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(Article begins on next page)

Chopping time of the FPU α-model

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November 24, 2017

Abstract

We study, both numerically and analytically, the time needed to observe the breaking of an FPU α-chain in two or more pieces, starting from an unbroken configuration at a given temperature. It is found that such a "chopping" time is given by a formula that, at low temperatures, is of the Arrhenius-Kramers form, so that the chain does not break up on an observable time-scale. The result explains why the study of the FPU problem is meaningful also in the ill-posed case of the α-model.

1 Introduction

As is well known, the so-called Fermi-Pasta-Ulam (FPU) model was introduced in 1954 [1], and consists in a one-dimensional chain of N identical particles, interacting through a nearest neighbor, non quadratic potential $V(x)$, x denoting the inter-particle distance. The problem FPU were interested in was the characterization of the relaxation path of the system to its micro-canonical equilibrium. Such an issue, known as the FPU problem, is related to, but is not the main focus of our work, and the interested reader is referred, for example, to the recent works [2]–[8].

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In the present paper we deal with the problem of determining the life-time of a chain with pairwise potential $V(x)$ that is not lower bounded. In particular, we study the so-called FPU α-model, i.e. the model with cubic potential

$$V(x) = \frac{1}{2}x^2 + \frac{\alpha}{3}x^3 \quad (\alpha \neq 0) \ , \tag{1}$$

which was among those originally considered by FPU [1] and widespread in the literature of the field since then. As is well known, potentials which are not bounded from below, pose problems from the point of view of both statistical mechanics and dynamics. Indeed, due to the lack of compactness of the constant energy surface, the micro-canonical (as well as the canonical) measure and the global (in time) solution of the equations of motion do not exist, with two unpleasant consequences:

i) the equilibrium thermodynamics of the system is not defined;

ii) the system is expected to (and actually does) blow-up in a finite time.

In fact, the cubic potential (1) displays a potential well of finite height $\Delta E = V(-1/\alpha) = (6\alpha^2)^{-1}$ on the left/right of $x = 0$, and tends to $-\infty$ as $x \to \mp\infty$, according to whether the sign of α is ± 1. This implies that, for total energy values above the threshold ΔE, at least one particle can escape to infinity, causing a local breakdown of the chain. Thus, if one works at fixed specific energy (energy per particle), for a sufficiently large number N of particles the chain breaks down into pieces of finite length, regardless of the specific energy value. Equivalently, if N is very large and one extracts the particle velocities from a Maxwell distribution at temperature $T = 1/\beta$, the kinetic energy of some particles will be larger than ΔE, so that, no matter how small T is, the chain should end up "chopped". On the other hand, there are many numerical studies in the literature, starting from that of FPU, devoted to this problem, where the chain is not observed to break down, and is even observed to reach and persists in a state characterized by quasi equipartition of the energy, at least when one starts with unbroken configurations of the chain and the temperature is small enough.

More in general, we stress that a chain would end up broken with any realistic, short range, interaction potential tending to a constant value out of a well of a finite depth and width, such as the Lennard-Jones and the Morse ones. That is why the study of the *chopping time* (i.e. the time needed to the chain to break up into two or more pieces) is of physical

relevance. Just to make a nontrivial example, think of the DNA dynamics [9, 10] where, if the temperature is low enough, the double helix does not unbind, notwithstanding it should do that by heuristic arguments similar to those reported above. This means that the system remains trapped in an unlikely state on a long term, which also displays analogies with the behavior of glasses; some comments about this point are deferred to the last Section.

Notice that, for the study of the chopping time, the choice of the unphysical FPU α-model is not "odd", but, on the contrary, benefits of certain advantages in numerical simulations, for example a clear cut determination of the blow-up, signaled by an overflow, as shown below. We observe moreover that the potential (1) is the third order expansion of any realistic potential around the minimum point of its attracting well. In this sense, the phenomenology of any chain chopping should be well described by the simple α-model.

The results we found are the following. By suitably choosing random initial conditions (to be specified below in Section 2), we estimate numerically the mean t_c and the standard deviation δt_c of the chopping time as a function of the inverse temperature β of the system, for two different (large) values of the number N of particles. Moreover, a theoretical estimate of the probability distribution of the chopping time is also obtained, which leads to the law

$$t_c = \frac{A}{1-(1-\mathsf{p})^N} = \frac{A}{1-e^{N\ln(1-\mathsf{p})}} \ , \tag{2}$$

where A is the free parameter of the theory, whereas p can be expressed in terms of the complementary error function[1] $\mathrm{erfc}(x)$ as follows

$$\mathsf{p} = \mathrm{erfc}\left(\sqrt{\beta\Delta E}\right) \ . \tag{3}$$

Here β is the inverse temperature of the system (determined by the initial conditions) and ΔE is the height of the potential well. The quantity p, defined in (3), will be shown to be the probability that a local blow-up takes place somewhere in the chain. The theoretical law (2) is plotted against the numerical data in Figure 1 below.

[1] We recall that the complementary error function is defined as

$$\mathrm{erfc}(x) = (2/\sqrt{\pi}) \int_x^{+\infty} e^{-t^2}\, \mathrm{d}t \ .$$

Notice that $t_c \to A$ both in the high temperature limit $\beta\Delta E \to 0$ (which implies $\mathsf{p} \to 1$), and $N \to +\infty$ at any fixed value of $\beta\Delta E$, so that the parameter A has the meaning of expected chopping time in the thermodynamic and/or high temperature limit. On the other hand, if $\beta\Delta E$ is so large that $N\mathsf{p} \ll 1$, one gets the asymptotic behavior

$$t_c \sim \frac{A}{N\mathsf{p}} \sim \frac{A}{N}\ \sqrt{\pi\beta\Delta E}\ e^{\beta\Delta E}\ , \tag{4}$$

i.e. a law of the Arrhenius-Kramers type. In other terms the chopping time increases exponentially fast with the inverse temperature β. This explains why any finite chain (also of a macroscopic size) may remain frozen in an unbroken state, for a sufficiently low (but finite) temperature.

According to the theory, the predicted standard deviation δt_c on the chopping time is

$$\delta t_c = A\ \frac{e^{N\ln\sqrt{1-\mathsf{p}}}}{1-e^{N\ln(1-\mathsf{p})}}\ . \tag{5}$$

Thus, when the chain chopping becomes a rare event ($N\mathsf{p} \ll 1$), the expected chopping time t_c undergoes very large fluctuations, with $\delta t_c \sim t_c$; on the other hand $\delta t_c \to 0$ very quickly in the limit $N \to \infty$ or $\beta\Delta E \to 0$. The theoretical law (5) is plotted against the numerical data in Figure 2 below.

It has to be stressed that, contrary to what might appear at a first glance, the condition $N\mathsf{p} \ll 1$ for the validity of the asymptotic formula (4), is completely meaningful from a physical point of view. Indeed, another way of stating it is $T \ll \Delta E/\ln N$. The latter, if the number of particles in the chain is $N = 10^\gamma$, reads $T \ll \Delta E/(\gamma \ln 10)$, the upper bound ranging from $\Delta E/53$ for ordinary matter ($\gamma = 23$) up to $\Delta E/14$ for a human gene ($\gamma = 6$, the limit numerically explored in the present paper). Thus, in dealing with macroscopic chains of a fixed size, there always exists an observable temperature below which the chain chopping, describing physical phenomena such as melting, denaturation and so on, takes place on extremely long timescales, on average.

Concerning the existing literature on the subject, an Arrhenius-like asymptotic law for the breaking time (or chopping time) of a Lennard-Jones chain has been obtained in [11], where the analysis is grounded in the Kramers method, requiring the use of viscosity and noise, which is different from the conservative case treated here. However, the chain break-down analysis is reduced, from a dynamical point of view, to the two body problem of nearby

particles: we do the same here (adding some probabilistic reasonings). In reference [12], the conservative dynamics of a nonlinear Klein-Gordon chain with on-site cubic (unbounded) potential, has been considered. The results of the latter paper are more qualitative in character, and an Arrhenius-like law can be deduced from the figures reported therein. However, we stress that the cubic Klein-Gordon model is completely different from the FPU α-model considered here: the former (with periodic boundary conditions) admits an exact spatially homogeneous solution, where all the particles oscillate in phase with the same amplitude, and the escape time (or chopping time) is there obtained by studying the exponential growth of slight perturbations of such a state, which leads to a parametric resonance problem; see also [13]. Nothing similar applies to the α-model (the homogeneous solution being simply the equilibrium one). We finally stress that our use of the term *chopping time* (breaking, or escape time in the literature) is consistent with its mathematical definition: it refers to the time the chain takes to breakdown in at least two pieces. Of course, as pointed out in reference [11], the probability that the chain simultaneously breaks down in three or more pieces, i.e. the probability that a blow-up occurs, at the same time, in the dynamics of two or more distinct pairs of particles, is expected to be very small.

The paper is organized as follows. In Section 2 the results obtained by numerical integrating the equation of motions for a system of $N = 65,535$ and one of $N = 1,048,575$ particles are reported, and the agreement with the law (2) for the chopping time is illustrated. Such a law is deduced in Section 3 by considering the dynamics of the chain at discrete time intervals and defining the probability P of chain chopping during each time step. A few plausible hypotheses on such a probability allow then to simply compute the expected chopping time. The constant A appearing in (2) cannot be deduced from the analytic computations, but it is nevertheless estimated by the numerical results of Section 2. Further comments are deferred to Section 4.

2 Numerical computations

To the purpose of numerical integration we have set $\alpha = 0.25(= 1/4)$ in the potential (1). Notice that such a value is by no means special because, by a suitable rescaling of the variables, one can always reduce to this case. Thus,

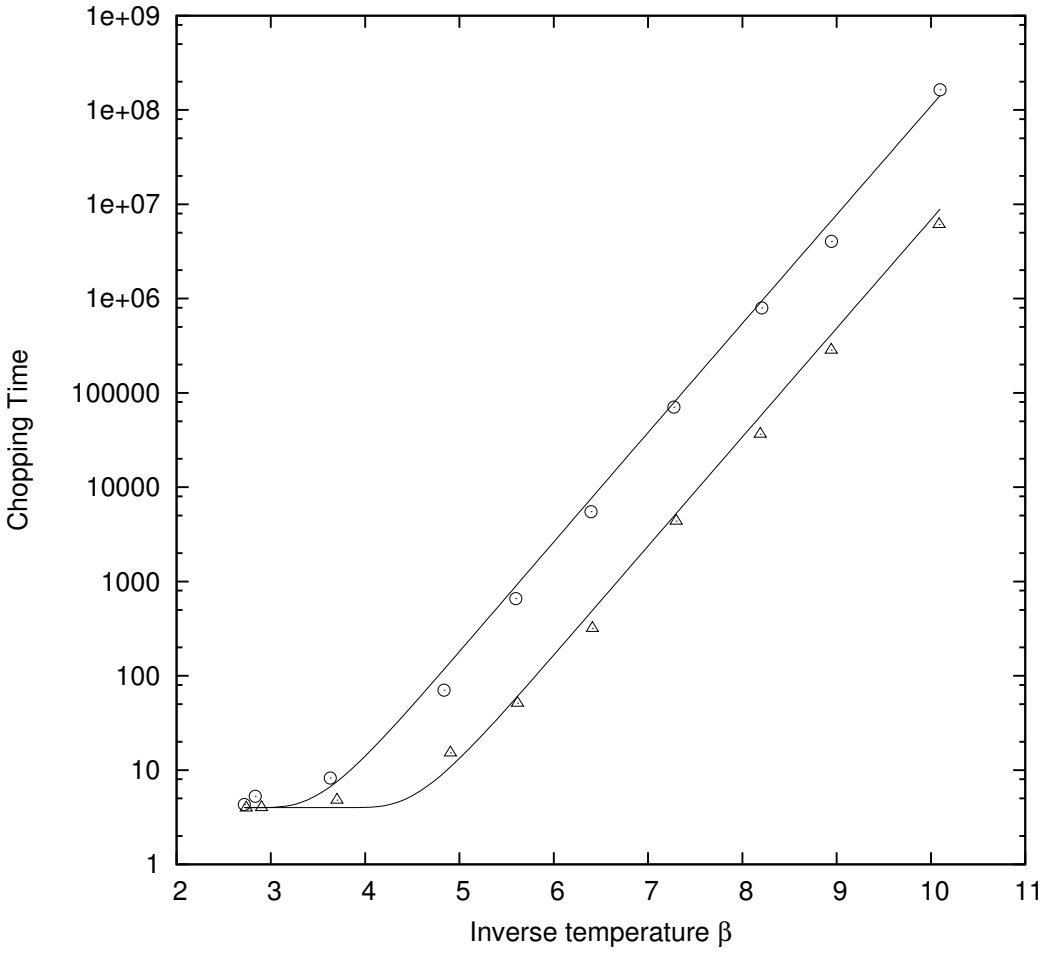

Figure 1: The chopping time t_c, as a function of β, in semi logarithmic scale. Circles refer to $N = 65,535$ particles, while triangles refer to $N = 1,048,575$. Solid lines are the plots of the analytic formula (2) with $\mathsf{p} = \mathrm{erfc}\left(\sqrt{\beta \Delta E}\right)$, $A = 4.0$ and $\Delta E = 2.57$.

the Hamiltonian studied is

$$H = \frac{1}{2}\sum_{j=1}^{N} p_j^2 + \frac{1}{2}\sum_{j=0}^{N}(q_{j+1} - q_j)^2 + \frac{1}{12}\sum_{j=0}^{N}(q_{j+1} - q_j)^3 \ ,$$

with fixed ends: $q_0 = q_{N+1} = 0$. The numerical integration of the equations of motion was performed by using the standard Verlet algorithm [14], with

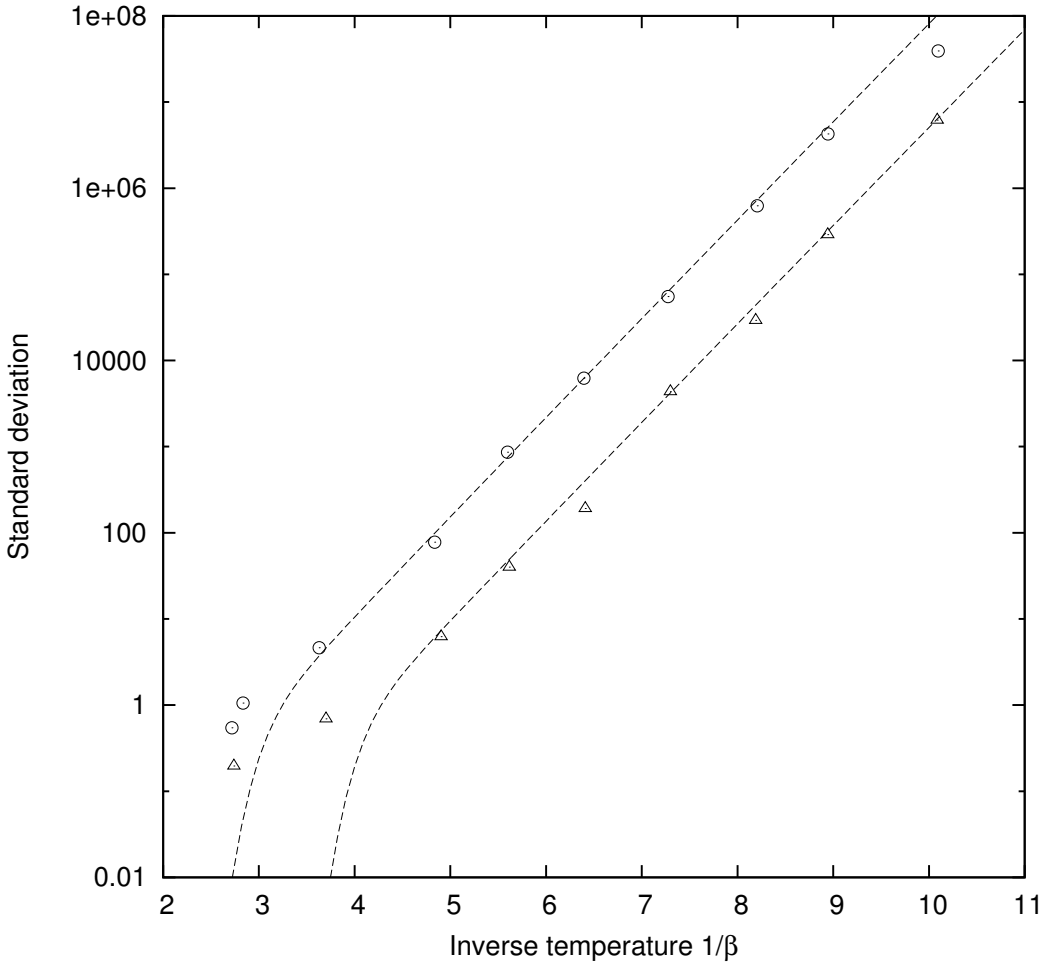

Figure 2: The standard deviation δt_c, as a function of β, in semi logarithmic scale. Circles refer to $N = 65,535$ particles, while triangles refer to $N = 1,048,575$. Dotted lines are the plots of the analytic formula (5), with $\mathsf{p} = \mathrm{erfc}\left(\sqrt{\beta \Delta E}\right)$, $A = 4.0$ and $\Delta E = 2.57$.

a time–step equal to 0.025, which ensures the energy conservation up to a relative error less than 10^{-3} in all the computations performed.

We considered two different numbers N of particles, namely $N = 65,535$ and $N = 1,048,575$ respectively, and specific energy values in the range $0.1 \div 1$. In dealing with such large numbers of particles, care has to be

taken in choosing the initial data, otherwise, in the chosen energy range, the chain is found to be almost immediately chopped. We remark that the chopping phenomenon takes place when the relative distance between a couple of neighboring particles is so large (namely larger than $|-1/\alpha| = 4$) that the force between them is repulsive and the two halves of the chain separate out. For such a reason we decided to set all the initial positions $q_j^0 = 0$, for all $j = 1, \ldots, N$, while the initial momenta p_j^0 are extracted from a Maxwell distribution at inverse temperature β, taking care to reject all those values with a kinetic energy too large. More precisely, if it happens that $\left(p_j^0\right)^2 > \Delta E$, we extract p_j^0 again and again until such a condition no longer holds. In this way, we are sure to start in the (unlikely) state in which the chain is unbroken. Then we begin the numerical simulation, going on with it up to the time $\tilde{t}$ such that

$$q_{j+1}(\tilde{t}\,) - q_j(\tilde{t}\,) < -6 \tag{6}$$

for at least one j. The threshold value -6 for the inter-particle distance is conventionally fixed among the possible ones smaller than the local maximum point $-1/\alpha = -4$. As we have just remarked, when this condition holds, the force between the two particles q_{j+1} and q_j becomes repulsive and the two pieces of the chain move apart from each other. For times longer than $\tilde{t}$ one always gets an overflow error very quickly, because, in our model, the repulsive force grows very fast as the distance increases. This means that there exists a local blow-up time $t_b \in \mathbb{R}$ such that

$$\lim_{t \to t_b^-} \sup_j |q_{j+1} - q_j| = +\infty \ .$$

The local blow-up time time t_b would be the actual chopping time of the chain. However, as just explained above, to all practical purposes, t_b is well approximated by the time $\tilde{t}$ defined by the relation (6), with the obvious advantage of avoiding to stop the computation at the overflow, which in turn allows to implement cyclical runs. Indeed, since the time $\tilde{t}$ (as well as t_b) depends on the initial data, it is a random variable varying from one numerical experiment to the other. As a consequence, we define the *expected chopping time* t_c as the average of $\tilde{t}$ with respect to the initial data. In practice, once fixed the value of the inverse temperature β, one repeats the numerical experiment with a set of M different initial conditions. Then one gets a sample of different values $\tilde{t}_k$, $k = 1, \ldots, M$, and estimates $\tilde{t}$ by the its

(sample) average

$$t_c = \frac{1}{M} \sum_{k=1}^{M} \tilde{t}_k \ .$$

In our simulations we use $M = 25$, which is the largest number we were able to reach with the computational power available.

The result are shown in Figure 1, where we report in semi-logarithmic scale the expected chopping time t_c as a function of β. The exponential behavior becomes evident for values of β larger than about 6. The solid lines are the plots of the formula (2), with $\mathsf{p} = \mathrm{erfc}(\sqrt{\beta \Delta E})$, for the two mentioned values of N and an empirical value $\Delta E = 2.57$, which agrees well with the theoretical one, namely $\Delta E = (6\alpha^2)^{-1} = 2.66$. The value of the constant A (a free parameter in the theory) turns out to be equal to 4.

In the same way, we compute the chopping time (sample) standard deviation δt_c defined by

$$\delta t_c = \sqrt{\frac{1}{M} \sum_{k=1}^{M} (\tilde{t}_k - t_c)^2}.$$

The result, shown in Figure 2, is particularly relevant. The standard deviation is of the same order of magnitude of the average when the chopping of the chain is a *rare event*. In other terms, the fluctuations become very large by decreasing the temperature, as predicted by the formula (5). However, the latter formula does not fit the numerical data at high temperatures. This is possibly due to different reasons; in any case the smallness of the sample prevents to compute small values of standard deviation with accuracy.

We finally stress that the small discrepancy between the optimal numerical value of ΔE and the theoretical one, amounting to about 3%, might partly depend on the fact that $\tilde{t} < t_b$ for any choice of the threshold value for the inter-particle distance, which we have fixed to -6. As a consequence, the chopping time t_c determined numerically turns out to be an underestimate of the true one (the nasty sample average of the overflow times). Another possible cause of such a discrepancy will be discussed at the end of the next Section.

3 Analytic estimate of t_c

Our analytic deduction of formula (2) is based on the following assumptions and reasonings. Let us consider the FPU α-chain with some measure on the initial conditions evolved on consecutive time intervals of length A. Let us call P_k the probability of the event E_k: *chain chopping occurs in the time interval* $\Delta t_k = [(k-1)A, kA]$. As anticipated above, by chain chopping we mean the occurrence of at least one local blow-up, namely the divergence, in a finite time, of at least one of the inter-particle distances $r_n := q_{n+1} - q_n$ to $-\infty$ (obviously, the probabilistic nature of the event E_k is inherited by the evolution in time of the measure chosen on the initial data). One has $P_k = 1 - Q_k$, where Q_k denotes the probability of the complementary event $\complement E_k$: *no chain chopping on the time interval* Δt_k *occurs*. The first simplifying hypothesis is introduced here, assuming that the local blow-up events giving rise to the chain chopping are mutually independent and occur with the same probability for each particle pair. In such a way one can write $Q_k = (\mathsf{q}_k)^N$, q_k denoting the probability that r_n is lower bounded on the time interval Δt_k, for any $n = 1, \ldots, N$. Such a hypothesis of statistical independence is more plausible for free ends or periodic boundary conditions, while for fixed ends (which is the case numerically considered here) some boundary effect is expected, with a vanishing contribution as N gets larger and larger. Now, writing $\mathsf{q}_k = 1 - \mathsf{p}_k$, one gets

$$P_k = 1 - (1 - \mathsf{p}_k)^N = 1 - e^{N \ln(1-\mathsf{p}_k)} \ , \tag{7}$$

where p_k denotes the probability that $r_n \to -\infty$ on the time interval Δt_k, for *some* $n = 1, \ldots, N$. A second fundamental hypothesis is here introduced, assuming that the probability p_k is independent of k, i.e. of the specific time interval Δt_k, depending instead only on its length $|\Delta t_k| = A$. This is clearly a Markov-like hypothesis, equivalent to assume that, up to the occurrence of the first local blow-up, the measure on the initial data is just slightly modified by the flow, so that the probability of local blow-up does not significantly change in the course of time. Thus $\mathsf{p}_k \simeq \mathsf{p}_1$ for any k, p_1 being the probability that a local blow-up occurs (i.e. $r_n \to -\infty$) on the time interval $[0, A]$, i.e. the probability, according to the measure on the initial data, that the local blow-up time is less than A. We shall see below how to compute $\mathsf{p}_1(A)$. The consequence of this second hypothesis is that the probability of chain chopping (7) on any time interval Δt_k is given by

$$P_k \simeq P_1 = 1 - e^{N \ln(1-\mathsf{p}_1)} \ . \tag{8}$$

The latter simplification allows us to get a simple expression for the probability π_n that the chain breaks down for the first time in the n-th time interval $\Delta t_n = [(n-1)A, nA]$ and not before, namely the geometric distribution [15]

$$\pi_n = (1 - P_1)^{n-1} P_1 \ . \tag{9}$$

The (mean) chopping time t_c is then naturally defined as the expected time one has to wait for the occurrence of the first local blow-up of the chain, namely

$$t_c := A\langle n \rangle := A \sum_{n \geq 1} n \pi_n \ . \tag{10}$$

An elementary computation, making use of the properties of the geometric series, yields

$$t_c = \frac{A}{P_1} = \frac{A}{1 - e^{N \ln(1-\mathsf{p}_1)}} \ , \tag{11}$$

which has the form (2). We stress here that the latter formula for the chopping time admits the two following limit expressions. The first one holds if p_1 is kept fixed and $N \to +\infty$, i.e. in the thermodynamic limit. In this case, since $\ln(1-\mathsf{p}_1) < 0$ one gets $P_1 \to 1$ and $t_c \to A$. Such a result is independent of any detail of the system and actually defines the up to now arbitrarily chosen time unit: *A is the chopping time of the infinite chain.* This is a quantity we are not able to compute analytically and is thus left as a free parameter of the theory, to be numerically determined. The other interesting limit of formula (11) is obtained when N is thought of as fixed, though as large as needed, while p_1 is so small that $N\mathsf{p}_1 \ll 1$ (which is possible because p_1 depends on the temperature). In this case one has $P_1 \simeq 1 - e^{-N\mathsf{p}_1} \simeq N\mathsf{p}_1$, and $t_c \simeq A/(N\mathsf{p}_1)$. The latter asymptotic expression is clearly of the form (4) when p_1 is of the form (3). Concerning the variance of the chopping time, it is given by

$$(\delta t_c)^2 := A^2 \left\langle (n - \langle n \rangle)^2 \right\rangle = A^2 \sum_{n \geq 1} (n - \langle n \rangle)^2 \ \pi_n \ . \tag{12}$$

Here again, an elementary computation based on the properties of the geometric distribution (9), yields $\delta t_c = A\sqrt{1 - P_1}/P_1$, so that the standard deviation of the chopping time turns out to be given by

$$\delta t_c = A \ \frac{e^{N \ln \sqrt{1-\mathsf{p}_1}}}{1 - e^{N \ln(1-\mathsf{p}_1)}} \ , \tag{13}$$

of the form (5) when p_1 is of the form (3). Notice that in the limit $N \to \infty$, p_1 being kept fixed, $\delta t_c \to 0$; on the other hand, if $N\mathsf{p}_1 \ll 1$, one gets $\delta t_c \sim t_c$: the chain chopping is a rare event and the fluctuations of the chopping time are comparable with its mean.

We finally pass to the computation of p_1, the probability, according to the measure on the initial data, that a local blow-up takes place in the chain on the time interval $[0, A]$, in order to show that p_1 is given by the expression (3) to a rather good approximation. Obviously, p_1 *is the measure of the initial data such that the local blow-up time is less than* A. In order to define the local blow-up time, let us consider the equations of motion of the FPU α-chain, with the pair potential $V(r) = r^2/2 + \alpha r^3/3$. The evolution equations of the chain in terms of the variables $r_n := q_{n+1} - q_n$ read

$$\ddot{r}_n = V'(r_{n+1}) + V'(r_{n-1}) - 2V'(r_n) \ , \tag{14}$$

whose form is valid for any potential V; as remarked above, we do not discuss boundary effects. Let us consider a specific pair of sites in the bulk, corresponding to $n = s$, where a blow-up event takes place, namely $r_s \to -\infty$ in a finite time. In such a case, under the hypothesis $|r_s| \gg |r_{s\pm1}|$, the main contribution to the force on the right hand side of equation (14) is provided by the last term, and one can consider the isolated two body problem ruled by the equation

$$\ddot{r}_s = -2V'(r_s) \ . \tag{15}$$

The latter equation, describing the relative dynamics of two nearby particles, is the Newton equation of a single particle of mass $1/2$, i.e. the reduced mass of two particles of unit mass, subject to the force $-V'(r)$. The measure on the initial conditions on the particles of the α-chain is

$$d\mu_0 := \left(\prod_{n=1}^{N} \sqrt{\frac{\beta}{\pi}} e^{-\beta p_n^2} \delta(r_n) \right) dr_1 \dots dr_N \ dp_1 \dots dp_N \ , \tag{16}$$

where $p_n = \dot{r}_n/2$ is the relative momentum of two nearby particles and $\delta(x)$ is the Dirac delta-function. The measure (16) corresponds to place all the particles in their equilibrium position with a relative momentum distributed according to the Maxwell-Boltzmann measure at temperature $T = \beta^{-1}$. Now, in the present specific case $V(r) = r^2/2 + \alpha r^3/3$, and exploiting the conservation of energy (at level ε), one easily finds that the blow-up time t_b of

equation (15), with initial condition $r_s(0) = 0$, $p(0) := \dot{r}_s(0)/2 = \pm\sqrt{\varepsilon}$, under the condition $\varepsilon > \Delta E := V(-1/\alpha) = 1/(6\alpha^2)$, is given by the formula

$$t_b(\varepsilon) = \int_{-\infty}^{0} \frac{dr}{2\sqrt{\varepsilon - V(r)}} + \theta(p(0)) \int_{0}^{r_\varepsilon} \frac{dr}{\sqrt{\varepsilon - V(r)}} \ , \tag{17}$$

where $\theta(x)$ is the Heaviside step function, whereas r_ε is the value of the right turning point coordinate, i.e. the (only) root of the equation $V(r) = \varepsilon$. The condition $\varepsilon > \Delta E$ is obvious: the blow-up occurs along the energy level curves that lie outside the homoclinic connection. Notice that the contribution of the second integral to the right hand side of formula (17) exists only when $p(0) = +\sqrt{\varepsilon}$, because in this case the "particle" starts to move to the right, reaches the turning point and then reverses the direction of motion and goes to $-\infty$; see Figure 3.

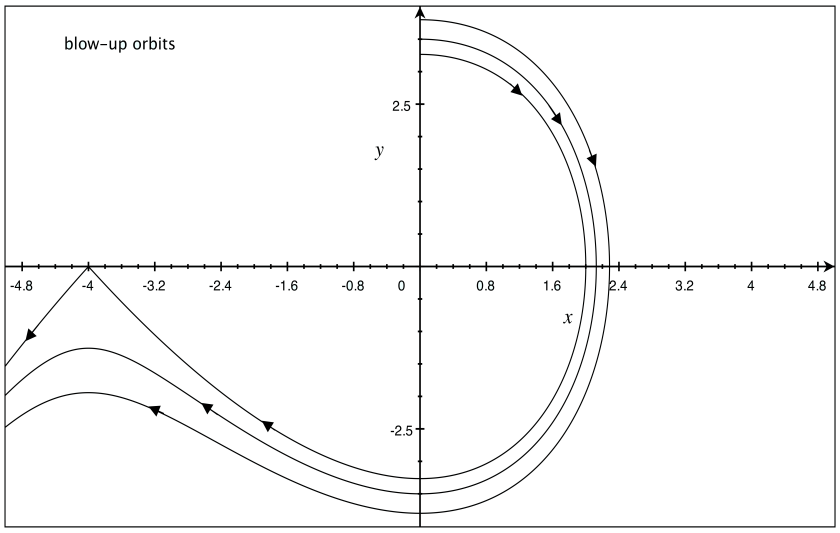

Figure 3: Three phase curves of system (15) corresponding to the initial condition $r(0) = 0$ and $\dot{r}(0) = +2\sqrt{\varepsilon}$. The most internal one corresponds to the homoclinic connection value $\varepsilon = \Delta E = 1/(6\alpha^2) = 2.\bar{6}$. The other two are blow-up curves, corresponding to $\varepsilon = 3.06$ and $\varepsilon = 3.61$.

Now we determine $\mathsf{p}_1(A)$ defined as the probability that $t_b(\varepsilon) < A$ according to the measure (16). Let us observe that the blow-up time t_b, given

by the formula (17), turns out to be a decreasing function of ε. This means that the condition $t_b(\varepsilon) < A$ is equivalent to $\varepsilon > \bar{\varepsilon}(A)$; moreover $\bar{\varepsilon} \to \Delta E^+$ when $A \to +\infty$. Recalling that the energy conservation law for problem (15) reads $p_s^2 + V(r_s) = \varepsilon$, making use of the initial measure (16) at the site of $n = s$, and omitting the site subscript s, one finds

$$\begin{aligned} \mathsf{p}_1(A) &= \int_{\{p^2+V(r)>\bar{\varepsilon}(A)\}} \sqrt{\frac{\beta}{\pi}} e^{-\beta p^2} \delta(r) dr dp = \\ &= \int_{\{p^2>\bar{\varepsilon}(A)\}} \sqrt{\frac{\beta}{\pi}}\, e^{-\beta p^2} dp = \frac{2}{\sqrt{\pi}} \int_{\sqrt{\beta\bar{\varepsilon}(A)}}^{+\infty} e^{-y^2} dy = \\ &= \operatorname{erfc}\left(\sqrt{\beta\bar{\varepsilon}(A)}\right) , \end{aligned} \tag{18}$$

where $\operatorname{erfc}(x) := (2/\sqrt{\pi}) \int_x^{+\infty} e^{-y^2} dy$ is the complementary error function. The relation (18) depends clearly on A. However, on the basis of the previous remark, the blow-up time (17) diverges on the homoclinic connection, which means that

$$t_b(\varepsilon) \sim f(\varepsilon - \Delta E) \tag{19}$$

as $\varepsilon \to \Delta E^+$, where $f(x)$ is a monotonically decreasing function such that $f(x) \to +\infty$ as $x \to 0^+$. As a consequence, if the time step A is large enough, the asymptotic behavior (19) yields an estimate for $\bar{\varepsilon}(A)$, namely

$$\bar{\varepsilon}(A) \sim \Delta E + f^{-1}(A) , \tag{20}$$

for large values of A. In the latter approximation, the deviation of the estimate (20) with respect to ΔE is small, since $f^{-1}(A) \to 0^+$ as $A \to +\infty$. In conclusion, one can reasonably choose $\bar{\varepsilon}(A) \simeq \Delta E$ in (18). As a consequence,

$$\mathsf{p}_1(A) \simeq \mathsf{p} := \operatorname{erfc}\left(\sqrt{\beta\Delta E}\right) , \tag{21}$$

which motivates the formula (3). Concerning the asymptotic expansion of p when $\beta\Delta E$ is large, this is readily obtained by the change of variable $y^2 = \varepsilon$, which yields

$$\begin{aligned} \mathsf{p} &= \frac{2}{\sqrt{\pi}} \int_{\sqrt{\beta\Delta E}}^{+\infty} e^{-y^2} dy = \frac{1}{\sqrt{\pi}} \int_{\beta\Delta E}^{+\infty} \frac{e^{-y}}{\sqrt{y}} dy = \\ &= \frac{1}{\sqrt{\pi}} \left[\frac{1}{(\beta\Delta E)^{1/2}} - \frac{1}{2(\beta\Delta E)^{3/2}} + O((\beta\Delta E)^{-5/2}) \right] e^{-\beta\Delta E} , \end{aligned} \tag{22}$$

which explains formula (4). The approximation of large A (whose actual numerical value is 4) is checked to hold a fortiori, by the good agreement of the theoretical formulas with the numerical data.

As already stressed at the end of the preceding Section, we find that the value of ΔE best fitting the numerical data in Figure 1 is $\Delta E = 2.57$, which is a bit lower than the theoretical one, namely 2.66. In addition to what remarked there, we here observe that the probability density of the r_n's is a delta function just at time $t = 0$. At later times, the average density will be some function $g(r)$ localized about $r = 0$. As an example, just to get an idea of the behavior of the above integral, one can consider the simple case of a constant density $g(r) = 1/(2\eta)$ inside the interval $[-\eta, \eta]$, and $g(r) = 0$ outside it, with $0 < \eta \ll 1$. In this case, the formula (18), in the limit $A \to +\infty$, becomes

$$\begin{aligned}
\mathsf{p}(\beta) &= \int_{\{p^2+V(r)>\Delta E\}} \sqrt{\frac{\beta}{\pi}} e^{-\beta p^2} g(r) dr dp = \\
&= \sqrt{\frac{\beta}{\pi}} \int_{\Delta E}^{+\infty} e^{-\beta\varepsilon} \left(\int_{-\infty}^{+\infty} e^{\beta V(r)} \frac{g(r)}{\sqrt{\varepsilon - V(r)}} \right) d\varepsilon \simeq \\
&\simeq \sqrt{\frac{\beta}{\pi}} \int_{\Delta E}^{+\infty} \frac{e^{-\beta(\varepsilon-\eta^2/2)}}{\sqrt{\varepsilon - \eta^2/2}} \, d\varepsilon = \mathrm{erfc}(\beta(\Delta E - \eta^2/2)) \ .
\end{aligned}$$

Thus, to the oscillation of the particles around their (initial) equilibrium position, there corresponds a lower value of the effective height of the energy barrier, as physical intuition would suggest.

4 Final comments

In the sequel, three issues related to the subject of the present work are discussed.

Concerning the dependence of the chopping time of the α-model on the initial conditions, in the present work we limited ourselves to consider "crystal-like" configurations, in order to start from a simple, unbroken state of the chain. The latter condition would be of course ensured by other interesting initial conditions. As an example, one might consider the initial excitation of one or a few long-wavelength Fourier modes, as traditionally done in the literature, from the original paper [1] on. As is well known,

in such a case, if the specific energy of the chain is small enough, no chain chopping is observed, and the system seems to behave as predicted by a micro-canonical statistics (which, we stress it once again, does not exist); see e.g. [3]. A qualitative explanation of the widespread lack of observed chain chopping of the FPU α-model in the literature goes as follows. One first observes that chain chopping may take place only when a considerable fraction of the energy has been transferred to shortest wavelength modes, so that at least one among the differences $q_{n+1} - q_n$ can become large and give rise to a local blow-up (the same differences are very small when only long wavelength modes are excited); as is well known, such an energy cascade leading to energy equipartition requires long times at low energies. When the system has reached a state of energy equipartition, so that a kind of temperature, identified with two times the mean kinetic energy per particle, can be defined, the theory here developed might apply. The consequence would be that, for such long-wavelength initial conditions, the chopping time can become so long to be unobservable. More specific estimates on this point are left to a future work.

The estimate here provided for the chopping time, could also be useful in the case of glasses. In the glassy state, one usually assumes that the microscopic dynamics remains trapped in a region of phase space, corresponding to the glass phase, without entering the "Boltzmann sea" corresponding to the crystal and/or the fluid phase. In fact particles are thought of as frozen in the local minima of the potential, being able to jump out only after a huge amount of time. A simple one–dimensional model in which this happens is described in paper [16]. We are hopefully thinking to adapt the present analytic treatment to the study of glasses.

Finally, we shortly discuss the possibility to approach the chain chopping problem with the theory developed by Kramers [17]. A possible line of reasoning is the following. The pair of particles where the chain breaks down is not an isolated system, being subject to the influence of the rest of the chain. According to the picture emerging from the famous work by Ford, Kac and Mazur [18], one may suppose that the rest of the chain acts on that pair of particles as an effective thermal bath, giving rise to a Langevin dynamics of their relative displacement. In such a case one would deal with what is known in the literature as a *Kramers problem*, namely the estimate of the escape time of a Brownian particle from a potential well (see [19] for a review on the subject). The rate w of escape over the potential barrier, first com-

puted by Kramers [17], turns out to be given by an Arrhenius-like formula: $w \propto e^{-\beta \Delta E}$, where $\beta = 1/T$ is the inverse temperature of the thermal bath (here proportional to the mean kinetic energy of the chain) and ΔE is the height of the potential barrier. On the other hand, in a chain of N sites, the rate of chain chopping would be $Nw \propto Ne^{-\beta \Delta E}$, whose inverse gives the chopping time, namely formula (4) up to a small correction (at small temperature). However, in so reasoning, one meets a major difficulty. Indeed, in the quoted work [18], a linear chain with a rather special frequency spectrum is considered, namely the only one rigorously leading, in the thermodynamic limit, to a Langevin equation for the the single particle with constant damping coefficient and gaussian noise. That deduction does not work for nearest neighbors potential, and an extension of those results to the FPU models is not known to us.

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