Symposium On Fractional Signals and Systems

IPC, Coimbra, Portugal
4 - 5 November 2011

Some Notes About the Fermi-Pasta-Ulam Problem

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1. Introduction

During 1953, at Los Alamos, Fermi, Pasta and Ulam (FPU) developed computer simulations of a mechanical system composed of masses and springs [1]. We should also refer Mary Tsingou that helped in the programming of the computer Maniac. The idea formulated by Enrico Fermi was to simulate the one-dimensional analogue of atoms in a crystal by mean of a chain of particles linked by springs fixed at the extreme points. The springs were modeled by a term following a linear model (Hooke's law) and a nonlinear term either quadratic (FPU - α), or cubic (FPU - β). These researchers found a dynamics considerably different from what linear systems would suggest. In fact, they thought that the system would exhibit "thermalization", that is, a behavior in which the influence of the initial modes of vibration would fade, becoming all modes excited equally. Nevertheless, the simulations revealed a complex quasi-periodic dynamics. They thought that the energy introduced into the first frequency mode (k = 1) should drift to the other modes until the equipartition of energy would be reached. For the first instants of the simulation the higher modes (k = 2, 3,…) were successively excited, reaching almost an equipartition state, but after some time they verified that almost all energy was back to the first mode. Further simulations revealed the repetition of this phenomenon and that a kind of recurrence emerges, being recovered replicas of the initial state [2-4].
The FPU experiment marked the beginning of the nonlinear physics and the age of computer simulations for analyzing scientific problems. It triggered important questions and motivated a huge volume of research during the last six decades [5-23].
The main goal of this paper is to address the FPU dynamics in the perspective of Fractional Calculus (FC). FC goes back to the beginning of the theory of differential calculus and deals with the generalization of standard integrals and derivatives to a non-integer order [24-26]. A wide range of potential fields of application are possible [27-35], but until recently, FC was considered an "exotic" mathematical tool, being present day interest due to the important developments in the area of nonlinear dynamics and chaotic systems. FC captures long range phenomena that are overlooked by standard differential calculus. Therefore, this property makes FC a natural tool for analyzing the dynamical phenomena that occur in the PFU problem.
Having these ideas in mind, section 2 formulates the problem, the adopted tools and algorithms and compares the results for integer and fractional order elements in the mechanical chain. Finally, section 4 draws the main conclusions.

2. A Fractional Perspective of the FPU Dynamics

We start by formulation the initial system designed by Fermi, Pasta and Ulam. The FPU - α and FPU - β equations of motion for N masses (Fig. 1) is:

$$\ddot{x}_n = (x_{n+1} - x_n) - (x_n - x_{n-1}) + \alpha\left[(x_{n+1} - x_n)^2 - (x_n - x_{n-1})^2\right] \tag{1a}$$

$$\ddot{x}_n = (x_{n+1} - x_n) - (x_n - x_{n-1}) + \beta\left[(x_{n+1} - x_n)^3 - (x_n - x_{n-1})^3\right] \tag{1b}$$

where $1 \le n \le N$ is the index representing each mass and the fixed extremes are represented by $n = 0$ and $n = N + 1$. For the string k-th mode the sum of the kinetic and potential energies is given by:

$$E_k = \frac{1}{2}\left(\dot{A}_k{}^2 + \omega_k{}^2 A_k{}^2\right) \tag{2}$$

where A_k is related to the displacements by the expression:

$$A_k = \sqrt{\frac{2}{N+1}} \sum_{n=1}^{N} x_n \sin\left(\frac{nk\pi}{N+1}\right) \tag{3}$$

and frequencies:

$$\omega_k = 2\sin\left(\frac{k\pi}{2(N+1)}\right) \quad (4)$$

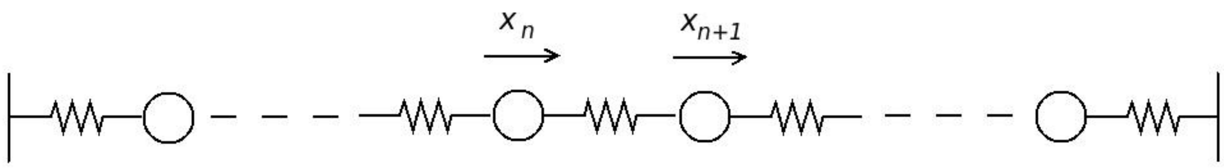


Figure 1 The mechanical system of the FPU problem.

During the simulations it is adopted a Runge-Kutta 4 numerical integration with time step $dt = 10^{-2}$ sec, $N = 32$ and the initial conditions formulated by Fermi, Pasta and Ulam, namely $x_n(0) = \sin\left(\frac{n\pi}{N+1}\right)$, $\dot{x}_n(0) = 0$.

Figure 2 depicts a typical time evolution of $E_k(t)$, $k = \{1, \cdots, 6\}$, for the FPU – α for a period of time of 10^4 sec, where is visible the recurrence phenomenon.

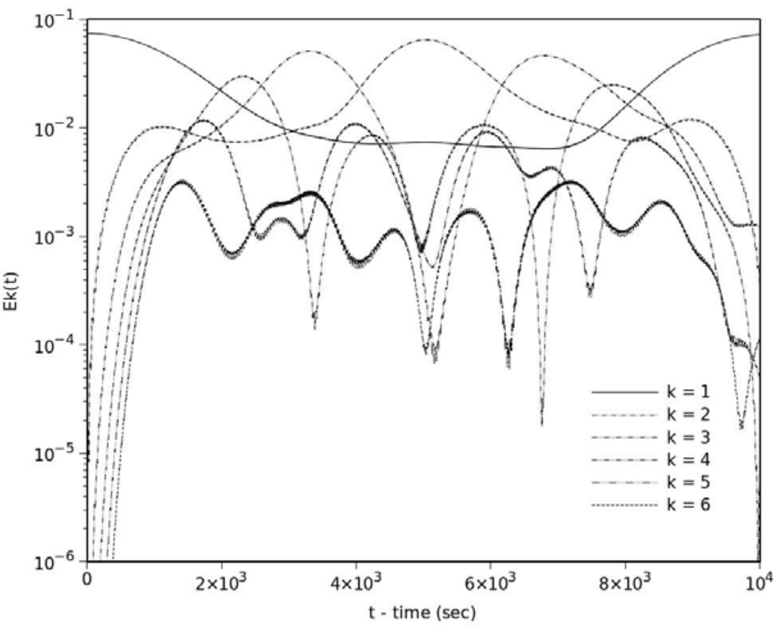
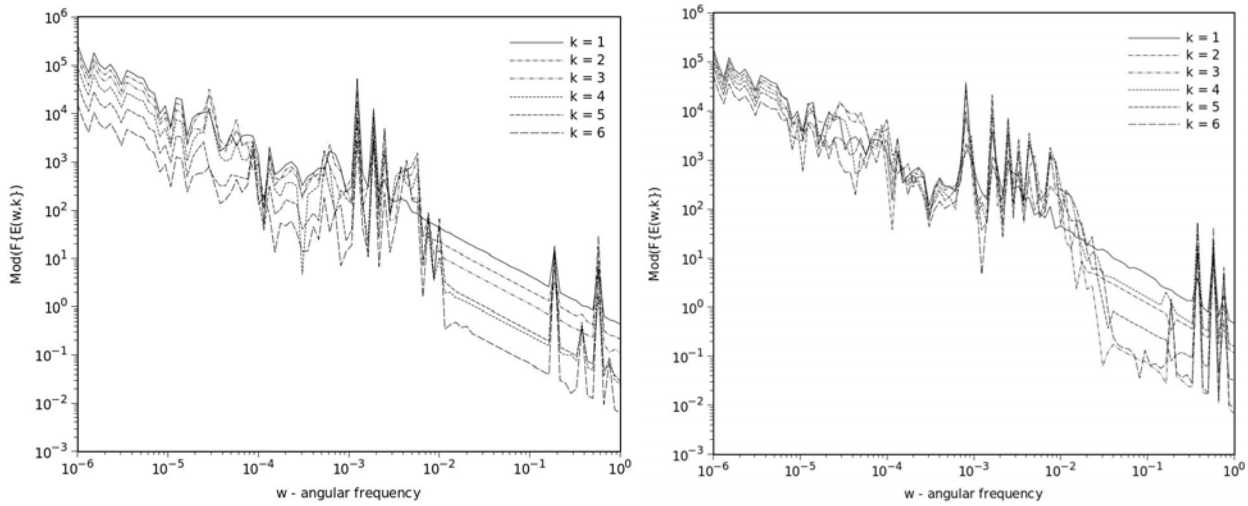


Figure 2 Time evolution of E_k , $k = \{1, \cdots, 6\}$, and the FPU - α problem.

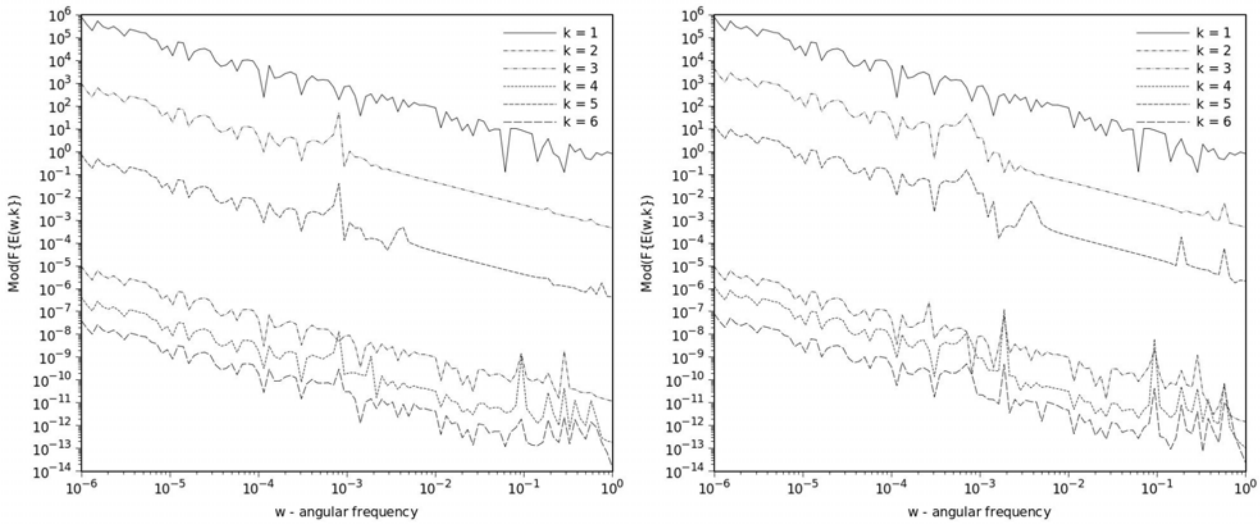
It is well known that the time representation poses visualization problems for long time periods, with distinct time scales for the quasi-periodic phenomena. Therefore, it is considered the representation in the frequency domain using a logarithmic scale. By other words, considering the Fourier transform $F\{E_k\} = \int_{-\infty}^{+\infty} E_k(t) e^{-i\omega t} dt$, $i = \sqrt{-1}$, where ω represents the angular frequency, the $E_k(t,k)$ representation is substituted by the $E_k(\omega,k)$ with a logarithmic scale in the ω -axis. Figure 3 shows $E_k(\omega,k)$, $k = \{1, \cdots, 6\}$, for the FPU - α and - β , with the Fourier transform calculated for a period of time of 10^6 sec, when $\alpha = \{0.25, 0.50\}$ and $\beta = \{0.25, 0.50\}$.

We observe the more complicated spectrum of the FPU - α and the emergence of peaks at several frequencies that characterize the quasi-periodic evolution. The ω^{-1} base line is due to the average value of $E_k(t,k)$. Furthermore, the higher the mode, the smaller its amplitude.



$\alpha = 0.25$ $\alpha = 0.50$

a)



$\beta = 0.25$ $\beta = 0.50$

b)

Figure 3 Locus of $\left|E_k(\omega, k)\right|$, $k = \{1, \cdots, 6\}$, and the a) FPU - α and b) FPU - β problems.

We observe that classical mechanics for the spring (Hooke's law), friction (viscous) and mass (Newton's law) follow a relationship between force $F(t)$ and displacement $x(t)$ of the type $F(t) = \alpha \cdot D^{\mu} x(t)$ with $\mu = \{0, 1, 2\}$. Therefore, bearing in mind the generalization of FC, we can evaluate the behavior of the FPU system for a fractional order spring (an element in between the classical spring and damping). For implementing the fractional derivative it is considered the Grünwald-Letnikov definition of a fractional derivative of order $0 \le \mu \le 1$ given by the expression:

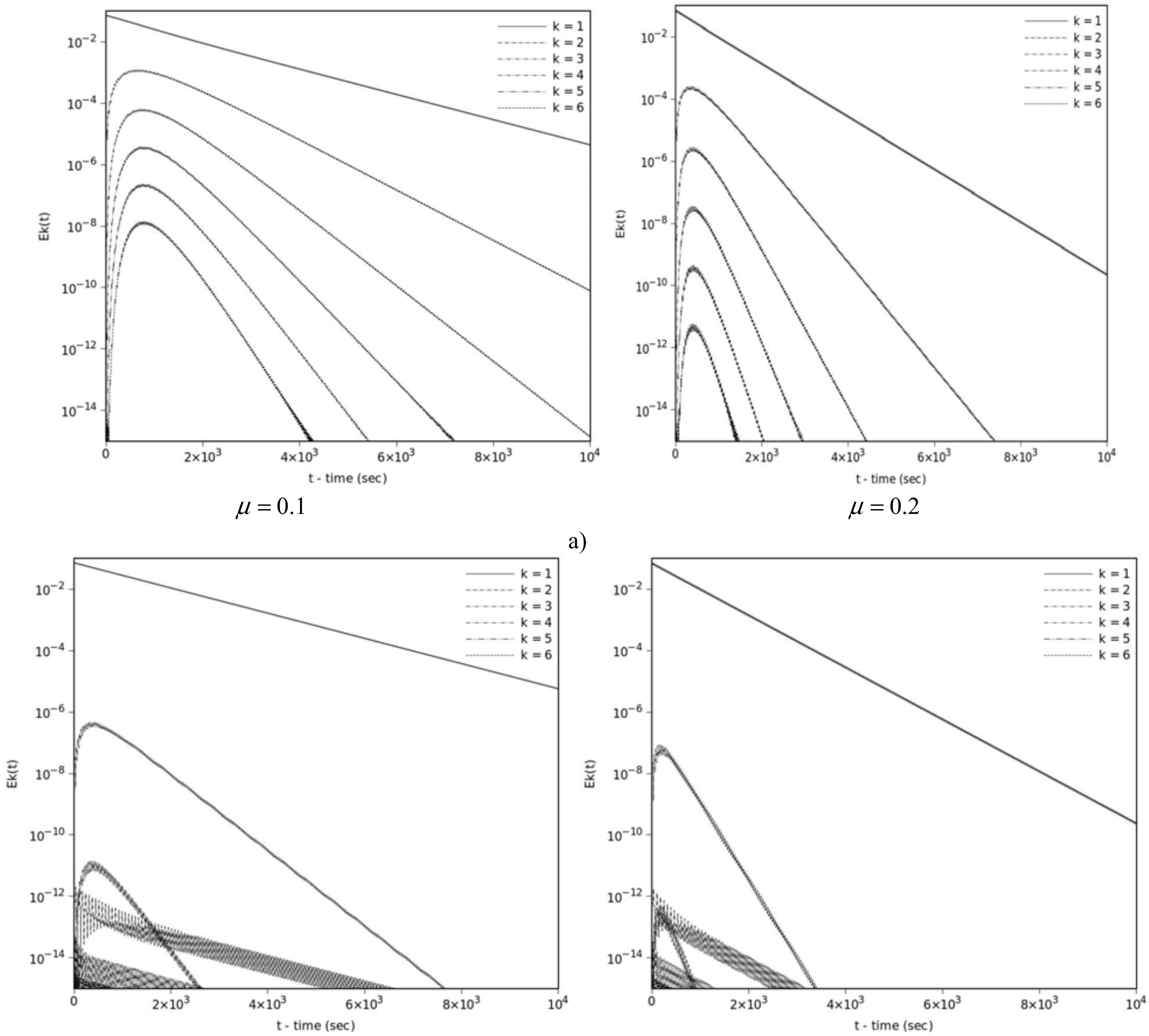
$$D^{\mu}[x(t)] = \lim_{h \to 0} \left[\frac{1}{h^{\mu}} \sum_{k=0}^{\infty} (-1)^k \frac{\Gamma(\mu + 1)}{k!\,\Gamma(\mu - k + 1)} x(t - kh) \right] \quad (5)$$

where Γ represents the gamma function and h the time increment.
For the computational implementation the time increment h is approximated by the T sampling period and the series is truncated at r terms yielding:

$$D^{\mu}[x(t)] \approx \lim_{h \to 0} \left[\frac{1}{T^{\mu}} \sum_{k=0}^{r} (-1)^k \frac{\Gamma(\mu + 1)}{k!\,\Gamma(\mu - k + 1)} x(t - kT) \right] \quad (6)$$

Figure 4 depicts a typical time evolution of $E_k(t)$, $k = \{1, \cdots, 6\}$, $\mu = \{0.1, 0.2\}$, $r = 100$, for the FPU - α and FPU - β

problems. It is visible a strong dissipation of the energy occurs the higher the value of the fractional derivative μ avoiding, therefore, the appearance of quasi periodic motions.



$\mu = 0.1$ $\mu = 0.2$

a)

$\mu = 0.1$ $\mu = 0.2$

b)

Figure 4 Time evolution of E_k , $k = \{1, \cdots, 6\}$, $\mu = \{0.1, 0.2\}$, $r = 100$, for the a) FPU - *α*, $\alpha = 0.25$, and b) FPU - *β*, $\beta = 0.25$, problems.

We observe some numerical instability at very low amplitudes that are not significant for the main conclusions. Finally, we conclude that the FPU - *α* dissipates the energy modes slower than the FPU – *β*.

3. Conclusions

In the last six decades the Fermi - Pasta - Ulam problem posed important challenges in the area of nonlinear dynamics. Nevertheless, in spite of the intense research many aspects remain to be clearly understood. Therefore, it is important to developed fresh approaches that can lead to new perspectives. Recently the theory of FC was proved to be a useful mathematical tool to model systems with long range dynamical properties. In this line of thought, this paper presented a novel approach based on the implementation of fractional order elements based on a series approximation of the Grünwald-Letnikov definition of fractional derivative. The comparison of integer and fractional order perspectives leads to clear conclusions motivating further research using the formalism of FC.

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