order to estimate the quantity $< (E_n - E_0)^2 >_T$ which appears in (1), one has to repeat the above procedure.

![Specific heat versus temperature](image_url)
a sufficient number $K$ of times, each time choosing the initial data for the FPU system at random from a Gibbs distribution at temperature $T$. Thus, one has $K$ initial energies $E_0^i$, $i = 1, \ldots, K$, and $K$ energy sequences $\{E_n^i\}$, each one corresponding to $n$ collisions, and finally one sets $\langle (E_n^i - E_0^i)^2 \rangle_T = \sum_{i=1}^K (E_n^i - E_0^i)^2 / K$.

An example of the results obtained in such a way is illustrated in Figure 1, where the quantity $\langle (E_n - E_0)^2 \rangle / 2NT^2$, which from now on will be called the “energy fluctuation” (but might rather be called mean squared “energy jump”) is plotted versus the number $n$ of collisions. The figure corresponds to the case of a FPU system with $N = 100$ moving particles, at temperature $T = 1$ (in our units), with $K = 640$. One sees that the energy fluctuation starts up growing from 0, and after a number $n \approx 3 \cdot 10^4$ of collisions appears to have attained an asymptotic value $\approx 0.95$. We recall that, for a purely quadratic FPU Hamiltonian, the equilibrium value of $C_V(T)$ is independent of temperature and equal to 1. To decide whether the observed “final value” agrees with the predictions of equilibrium statistical mechanics, the canonical value of $C_V$ at $T = 1$ corresponding to the full anharmonic FPU system $H_f$ has to be evaluated.

In order to illustrate how this was performed, we start describing how the anharmonic contribution was taken into account in the related problem of extracting the initial data according to the Gibbs distribution proportional to $\exp(-H_f(p, q)/T)$. To this end we make use of the so called “rejection method”. Namely, we start considering only the quadratic part (say $H_2(p, q)$) of the FPU Hamiltonian $H_f(p, q)$, because in such a case the normal modes are distributed as independent gaussian variables. Having extracted the values for the normal modes according to the harmonic Hamiltonian, we then read the numbers $E_0 = H_f(p, q)$ and $\tilde{E}_0 = H_2(p, q)$. The values are rejected if, having chosen at random a value $z$ in $(0, 1)$, one has $z > \exp((\tilde{E}_0 - E_0)/T)$, while they are accepted in the opposite case. The sequence of accepted values is known to be distributed according to a density proportional to $\exp(-H_f(p, q)/T)$. In this way we are also able to numerically evaluate the canonical specific heat for the full Hamiltonian $H_f$, by just evaluating at each temperature $T$ the standard deviation of the distribution and using the familiar canonical formula relating standard deviation and specific heat.

The results of such a procedure are reported in Fig-
The best fit gives $A_T$ reported. First we considered a temperature larger than temperatures; the above mentioned interpolations are also relaxed to a smaller value than at $T = 1$. The dynamical energy fluctuation reported in Figure 1 actually turns out to be so steep, that we cannot afford to approach the harmonic equilibrium value is followed also by the dynamical asymptotic value at $T = 0.1$, as the results of Figure 5 show. One will notice that the computations were performed in such a case only for a rather short time. The reason was that the computer times become formidable with decreasing temperatures. So we decided that the indications available at $T = 0.1$ were sufficient, and concentrated our attention to the case $T = 0.05$, with a run that, as mentioned above, took one month of computation. The results were however quite rewarding. Indeed, here too a rather good approach to some asymptotic value is obtained. But there is however an inversion in the trend of the asymptotic value because the present one, instead of being still nearer to 1, turns out to have sensibly diminished, being $\simeq 0.75$.

We interpret this result as a strong indication that a metastable state has been attained. Indeed here too, in analogy with the case of initial excitations of a few low–frequency modes, we may expect that the energy fluctuation will eventually attain the equilibrium canonical limit. But the results of Figure 5 suggest that at $T = 0.05$ the final relaxation would require a number of collisions much larger than $n_0(T)$. In other terms, the time–scale to the final equilibrium is expected to be much larger than the one leading to the relaxation observed here. Such an occurring of (at least) two different time–scales indeed is a characteristic feature of metastability phenomena. Our numerical results thus appear to be a direct indication that, below a certain critical temperature ($T = 0.05$ in our units), two time–scales, and thus a metastability phenomenon, do show up for initial data of full measure, in connection with measurements of the specific heat. For a previous indication see [7]. It would now be interesting to explore the region of lower temperatures. The situation is however rather hard, because unfortunately, as typical of all metastability phenomena, the critical temperature also constitute an actual bound for possible numerical experiments.

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