Dynamics and Stability in Fermi Pasta Ulam Chain

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INTRODUCTION

Dynamics of β-Fermi Pasta Ulam potential in 1 dimensional N particle leads to discrete non-linear equation of motion. For nearest neighbouring interaction we can categorize the equation of motion which leads to periodic solutions in to 6 groups, all these different groups lead to different elliptic solutions and a different 1 -d lattice arrangement. Only these 6 groups belonging to 6 distinct lattice arrangements will give a elliptic periodic solutions. Energy per particle of each group is calculated in terms of elliptic modulus 'κ' and non linearity coefficient 'β'. The stability of these solutions is analysed using Floquet theory and stability zones are plotted for different elliptic modulus value.

THEORETICAL FORMALISM

We study the dynamics and stability properties of simple periodic orbits of the β-Fermi-Pasta-Ulam (FPU) lattice. We consider the β-FPU Hamiltonian,

$$H = \frac{1}{2}\sum_{j=1}^{N}\dot{x}_j^2 + \sum_{j=0}^{N}\left(\frac{1}{2}(x_{j+1}-x_j)^2 + \frac{1}{4}\beta(x_{j+1}-x_j)^4\right) = E$$

where β is a positive real constant, N is the total number of particles and x_j denotes the displacement of the jth particle from its equilibrium position. If we consider nearest-neighbour interaction, we get equations of motion as follows:

$$\begin{aligned}\ddot{x}_j &= -\frac{\partial V_j}{\partial x_j}\\ &= x_{j+1} + x_{j-1} - 2x_j + \beta\left[(x_{j+1}-x_j)^3 - (x_j - x_{j-1})^3\right]\end{aligned}$$

where

$$V_j = \frac{1}{2}\left[(x_{j+1}-x_j)^2 + (x_j - x_{j-1})^2\right] + \frac{1}{4}\beta\left[(x_{j+1}-x_j)^4 + (x_j - x_{j-1})^4\right].$$

We can apply periodic boundary condition (PBC),

$$x_j(t) = x_{j+N}(t)$$

SIMPLE PERIODIC ORBITS

For an N-particle system, enumeration of periodic orbits is a difficult task. In the following, we restrict ourselves to what can be termed as 'Simple periodic orbits' as all the individual particles satisfy the same equation:

$$\ddot{x}_j = f(x_j)$$

for any J. We enumerate possible phase-relationships of particles on a 1-D β-FPU lattice such that the motion of all the particles are governed by a single equation of motion. As we consider only nearest-neighbour interaction, we group these basic arrangements of triplets ((j-1)$^{\text{th}}$, j$^{\text{th}}$, (j+1)$^{\text{th}}$ particles) that yield periodic solution on repetition. Six such arrangements are noted below.

Case I :

↑ ↑ ↑ ↑ ↑ ↑ ↑ ↑ ↑ ↑ ↑ ↑
1 2 3 4 5 6 7 8 9 10 11 12

When x_{j-1}, x_j and x_{j+1} are in phase, and, the magnitudes of their displacement are equal, we get a trivial equation of motion-that of their centre of mass:

$$\ddot{x}_j = 0$$

for $j = 1, 2, \ldots, N$.

Case II :

↑ ↑ 3 4 ↑ ↑ 7 8 ↑ ↑ 11 12
1 2 ↓ ↓ 5 6 ↓ ↓ 9 10 ↓ ↓

When x_{2j-1}, x_{2j} are in phase and x_{2j}, x_{2j+1} are out of phase, and, the magnitudes of their displacement are equal, we get an equation of motion

$$\ddot{x}_j = -2x_j - 8\beta x_j^3$$

for $j = 1, 2, \ldots, N/2$ and $N = 4n$ where $n = 1, 2, 3 \ldots$.

Case III :

↑ ↑ o 4 5 o ↑ ↑ o 10 11 o
1 2 3 ↓ ↓ 6 7 8 9 ↓ ↓ 12

When x_{3j-2}, x_{3j-1} are in phase and x_{3j-1}, x_{3j+1} are out of phase, and, the magnitudes of their displacement are equal.x_{3j} is at rest, we get an equation of motion

$$\ddot{x}_j = -x_j - \beta x_j^3$$

for $j = 1, 2, \ldots, N/3$ and $N = 3n$, even values where $n = 2, 4 \ldots$.

Case IV :

↑ 2 o ↑ 5 o ↑ 8 o ↑ 11 o
1 ↓ 3 4 ↓ 6 7 ↓ 9 10 ↓ 12

When x_{3j-2}, x_{3j-1} are out of phase and x_{3j-1}, x_{3j+1} are also out of phase, and, the magnitudes of their displacement are equal. x_{3j} is at rest, we get an equation of motion

$$\ddot{x}_j = -3x_j - 9\beta x_j^3$$

for $j = 1, 2, \ldots, N/3$ and $N = 3n$, where $n = 1, 2, \ldots$.

Case V :

↑ o 3 o ↑ o 7 o ↑ o 11 o
1 2 ↓ 4 5 6 ↓ 8 9 10 ↓ 12

When x_{2j-1}, x_{2j+1} are out of phase, and, the magnitudes of their displacement are equal. x_{2j} is at rest, we get an equation of motion

$$\ddot{x}_j = -2x_j - 2\beta x_j^3$$

for $j = 1, 2, \ldots, N/2$ and $N = 4n$, where $n = 1, 2, \ldots$.

Case VI :

↑ 2 ↑ 4 ↑ 6 ↑ 8 ↑ 10 ↑ 12
1 ↓ 3 ↓ 5 ↓ 7 ↓ 9 ↓ 11 ↓

When x_j, x_{j+1} are out of phase, and, the magnitudes of their displacement are equal, we get an equation of motion

$$\ddot{x}_j = -4x_j - 16\beta x_j^3$$

for $j = 1, 2, \ldots, N$ and $N = 2n$, where $n = 1, 2, \ldots$.

RESULTS AND DISCUSSIONS

Characterization

We present explicit solutions of the EOM for Case II, following the earlier works . The EOM for all the SPOs is the same, thus all the solutions can be explicitly written down. This section will eventually complete the enumeration and characterization of all the SPOs. The EOM for Case II is

$$\ddot{x}_j = -2x_j - 8\beta x_j^3.$$

This admits well-known solution in term of Jacobian elliptic function ,

$$x(t) = C\,\mathrm{cn}(\lambda t, k^2)$$

with elliptic modulus, k, and

$$C^2 = \frac{k^2}{2\beta(1-2k^2)},$$
$$\lambda^2 = \frac{2}{(1-2k^2)}.$$

This solution is periodic in time with period,$4K$.

$$\frac{E}{N} = \frac{1}{2}\frac{k^2(1-k^2)}{\beta(1-2k^2)^2}$$

The energy per particle is constant. Thus there is equipartition of energy in the mode.

Stability Analysis

We perform the linear stability analysis of periodic orbits, employing Floquet theory . To illustrate, we consider Case II again and perturb the solution x_j to

$$x_j = x + y_j.$$

The instantaneous position of the j^{th} particle is displaced y_j from the periodic solution, it satisfies the (EOM), (2):

$$\ddot{y}_{2j} = \left(1 + 12\beta x^2\right)y_{2j+1} - \left(2 + 12\beta x^2\right)y_{2j} + y_{2j-1}$$
$$\ddot{y}_{2j-1} = y_{2j} - \left(2 + 12\beta x^2\right)y_{2j-1} + \left(1 + 12\beta x^2\right)y_{2j-2}$$

To be explicit, we specialize to $N = 12$ and write EOM in vectorial form: $\ddot{\vec{y}} = M\vec{y}$ We get following distinct eigenvalues :

$$\lambda_1 = 0, \lambda_2 = -2, \lambda_3 = -2\left(1 + 12\beta x^2\right), \lambda_4 = -4\left(1 + 6\beta x^2\right),$$
$$\lambda_{5,6} = -2(1 + 6\beta x^2) \mp \sqrt{3(1 + 12\beta x^2 + 48\beta^2 x^4)},$$
$$\lambda_{7,8} = -2(1 + 6\beta x^2) \mp \sqrt{1 + 12\beta x^2 + 144\beta^2 x^4}.$$

For each distinct eigenvalue, we solve the eigenvalue equation to find eigenfunction $z_j(t)$. Using the solution (11) and defining $u = \lambda t$, we get the Lamé equation for $z_j(u)$:

$$\ddot{z}_j(u) + Q(u)z_j(u) = 0$$

The function $z_j(u)$ is a linear combination of y_j and

$$\dot{z}_j(u) = \frac{dz_j(u)}{du},$$

for each distinct eigenvalue. The function $Q(u)$ takes distinct forms for each eigenvalue. According to the Floquet theory, $Q(u)$ is a periodic function. For Case II, $Q(u)$ is $2K$-periodic, i.e.

$$Q(u) = Q(u + 2K).$$

The stability of the solution is determine by the boundedness of motion. We express $Q(u)$ and $z(u)$ in Fourier series,

$$Q(u) = \sum_{n'=-\infty}^{+\infty} a_{n'} \exp\left(\frac{in'\pi u}{K}\right),$$
$$z(u) = \sum_{n=-\infty}^{+\infty} \phi_n \exp\left(\frac{in\pi u}{K}\right)\exp(\gamma u),$$

where γ is the Floquet exponent.

Putting it in the Hill's equation and equating the coefficients we get an infinite-dimensional matrix. $D[i\gamma]$ represents the matrix with elements as follows,

$$D[i\gamma]_{n,m} = a_{n-m} \quad \ldots n \neq m,$$
$$D[i\gamma]_{n,m} = a_0 - \left(i\gamma - \left(\frac{n\pi}{K}\right)\right)^2$$

We define new matrix,

$$\Delta = [A_{m,n}]$$
$$with\ A_{m,m} = \frac{\left[\left(\frac{n\pi}{K} - i\gamma\right)^2\right] - a_0}{\frac{n^2\pi^2}{K^2} - a_0}$$
$$and\ A_{m,n} = \frac{-a_{m-n}}{\frac{n^2\pi^2}{K^2} - a_0} \quad \ldots for\ m \neq n.$$

Further simplifying it we get the stability condition,

$$\cos(2Ki\gamma) = \left|1 - 2\sin^2(Ka_0)\Delta(0)\right|$$

putting $i\gamma = \alpha$, we get,

$$\cos(2\alpha K) = \left|1 - 2\sin^2(K\sqrt{a_0})\Delta(0)\right|.$$

For Case II, we have plotted the stability regions for eigenvalues λ_3, λ_4 respectively.

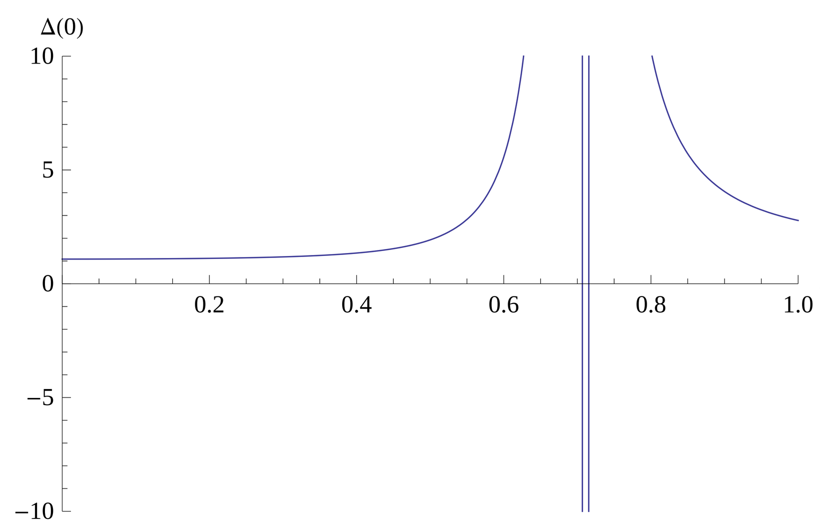

Figure 1: $\lambda_3 = -2(1 + 12\beta x^2)$

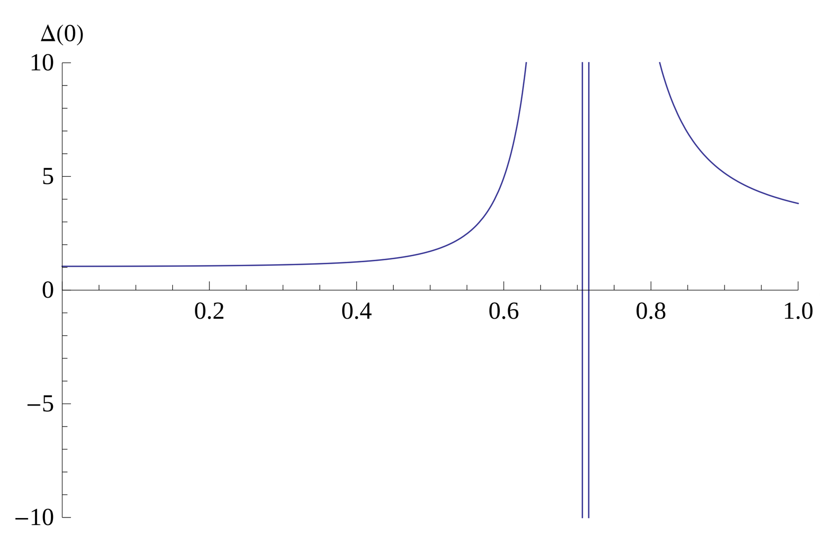

Figure 2: $\lambda_4 = -4(1 + 6\beta x^2)$

$\Delta(0)$ plotted on y-axis, decides the stability condition. It is an infinite-dimensional matrix, but we have approximated it by 3x3 matrix. It has been verified that it is a very good approximation.

References

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