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Dynamics, stability analysis and quantization of β-Fermi–Pasta–Ulam lattice

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Abstract. We study the well-known one-dimensional problem of N particles with nonlinear interaction. The β-Fermi–Pasta–Ulam model is the special case of quadratic and quartic interaction potential among nearest neighbours. We enumerate and classify the simple periodic orbits for this system and find the stability zones, employing Floquet theory. We quantize the nonlinear normal modes and construct a wavefunction for what we believe is a primitive nonlinear analogue of a 'phonon'.

Keywords. Phonon; Fermi–Pasta–Ulam lattice; Floquet theory; semiclassical quantization.

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1. Introduction

Some of the fundamental questions underlying equilibrium statistical mechanics are related to equipartition and ergodicity [1]. These questions for macroscopic systems are intimately linked to the dynamical behaviour of the microscopic systems. One of the most popular systems is chains of particles attached by 'springs'. The 'springs' correspond to linear and nonlinear forces and these give rise to a set of nonlinear coupled equations whose analytic solutions are rare. Thus, numerical studies have been carried out for a large class of these systems, the foremost being the Fermi–Pasta–Ulam (FPU) system [2]. The breakdown of recurrences due to overlapping resonances [3] and the appearance of ergodicity with large-scale chaos are quite well-understood [4,5]. A lot of work was done to study the existence of discrete breathers in the lattice systems [6–8]. Flach and coworkers [9–11] have studied all the periodic orbits, which are exponentially localized in q-space of normal modes, where q is the wave number. These periodic orbits are termed as 'q-breathers'. By continuing the periodic orbit for the linear system into the domain of non-zero nonlinearity, for fixed energy, they numerically calculated all exact q-breathers.

Further, they also carried out stability analysis for these q-breathers by employing Floquet method [20].

Here, we study the dynamics and stability properties of simple periodic orbits (SPOs) of the β-FPU lattice. The normal modes employed to study the lattice systems inherently assume linearity of the Hamiltonians, unless one arbitrarily discards the particle non-conserving terms. We present nonlinear normal modes having the form of elliptic functions, in spirit of the earlier work by Budinsky and Bountis [12]. These are extended over all the modes and are valid for all values of β. The nearest-neighbour interaction allows only a certain number of modes which are listed here. The stability of these modes is then presented using the standard analysis. In ref. [13], Lakshmanan and Saxena have also obtained several static and moving periodic soliton solutions for a classical anisotropic, discrete Heisenberg spin chain using Jacobi elliptic function. These studies are important for understanding the equilibration of energy on the one hand, and for quantization in terms of recurrent patterns on the other hand. These are also of a great interest in nonlinear lattice dynamics [14].

As pointed out in [7], quantization of these systems is rather difficult. One of the possibilities is, of course, a generalization of Gutzwiller's periodic orbit theory [15] for this system of many particles. This requires all the periodic orbits with their stability properties. We are not even close to anything like this. However, we believe that the orbits (usually called as SPOs) studied here will bring us slightly closer to the Gutzwiller quantization. The quantization of these systems has been attempted using the Einstein–Brillouin–Keller (EBK) method in refs [7,16]. Schulman [16] has presented a generalized EBK method and employed path integral formalism to evaluate the semiclassical wavefunctions. We present our rather simple and straightforward generalization of quantization of nonlinear normal modes from what is done in constructing phonons from linear normal modes. The number of nonlinear normal modes and the number of particles for a nonlinear one-dimensional system will not match in general as a chaotic system is certainly non-integrable.

We consider the β-FPU Hamiltonian,

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

where β is a 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:

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

where

$$V_j = \frac{1}{2}\left((x_{j+1}-x_j)^2 + (x_j - x_{j-1})^2\right) + \frac{1}{4}\beta\left((x_{j+1}-x_j)^4 + (x_j-x_{j-1})^4\right). \tag{3}$$

We can apply periodic boundary condition (PBC),

$$x_j(t) = x_{j+N}(t), \tag{4}$$

or fixed boundary condition (FBC),

$$x_0(t) = x_{N+1}(t) = 0 \ \forall \ t. \tag{5}$$

We can transform the fixed boundary condition into periodic boundary condition in the following manner. If N' is the total number of degrees of freedom or total number of particles in the problem with FBC and N is the total number of degrees of freedom or total number of particles for the same Hamiltonian subjected to PBC, then it can be shown that [17]

$$\begin{aligned} &N = 2N' + 2 \\ &x_{n+N'+1} = -x_n, \qquad n = 1, 2, \ldots, N' + 1. \end{aligned}$$

2. Periodic solutions and their stability

We find out all possible SPOs of one-dimensional β-FPU lattice such that all the particles are governed by a common equation of motion. As we consider only nearest-neighbour interaction, we group these basic arrangements of triplets (jth, $j+1$th, $j-1$th particles) that yield periodic solution on repetition. We describe the possible arrangements and the stability of the periodic solutions ensuing therefrom.

2.1 *Case* I

$$\begin{array}{cccccccccccc} \uparrow & \uparrow & \uparrow & \uparrow & \uparrow & \uparrow & \uparrow & \uparrow & \uparrow & \uparrow & \uparrow & \uparrow \\ 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & 10 & 11 & 12 \end{array}$$

When x_j, x_{j+1} and x_{j-1} are in same phase with equal magnitude of displacement, we get a trivial equation of motion

$$\ddot{x}_j = 0, \tag{6}$$

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

2.2 *Case* II

$$\begin{array}{cccccccccccc} \uparrow & \uparrow & 3 & 4 & \uparrow & \uparrow & 7 & 8 & \uparrow & \uparrow & 11 & 12 \\ 1 & 2 & \downarrow & \downarrow & 5 & 6 & \downarrow & \downarrow & 9 & 10 & \downarrow & \downarrow \end{array}$$

When x_{2j}, x_{2j-1} are in same phase and x_{2j}, x_{2j+1} are in opposite phase with equal magnitude of displacement, we get an equation of motion

$$\ddot{x}_j = -2x_j - 8\beta x_j^3, \tag{7}$$

for $j = 1, 2, \ldots, N/2$ and $N = 4n$, where $n = 1, 2, 3, \ldots$. This admits an elliptic solution of period $4K$ [5,18],

$$x(t) = C\mathrm{cn}(\lambda t, k^2), \tag{8}$$

where k^2 is the elliptic modulus, and

$$C^2 = \frac{k^2}{2\beta(1-2k^2)}, \tag{9}$$

$$\lambda^2 = \frac{2}{(1-2k^2)}. \tag{10}$$

For $\beta < 0$, the solution is

$$r(t) = S\mathrm{sn}(\Lambda t, k^2), \tag{11}$$

with

$$S^2 = \frac{-k^2}{2\beta(1+k^2)},$$

$$\Lambda^2 = \frac{2}{(1+k^2)}. \tag{12}$$

To find energy per particle, substitute (7) in (1), and let us rewrite the Hamiltonian as

$$\begin{aligned} H &= \frac{1}{2}\sum_{j=1}^{N}\dot{x}_j^2 + \sum_{j=0}^{N}\left(\frac{1}{2}(x_{j+1}-x_j)^2 + \frac{1}{4}\beta(x_{j+1}-x_j)^4\right) \\ &= \sum_{j=1}^{N/2}\left[\dot{x}_{2j}^2 + 2x_{2j}^2 + 4\beta x_{2j}^4\right]. \end{aligned} \tag{13}$$

Using eqs (8), (9),

$$\dot{x}_{2j} = -C\lambda\mathrm{sn}(\lambda t, k^2)\mathrm{d}n(\lambda t, k^2). \tag{14}$$

Substituting the solution and its derivatives, we get the following expression for the energy per particle:

$$\frac{E}{N} = \frac{1}{2}\frac{k^2(1-k^2)}{\beta(1-2k^2)^2}. \tag{15}$$

2.2.1 *Stability.* We would like to find out whether the periodic solution given here is stable. For determining this, we must perform the linear stability analysis for the periodic orbit employing Floquet theory [20]. To briefly summarize the method [19], stability is found by perturbing this many-particle orbit, and checking if the perturbed orbit remains in the vicinity of the original SPO. This complex multidimensional motion is then quantified by the Floquet exponents. Finally, a stability condition gives us the zones in the parameter-space, where the orbit is stable. Thus, let us begin by perturbing the SPO, $\hat{x}_j$ to

$$x_j = \hat{x}_j + y_j, \tag{16}$$

and substitute in (7). We get

$$\ddot{y}_{2j} = \left(1 + 12\beta\hat{x}^2\right)y_{2j+1} - \left(2 + 12\beta\hat{x}^2\right)y_{2j} + y_{2j-1} \tag{17}$$

and

$$\ddot{y}_{2j-1} = y_{2j} - \left(2 + 12\beta\hat{x}^2\right) y_{2j-1} + \left(1 + 12\beta\hat{x}^2\right) y_{2j-2}. \tag{18}$$

In this paper, we are presenting the calculation for $N = 12$, as various distinct SPOs are shown by taking this many particles. We get

$$\begin{pmatrix} \ddot{y}_1 \\ \ddot{y}_2 \\ \ddot{y}_3 \\ \ddot{y}_4 \\ \ddot{y}_5 \\ \ddot{y}_6 \\ \ddot{y}_7 \\ \ddot{y}_8 \\ \ddot{y}_9 \\ \ddot{y}_{10} \\ \ddot{y}_{11} \\ \ddot{y}_{12} \end{pmatrix} = \begin{pmatrix} -\left(2+12\beta\hat{x}^2\right) & 1 & 0 & 0 & \cdots & 0 & \left(1+12\beta\hat{x}^2\right) \\ 1 & -\left(2+12\beta\hat{x}^2\right) & \left(1+12\beta\hat{x}^2\right) & 0 & \cdots & 0 & 0 \\ 0 & \left(1+12\beta\hat{x}^2\right) & -\left(2+12\beta\hat{x}^2\right) & 1 & \cdots & 0 & 0 \\ 0 & 0 & 1 & -\left(2+12\beta\hat{x}^2\right) & \cdots & 0 & 0 \\ 0 & 0 & 0 & \left(1+12\beta\hat{x}^2\right) & \cdots & 0 & 0 \\ 0 & 0 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 0 & 0 & \cdots & \left(1+12\beta\hat{x}^2\right) & 0 \\ 0 & 0 & 0 & 0 & \cdots & -\left(2+12\beta\hat{x}^2\right) & 1 \\ \left(1+12\beta\hat{x}^2\right) & 0 & 0 & 0 & \cdots & 1 & -\left(2+12\beta\hat{x}^2\right) \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \\ y_5 \\ y_6 \\ y_7 \\ y_8 \\ y_9 \\ y_{10} \\ y_{11} \\ y_{12} \end{pmatrix}.$$

We get the following distinct eigenvalues:

$$\begin{aligned} \lambda_1 &= 0, \\ \lambda_2 &= -2, \\ \lambda_3 &= -2\left(1 + 12\beta\hat{x}^2\right), \\ \lambda_4 &= -4\left(1 + 6\beta\hat{x}^2\right), \\ \lambda_5 &= -2(1 + 6\beta\hat{x}^2) - \sqrt{3}\sqrt{1 + 12\beta\hat{x}^2 + 48\beta^2\hat{x}^4}, \\ \lambda_6 &= -2(1 + 6\beta\hat{x}^2) + \sqrt{3}\sqrt{1 + 12\beta\hat{x}^2 + 48\beta^2\hat{x}^4}, \\ \lambda_7 &= -2(1 + 6\beta\hat{x}^2) - \sqrt{1 + 12\beta\hat{x}^2 + 144\beta^2\hat{x}^4}, \\ \lambda_8 &= -2(1 + 6\beta\hat{x}^2) + \sqrt{1 + 12\beta\hat{x}^2 + 144\beta^2\hat{x}^4}. \end{aligned}$$

For each distinct eigenvalue, we solve the eigenvalue equation to find the corresponding eigenfunction. Using the solution (8), (9) and $u = \lambda t$, we get the Lamé equation, which is an example of the Hill's equation,

$$\ddot{z}_j(u) + Q(u)z(u) = 0. \tag{19}$$

The eigenfunctions $z(u)$ are linear combination of y_j and

$$\dot{z}_j(u) = \frac{\mathrm{d}z_j(u)}{\mathrm{d}u}. \tag{20}$$

For each distinct eigenvalue, the function $Q(u)$ takes distinct forms. According to Floquet theory, $Q(u)$ is a T-periodic function with $T = 2K$, i.e.

$$Q(u) = Q(u + 2K). \tag{21}$$

Depending on the nature of solutions of (19), whether they are bounded or not, the stability is determined. We express $Q(u)$ and $z(u)$ in Fourier series [20] as

$$Q(u) = \sum_{n'=-\infty}^{+\infty} a_{n'} \exp\left(\frac{in'\pi u}{K}\right), \tag{22}$$

$$z(u) = \sum_{n=-\infty}^{+\infty} \phi_n \exp\left(\frac{in\pi u}{K}\right) \exp(\gamma u), \tag{23}$$

where γ is the Floquet exponent. Substituting (22) in the Hill's equation (19) and equating the corresponding coefficients, we get an infinite order matrix, $D[i\gamma]$ with elements as follows:

$$\begin{aligned} D[i\gamma]_{n,m} &= a_{n-m} \ldots n \neq m, \\ D[i\gamma]_{n,m} &= a_0 - \left(i\gamma - \left(\frac{n\pi}{K}\right)\right)^2. \end{aligned} \tag{24}$$

We define another matrix,

$$\Delta = [A_{m,n}],$$

with

$$\begin{aligned} A_{m,m} &= \frac{[((n\pi/K) - i\gamma)^2] - a_0}{n^2\pi^2/K^2 - a_0}, \\ A_{m,n} &= \frac{-a_{m-n}}{(n^2\pi^2/K^2) - a_0}. \end{aligned}$$

Also we define,

$$\begin{aligned} &\Delta_1(i\gamma) = [B_{m,n}], \\ &B_{m,m} = 1, \\ &B_{m,n} = \frac{-a_{m-n}}{((m\pi/K) - i\gamma)^2 - a_0}\ m \neq n. \end{aligned}$$

Now,

$$\Delta(i\gamma) = \Delta_1(i\gamma) \lim_{P\to\infty} \prod_{n=-P}^{P} \left(\frac{a_0 - (i\gamma - (n\pi/K))^2}{a_0 - (n^2\pi^2/K^2)}\right),$$

$$\sin(x) = x \prod_{n=1}^{\infty} \left(\frac{n^2\pi^2 - x^2}{n^2\pi^2}\right). \tag{25}$$

Using 'sin(x)' expansion, we can write

$$\Delta(i\gamma) = -\Delta_1(i\gamma) \frac{\sin(K(i\gamma - \sqrt{a_0}))\sin(K(i\gamma + \sqrt{a_0}))}{\sin^2(K\sqrt{a_0})}, \tag{26}$$

putting $\gamma = 0$ for $\Delta(0)$ and further simplifying, we get

$$\Delta(i\gamma) = \Delta(0) - \frac{\sin^2(Ki\gamma)}{\sin^2(K\sqrt{a_0})}, \tag{27}$$

to find roots of the above equation,

$$\begin{aligned} &\Delta(i\gamma) = 0, \\ &\sin^2(Ki\gamma) = \Delta(0) \cdot \sin^2(K\sqrt{a_0}). \end{aligned} \tag{28}$$

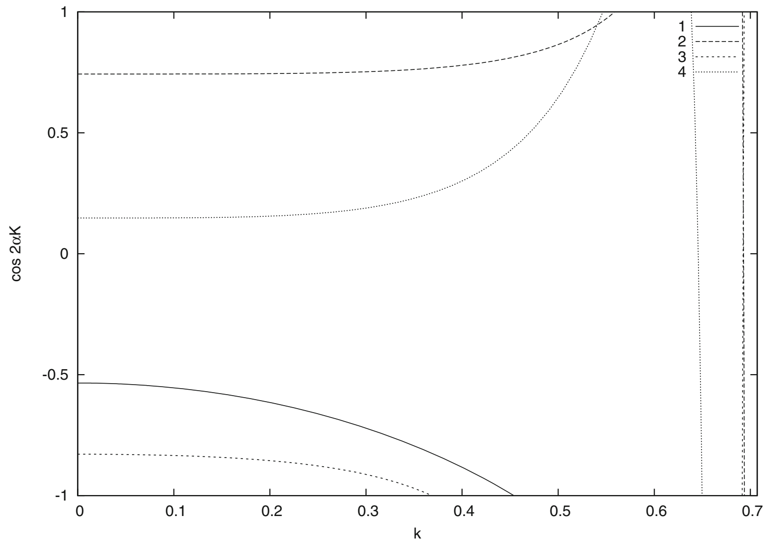

Figure 1. The plot of $\cos 2\alpha K$ vs. the elliptic modulus k brings out the regions of stability. The curves marked '1', '2', '3', '4' respectively, correspond to the $Q(u)$'s equal to $2(1+12\beta\hat{x}^2)$, $2+12\beta\hat{x}^2-\sqrt{3(1+12\beta\hat{x}^2+48\beta^2\hat{x}^4)}$, $2+12\beta\hat{x}^2+\sqrt{1+12\beta\hat{x}^2+144\beta^2\hat{x}^4}$, $2+12\beta\hat{x}^2-\sqrt{1+12\beta\hat{x}^2+144\beta^2\hat{x}^4}$; the regions of stability are given in table 1.

Table 1. Stability zones in k-space.

Eigenvalue	Stability region in k
$2(1+12\beta\hat{x}^2)$	[0, 0.4479]
$2+12\beta\hat{x}^2+\sqrt{3(1+12\beta\hat{x}^2+48\beta^2\hat{x}^4)}$	[0, 0.5547] and [0.6918, 0.6935]
$2+12\beta\hat{x}^2+\sqrt{1+12\beta\hat{x}^2+144\beta^2\hat{x}^4}$	[0, 0.3603] and [0.6916, 0.6930]
$2+12\beta\hat{x}^2-\sqrt{1+12\beta\hat{x}^2+144\beta^2\hat{x}^4}$	[0, 0.5335] and [0.6385, 0.6494]

Simplifying it further, we get the stability condition,

$$\cos(2Ki\gamma) = 1 - 2\sin^2(K\sqrt{a_0})\Delta(0). \tag{29}$$

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

$$\cos(2\alpha K) = 1 - 2\sin^2(K\sqrt{a_0})\Delta(0). \tag{30}$$

From figure 1, we can find the regions of stability corresponding to each eigenvalue. These are summarized in table 1 .

2.3 *Case* III

$\uparrow$	$\uparrow$	o	4	5	o	$\uparrow$	$\uparrow$	o	10	11	o
1	2	3	$\downarrow$	$\downarrow$	6	7	8	9	$\downarrow$	$\downarrow$	12

When x_{3j-1}, x_{3j-2} are in same phase and x_{3j-1}, x_{3j+1} are in opposite phase with equal magnitude of displacement and x_{3j} is at rest, we get an equation of motion

$$\ddot{x}_j = -x_j - \beta x_j^3, \tag{31}$$

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

$$x(t) = C\mathrm{cn}(\lambda t, k^2), \tag{32}$$

with k as elliptic modulus.

$$\begin{aligned} C^2 &= \frac{2k^2}{\beta(1-2k^2)}, \\ \lambda^2 &= \frac{1}{(1-2k^2)}. \end{aligned} \tag{33}$$

For $\beta < 0$, the solution is

$$r(t) = S\mathrm{sn}(\Lambda t, k^2), \tag{34}$$

with

$$\begin{aligned} S^2 &= \frac{-2k^2}{\beta(1+k^2)} \\ \Lambda^2 &= \frac{1}{(1+k^2)}. \end{aligned} \tag{35}$$

To find energy per particle, substituting the solution and its derivative in (1):

$$\frac{E}{N} = \frac{2}{3}\frac{k^2(1-k^2)}{\beta(1-2k^2)^2}. \tag{36}$$

2.3.1 *Stability.* Following the same method as earlier, we get different Hill's determinants, with distinct eigenvalues as follows:

$$\begin{aligned} \lambda_1 &= 0, \\ \lambda_2 &= -1 - 3\beta\hat{x}^2, \\ \lambda_3 &= -3\left(1 + \beta\hat{x}^2\right), \\ \lambda_4 &= -3\left(1 + 3\beta\hat{x}^2\right), \\ \lambda_5 &= -\frac{1}{2}(5 + 9\beta\hat{x}^2) + \sqrt{9 + 42\beta\hat{x}^2 + 81\beta^2\hat{x}^4}, \\ \lambda_6 &= -\frac{1}{2}(5 + 9\beta\hat{x}^2) - \sqrt{9 + 42\beta\hat{x}^2 + 81\beta^2\hat{x}^4}. \end{aligned} \tag{37}$$

The stability zones are found as shown in figure 2 and table 2.

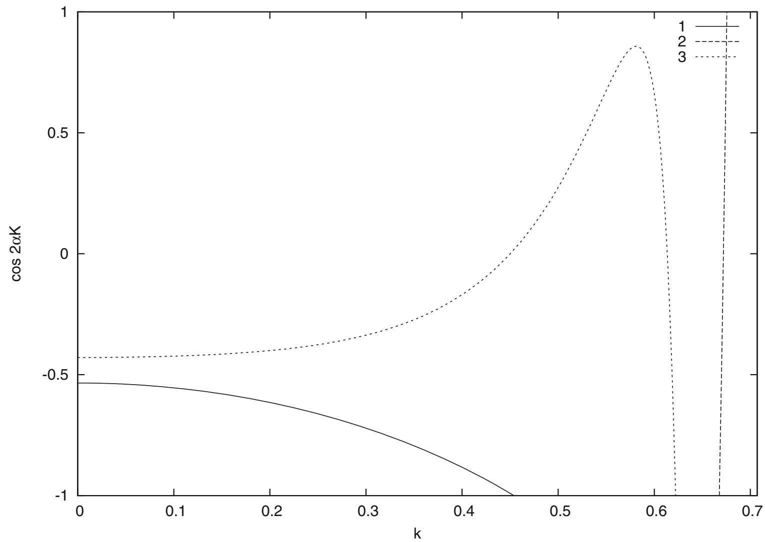

Figure 2. The plot of $\cos 2\alpha K$ vs. the elliptic modulus k brings out the regions of stability. The curves marked '1', '2', '3' respectively, correspond to the $Q(u)$'s equal to $1 + 3\beta\hat{x}^2$, $(1/2)(5 + 9\beta\hat{x}^2 + \sqrt{9 + 42\beta\hat{x}^2 + 81\beta^2\hat{x}^4})$, $(1/2)(5 + 9\beta\hat{x}^2 - \sqrt{9 + 42\beta\hat{x}^2 + 81\beta^2\hat{x}^4})$; the regions of stability are given in table 2.

Table 2. Stability zones in k-space.

Eigenvalue	Stability region in k
$1 + 3\beta\hat{x}^2$	[0, 0.4479]
$(1/2)(5 + 9\beta\hat{x}^2 + \sqrt{9 + 42\beta\hat{x}^2 + 81\beta^2\hat{x}^4})$	[0.6683, 0.6739]
$(1/2)(5 + 9\beta\hat{x}^2 - \sqrt{9 + 42\beta\hat{x}^2 + 81\beta^2\hat{x}^4})$	[0, 0.6221]

2.4 *Case* IV

$$
\begin{array}{cccccccccccc}
\uparrow & 2 & \mathrm{o} & \uparrow & 5 & \mathrm{o} & \uparrow & 8 & \mathrm{o} & \uparrow & 11 & \mathrm{o} \\
1 & \downarrow & 3 & 4 & \downarrow & 6 & 7 & \downarrow & 9 & 10 & \downarrow & 12
\end{array}
$$

When x_{3j-1}, x_{3j-2} are in opposite phase and x_{3j-1}, x_{3j+1} are also in opposite phase with equal magnitude of displacement and x_{3j} is at rest, we get an equation of motion

$$\ddot{x}_j = -3x_j - 9\beta x_j^3, \tag{38}$$

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

$$x(t) = C\mathrm{cn}(\lambda t, k^2), \tag{39}$$

with k as elliptic modulus.

$$\begin{aligned} C^2 &= \frac{2k^2}{3\beta(1-2k^2)}, \\ \lambda^2 &= \frac{3}{(1-2k^2)}. \end{aligned} \tag{40}$$

For $\beta < 0$, the solution is

$$r(t) = S\mathrm{sn}(\Lambda t, k^2), \tag{41}$$

with

$$\begin{aligned} S^2 &= \frac{-2k^2}{3\beta(1+k^2)} \\ \Lambda^2 &= \frac{3}{(1+k^2)}. \end{aligned} \tag{42}$$

To find energy per particle, substituting the solution and its derivative in (1):

$$\frac{E}{N} = \frac{2}{3}\frac{k^2(1-k^2)}{\beta(1-2k^2)^2}. \tag{43}$$

2.4.1 *Stability.* Solving the Hill's determinant in this case, we get distinct eigenvalues as follows:

$$\begin{aligned} \lambda_1 &= 0, \\ \lambda_2 &= -1 - 3\beta\hat{x}^2, \\ \lambda_3 &= -3\left(1 + 3\beta\hat{x}^2\right), \\ \lambda_4 &= -3\left(1 + 9\beta\hat{x}^2\right), \\ \lambda_5 &= -\frac{1}{2}(5 + 33\beta\hat{x}^2) + 3\sqrt{1 + 10\beta\hat{x}^2 + 57\beta^2\hat{x}^4}, \\ \lambda_6 &= -\frac{1}{2}(5 + 33\beta\hat{x}^2) - 3\sqrt{1 + 10\beta\hat{x}^2 + 57\beta^2\hat{x}^4} \end{aligned} \tag{44}$$

The stability zones are found as shown in table 3 and figure 3.

Table 3. Stability zones in k-space.

Eigenvalue	Stability region in k
$1 + 3\beta\hat{x}^2$	$[0, 1/\sqrt{2}]$
$3\left(1 + 3\beta\hat{x}^2\right)$	$[0, 1/\sqrt{2}]$
$3\left(1 + 9\beta\hat{x}^2\right)$	[0, 0.4479]
$(1/2)(5 + 33\beta\hat{x}^2) + 3\sqrt{1 + 10\beta\hat{x}^2 + 57\beta^2\hat{x}^4}$	[0, 0.3752] and [0.6984, 0.6993]
$(1/2)(5 + 33\beta\hat{x}^2) - 3\sqrt{1 + 10\beta\hat{x}^2 + 57\beta^2\hat{x}^4}$	[0, 0.5875] and [0.6693, 0.6744]

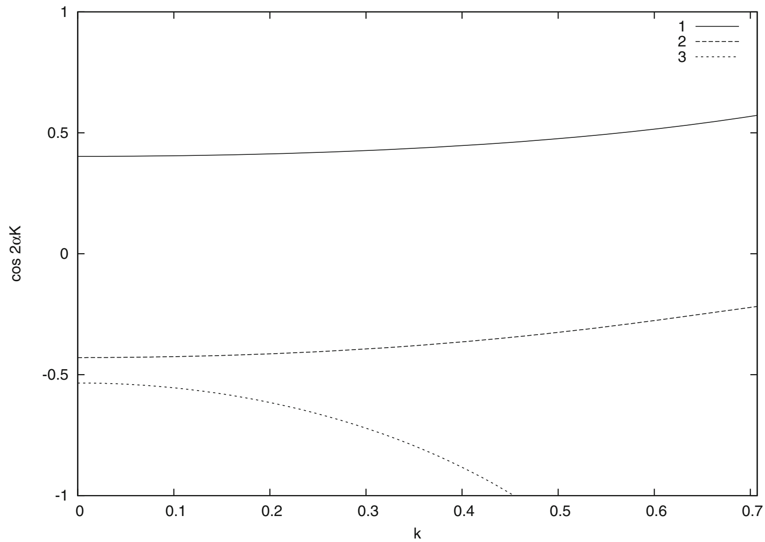

Figure 3. The plot of $\cos 2\alpha K$ vs. the elliptic modulus k brings out the regions of stability. The curves marked '1', '2', '3', '4', '5' respectively, correspond to $Q(u)$'s equal to $1+3\beta\hat{x}^2$, $3\left(1+3\beta\hat{x}^2\right)$, $3\left(1+9\beta\hat{x}^2\right)$, $1/2(5+33\beta\hat{x}^2)+3\sqrt{1+10\beta\hat{x}^2+57\beta^2\hat{x}^4}$, $1/2(5+33\beta\hat{x}^2)-3\sqrt{1+10\beta\hat{x}^2+57\beta^2\hat{x}^4}$; the regions of stability are given in table 3.

2.5 *Case* V

$\uparrow$	o	3	o	$\uparrow$	o	7	o	$\uparrow$	o	11	o
1	2	$\downarrow$	4	5	6	$\downarrow$	8	9	10	$\downarrow$	12

When x_{2j+1}, x_{2j-1} are in opposite phase with equal magnitude of displacement and x_{2j} is at rest, we get an equation of motion

$$\ddot{x}_j = -2x_j - 2\beta x_j^3, \tag{45}$$

for $j = 1, 2, ..., N/2$ and $N = 4n$, where $n = 1, 2, ...,$. The solution is

$$x(t) = C\mathrm{cn}(\lambda t, k^2), \tag{46}$$

with k as elliptic modulus.

$$C^2 = \frac{2k^2}{\beta(1-2k^2)},$$
$$\lambda^2 = \frac{2}{(1-2k^2)}. \tag{47}$$

For $\beta < 0$, the solution is

$$r(t) = S\mathrm{sn}(\Lambda t, k^2), \tag{48}$$

with

$$S^2 = \frac{-2k^2}{\beta(1+k^2)},$$
$$\Lambda^2 = \frac{2}{(1+k^2)}. \tag{49}$$

To find energy per particle, substituting solution and its derivative in (1):

$$\frac{E}{N} = \frac{k^2(1-k^2)}{\beta(1-2k^2)^2}. \tag{50}$$

2.5.1 *Stability.* Solving the Hill's determinant in this case, we get distinct eigenvalues as follows:

$$\lambda_1 = 0,$$
$$\lambda_2 = -1 - 3\beta\hat{x}^2,$$
$$\lambda_3 = -2\left(1+3\beta\hat{x}^2\right),$$
$$\lambda_4 = -3\left(1+3\beta\hat{x}^2\right),$$
$$\lambda_5 = -4\left(1+3\beta\hat{x}^2\right),$$
$$\lambda_6 = -(2+\sqrt{3})\left(1+3\beta\hat{x}^2\right),$$
$$\lambda_7 = -(2-\sqrt{3})\left(1+3\beta\hat{x}^2\right). \tag{51}$$

The stability zones are found as shown in figure 4 and table 4.

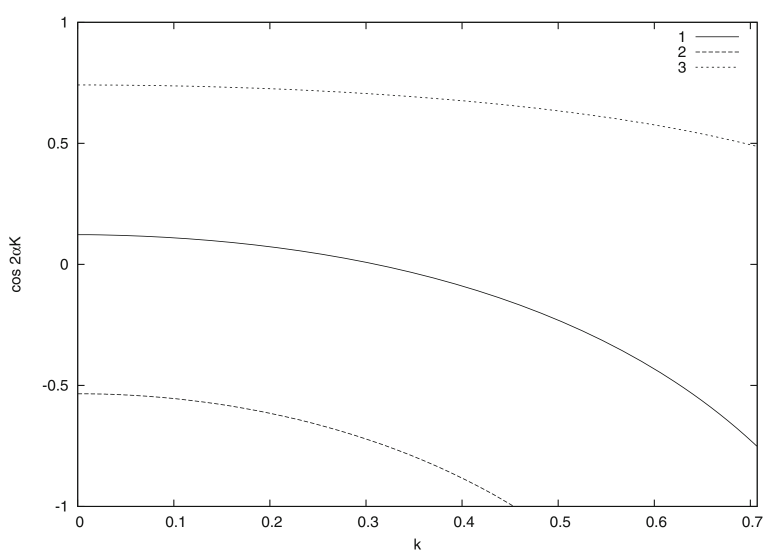

Figure 4. The plot of $\cos 2\alpha K$ vs. the elliptic modulus k brings out the regions of stability. The curves marked '1', '2', '3' respectively, correspond to the $Q(u)$'s equal to $1+3\beta\hat{x}^2$, $2(1+3\beta\hat{x}^2)$, $(2-\sqrt{3})\left(1+3\beta\hat{x}^2\right)$; the regions of stability are given in table 4.

Table 4. Stability zones in k-space.

Eigenvalue	Stability region in k
$1 + 3\beta\hat{x}^2$	$[0, 1/\sqrt{2}]$
$2(1 + 3\beta\hat{x}^2)$	$[0, 0.4479]$
$(2 - \sqrt{3})\left(1 + 3\beta\hat{x}^2\right)$	$[0, 1/\sqrt{2}]$

2.6 *Case* VI

$\uparrow$	2	$\uparrow$	4	$\uparrow$	6	$\uparrow$	8	$\uparrow$	10	$\uparrow$	12
1	$\downarrow$	3	$\downarrow$	5	$\downarrow$	7	$\downarrow$	9	$\downarrow$	11	$\downarrow$

When x_j, x_{j+1} are in opposite phase with equal magnitude of displacement, we get an equation of motion

$$\ddot{x}_j = -4x_j - 16\beta x_j^3, \tag{52}$$

for $j = 1, 2, ..., N$ and $N = 2n$, where $n = 1, 2, ...$. The solution is

$$x(t) = C\mathrm{cn}(\lambda t, k^2), \tag{53}$$

with k as elliptic modulus.

$$\begin{aligned} C^2 &= \frac{k^2}{2\beta(1-2k^2)}, \\ \lambda^2 &= \frac{4}{(1-2k^2)}. \end{aligned} \tag{54}$$

For $\beta < 0$, the solution is

$$r(t) = S\mathrm{sn}(\Lambda t, k^2), \tag{55}$$

with

$$\begin{aligned} S^2 &= \frac{-k^2}{2\beta(1+k^2)}, \\ \Lambda^2 &= \frac{4}{(1+k^2)}. \end{aligned} \tag{56}$$

To find energy per particle, substituting solution and its derivative in (1):

$$\frac{E}{N} = \frac{k^2(1-k^2)}{\beta(1-2k^2)^2}. \tag{57}$$

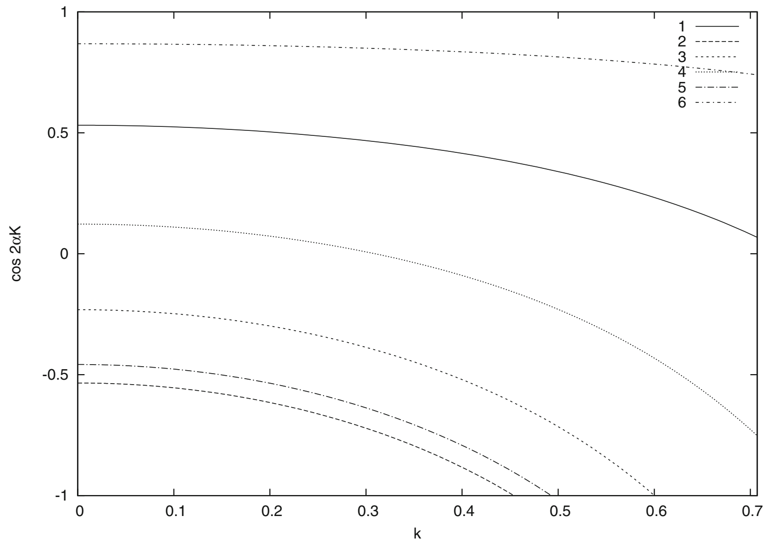

Figure 5. The plot of $\cos 2\alpha K$ vs. the elliptic modulus k brings out the regions of stability. The curves marked '1', '2', '3', '4', '5', '6' respectively, correspond to the $Q(u)$'s equal to $1 + 12\beta\hat{x}^2$, $2\left(1 + 12\beta\hat{x}^2\right)$, $3\left(1 + 12\beta\hat{x}^2\right)$, $4\left(1 + 12\beta\hat{x}^2\right)$, $(2 + \sqrt{3})\left(1 + 12\beta\hat{x}^2\right)(2 - \sqrt{3})\left(1 + 12\beta\hat{x}^2\right)$; the regions of stability are given in table 5.

Table 5. Stability zones in k-space.

Eigenvalue	Stability region in k
$1 + 12\beta\hat{x}^2$	$[0, 1/\sqrt{2}]$
$2\left(1 + 12\beta\hat{x}^2\right)$	$[0, 1/\sqrt{2}]$
$3\left(1 + 12\beta\hat{x}^2\right)$	$[0, 1/\sqrt{2}]$
$4\left(1 + 12\beta\hat{x}^2\right)$	$[0, 1/\sqrt{2}]$
$(2 + \sqrt{3})\left(1 + 12\beta\hat{x}^2\right)$	$[0, 1/\sqrt{2}]$
$(2 - \sqrt{3})\left(1 + 12\beta\hat{x}^2\right)$	$[0, 1/\sqrt{2}]$

2.6.1 *Stability.* Solving the Hill's determinant in this case, we get distinct eigenvalues as follows:

$$\begin{aligned}
\lambda_1 &= 0,\\
\lambda_2 &= -1 - 12\beta\hat{x}^2,\\
\lambda_3 &= -2\left(1 + 12\beta\hat{x}^2\right),\\
\lambda_4 &= -3\left(1 + 12\beta\hat{x}^2\right),\\
\lambda_5 &= -4\left(1 + 12\beta\hat{x}^2\right),\\
\lambda_6 &= -(2 + \sqrt{3})\left(1 + 12\beta\hat{x}^2\right),\\
\lambda_7 &= -(2 - \sqrt{3})\left(1 + 12\beta\hat{x}^2\right).
\end{aligned} \tag{58}$$

The stability zones are found as shown in figure 5 and table 5.

3. Quantization

We would like to recall the construction of the wavefunction of phonons very briefly before we write down the wavefunctions in the present case. In the case of a harmonic chain, the Schrödinger equation is written in terms of normal mode coordinates with corresponding frequencies. To recapitulate, we recall this for two masses (mass, m) attached to two ends by springs and also coupled by an identical spring. The transverse motion of these masses is quantified by two position coordinates, $q_1,\ q_2$ and the conjugate momenta $p_1,\ p_2$. The coupled equations satisfied by the coordinates can be uncoupled by making a transformation to the normal coordinates, $Q_1 = (q_1 + q_2)/\sqrt{2}$ and $Q_2 = (q_2 - q_1)/\sqrt{2}$. Quantum wavefunction $|\psi(t)\rangle$ satisfies the time-dependent Schrödinger equation with the Hamiltonian expressed in normal mode coordinates. This Hamiltonian is separable, whereas the Hamiltonian in $\hat{q}_1,\ \hat{q}_2$ is non-separable. Due to separability, the ground-state wavefunction can be expressed as

$$\psi(Q_1, Q_2) = \psi_0(Q_1)\psi_0(Q_2). \tag{59}$$

Due to the fact that normal modes could be found, an effective separability is achieved and consequently, a product wavefunction is realized. These correspond to phonons, and for a beautiful illustration, see ref. [21].

For the nonlinear problem at hand, we have found nonlinear normal modes. We would now construct the ground-state wavefunction labelled by the quanta corresponding to these modes. Unlike the linear case, we do not have the same number of coordinates as the number of particles and so the problem cannot be separated completely. But these modes are the ones in terms of which we can write some of the quantum states, if not all. Elaborate discussion on nonlinear normal mode and quanta of β-FPU lattice can be found in [27]. It is rare to be able to write down even approximate solutions of nonlinear many-body problems. For an example of a system, where in spite of chaos, some eigenfunctions have been written analytically, see ref. [25]. An interesting semiclassical study of some exact intrinsic localized mode solutions of a one-dimensional anisotropic Heisenberg ferromagnetic spin chain can be found in ref. [28].

3.1 *Semiclassical wavefunctions*

As explained above, we shall take each mode and then write the wavefunction in a product form as each of the mode is independent. The total wavefunction is then written as a product wavefunction in the two coordinates. Thus, we need to quantize the quartic oscillators underlying each of the modes obtained in the last section. We illustrate this for one mode, and write the final result.

For Case II, the underlying Hamiltonian is

$$H_I(p, x) = \frac{p^2}{2} + x^2 + 2\beta x^4 = \text{const.},\ E_{\mathrm{I}}, \tag{60}$$

where p is the momentum canonically conjugate to x. The Schrödinger equation is

$$\frac{\partial^2 \psi_I}{\partial x^2} + \frac{2}{\hbar^2}(E_{\rm I} - x^2 - \beta x^4)\psi_{\rm I} = 0, \tag{61}$$

subjected to the boundary condition that the solution must vanish at infinity. The solution can be written to a leading order [24]:

$$\psi_{\rm I}(x) \;=\; N_{\rm I}\frac{1}{k_{\rm I}(x)^{1/4}} \exp\left[\pm i \int^x k_{\rm I}(u){\rm d}u\right],$$

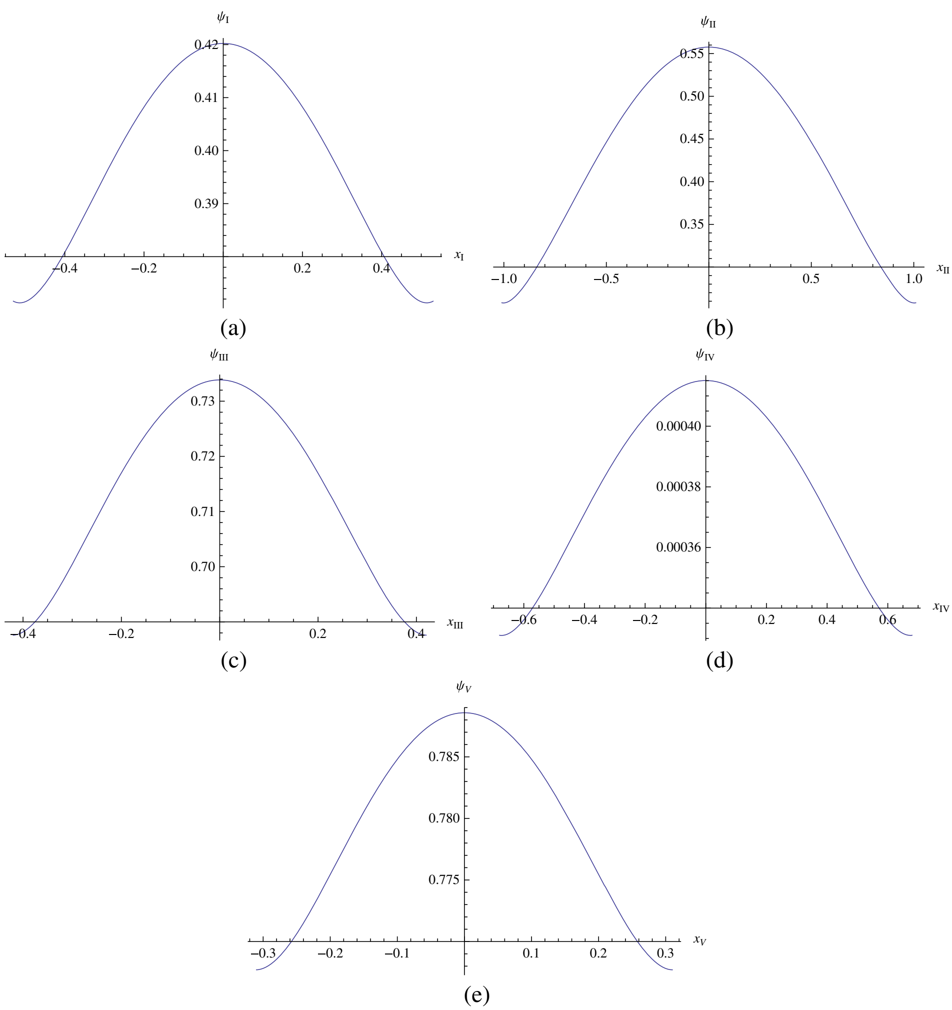

Figure 6. Wavefunctions calculated semiclassically for each of the modes, shown here as a function of the variable defining the mode, x_i, $i = {\rm I, II}, \ldots, {\rm V}$ by figures (**a**), (**b**), (**c**), (**d**) and (**e**) respectively.

where

$$k_{\mathrm{I}}(u) = \sqrt{\frac{2}{\hbar^2}(E_{\mathrm{I}} - u^2 - 2\beta u^4)}. \tag{62}$$

Similarly, we can write wavefunctions for all the cases. Finally, the wavefunction is

$$\Psi(x_{\mathrm{I}}, x_{\mathrm{II}}, ..., x_{\mathrm{V}}) = \psi_{\mathrm{I}}(x_{\mathrm{I}})\psi_{\mathrm{II}}(x_{\mathrm{II}})\psi_{\mathrm{III}}(x_{\mathrm{III}})\psi_{\mathrm{IV}}(x_{\mathrm{IV}})\psi_{\mathrm{V}}(x_{\mathrm{V}}). \tag{63}$$

The product form requires N coordinates for N particles. Thus, the final wavefunction is a function of all the coordinates. Here, we have integrated the equation representing Hamiltonian of each case as shown in eq. (60) for Case II. Using the boundary condition of solution in eq. (62), we then calculated wavefunction for all six cases, i.e. normal modes. We can show various sections by making projections (figures 7–9). We show three projections by integrating out the other coordinates. These are contour plots with lightest colour being maximum.

These contour plots of the product of wavefunctions in the respective normal mode coordinate planes show the maximum at zero. This is also reflected in figure 6, wherein the maximum of each wavefunction, plotted against its respective normal mode coordinate, is at zero. Turning points of each wavefunction are calculated by solving the EOM of each mode, which can also be seen in figure 6.

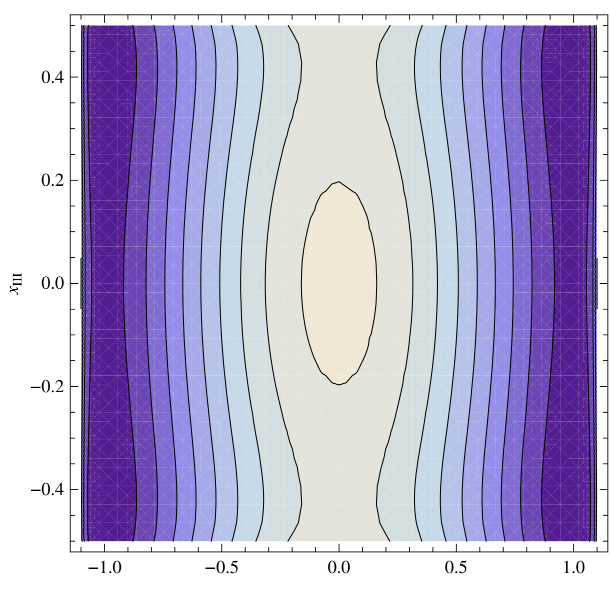

Figure 7. Contour plot of wavefunction in the (x_{II}–x_{III}) plane. The lighter regions correspond to larger positive values. Thus, we see that the system is ‘bound’ in a certain region. Of course, the state is residing in a five-dimensional space, each dimension being taken to build a nonlinear normal mode.

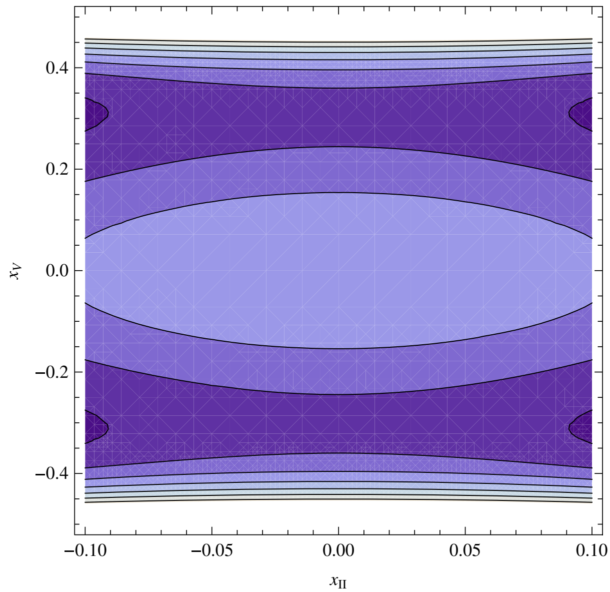

Figure 8. Contour plot of wavefunction in the (x_{II}–x_{V}) plane.

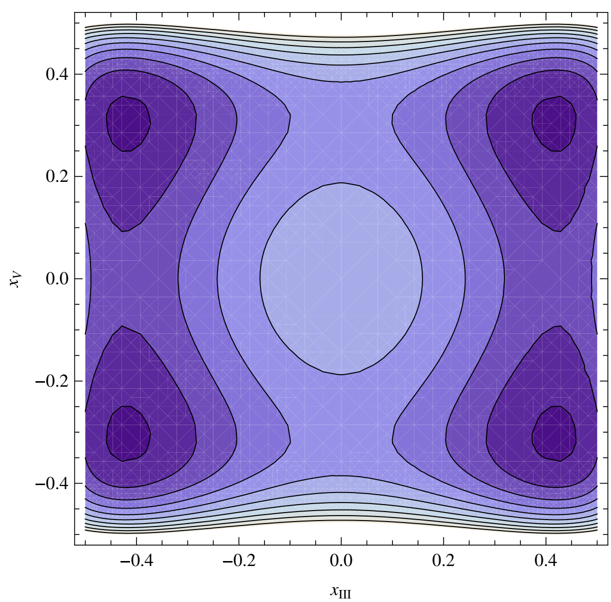

Figure 9. Contour plot of wavefunction in the (x_{III}–x_{V}) plane.

4. Concluding remarks

In this paper, we have considered 12-particle β-FPU lattice with quadratic and quartic potentials subjected to periodic boundary conditions. Allowing only nearest-neighbouring interaction, we have enumerated all possible simple periodic orbits. Further, we have characterized each of these simple periodic orbit or mode by solving the equation of motion corresponding to each distinct mode. We have obtained cn and sn Jacobian elliptic functions as solutions for $\beta > 0$ and $\beta < 0$ regions, respectively. Energy per particle for each mode is calculated in terms of the elliptic modulus k and β. We have carried out the linear stability analysis for 'cn elliptic function' by employing Floquet theory. By solving the Hill's equation corresponding to each distinct eigenvalue of all the modes, we have found the stability regions in 'k-space'. Some of these simple periodic orbits (Cases IV, V and VI) have been previously studied and characterized by Antonopoulos, Budinsky and Bountis [5,12]. They have found elliptic solutions for $\beta > 0$ and stability analysis was carried out for some modes.

In §3, we have semiclassically quantized β-FPU Hamiltonian of Case II using nonlinear normal modes. Among the various previous attempts, Aubry [7] has done quantization of the classical breather in quantum Boson–Hubbard model with boson conservation using Einstein–Brillouin–Keller (EBK) method, resulting in narrow bands of many bound bosons. Schulman [26] has studied one-dimensional FPU chain along the Jahn–Teller distortion axis to explain the anomaly in the relaxation of alkali metal halide crystals due to the existence of classical breather and quantized [16] it using the generalized EBK method. Ivic and Tsironis [23] quantized the β-FPU model using boson quantization rule retaining only the number conserving terms. They have identified on-site and nearest-neighbouring site biphonons within the mean-field approximation. Recently, Riseborough [22] calculated the lowest energy quantized breather excitation for β and α-FPU lattice using two-phonon propagators keeping the phonon non-conserving terms of the Hamiltonian. In §3.1, we have plotted various sections of wavefunctions in the corresponding normal mode coordinates. The calculations are based on the local analysis of the Schrödinger equation, and the plots show that each of those are the lowest states. Thus, the product represents the ground state.

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