Stability properties of the $N/4$ ($\pi/2$-mode) one-mode nonlinear solution of the Fermi-Pasta-Ulam-β system

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(Received 15 March 2007; published 24 July 2007)

We present a detailed numerical and analytical study of the stability properties of the $N/4$ ($\pi/2$-mode) one-mode nonlinear solution of the Fermi-Pasta-Ulam-β system. The numerical analysis is made as a function of the number N of the particles of the system and of the product $\lambda=\varepsilon\beta$, where ε is the energy density and β is the parameter characterizing the nonlinearity. It is shown that, both for $\beta>0$ and $\beta<0$, the instability threshold value $|\lambda_t(N)|$ converges, with increasing N, to the same value $2\pi^2/(3N^2)$, that for $\beta>0$ $|\lambda_t N^2|$ is a decreasing function of N as in the π-*mode*, whereas, for $\beta<0$, it is an increasing one. The asymptotic behavior of $|\lambda_t|$ for large values of N is analytically obtained in both cases with a Floquet analysis of the stability.

DOI: 10.1103/PhysRevE.76.016216 PACS number(s): 05.45.−a, 63.20.Pw, 63.20.Ry

I. INTRODUCTION

The study of the stability properties of one-dimensional anharmonic lattices, started by Fermi, Pasta, and Ulam [1] is of great interest to understand the energy distribution process among the normal modes and, in general, the statistical properties of a system in the thermodynamic limit. In particular, for the Fermi-Pasta-Ulam (FPU) β-model, there are many analytical and numerical results concerning the study of the stability properties of nonequilibrium motions in the case of a single-mode or narrow-packet modes excitation, against both the energy density and the excited mode's wave number [2–15].

In this paper we tackle the problem of the stability of a particular one-mode solution of the system. It is in fact well-known that, for a periodic FPU-β chain with a number N of oscillators and periodic conditions, there are exact one-mode solutions (OMSs) [8,12,14] corresponding to the values of mode number n (of course when n is an integer):

$$n=\frac{N}{4},\ \frac{N}{3},\ \frac{N}{2},\ \frac{2}{3}N,\ \frac{3}{4}N, \tag{1}$$

such that, if only one of these modes is initially excited, it evolves without transferring energy to any other mode. An important problem is the stability of these solutions against a generic perturbation. The stability of the $N/2$ mode (zone-boundary mode solution, π-mode) was studied by Boudinsky and Bountis [3]. They found that this mode is unstable above an energy threshold E_t that scales like $1/N$. This result was later and independently confirmed by Flach [7] and Poggi *et al.* [8], who also obtained the correct factor in the large N-limit, by a direct linear stability analysis around the periodic orbit corresponding to the mode.

A group theoretical approach, based on the concept of "bushes" (invariant manifolds in the modal space) of normal modes in mechanical systems with discrete symmetry, has been recently applied both to α and β models of the FPU system by Chechin *et al.* [11,14] and Rink [16].

In two recent papers [17,18] we have revisited the problem of stability of the $N/2$ mode. In [17] we made a numerical and analytical study of the stability of this mode as a function of the number N of particles and of the product $\lambda=\varepsilon\beta$, where ε is the energy density and $\beta>0$ is the parameter of nonlinearity in the Hamiltonian of the system. In the numerical analysis, based on the numerical integration of the nonlinear FPU model, no external perturbation for the solution was considered, the only perturbation being that introduced by computational errors in the numerical integration of motion equations. This simple method works very well and confirms the previous result [8] on the energy density threshold that asymptotically $\lambda_t N^2=\pi^2/3$. In [18] a thorough explanation of the behavior of λ_t as a function of N, for $\beta<0$, has been given on the base of Bogoliubov-Krylov method of averaging.

In this paper we continue the study of the OMSs by tackling the problem of the stability of the OMS corresponding to $n=N/4$ ($\pi/2$-mode). For the numerical analysis we apply the numerical method used in [17]. The main results obtained both for $\beta>0$ and $\beta<0$, $|\lambda_t|$ decreases asymptotically with N as $2\pi^2/3N^2$; for $\beta>0$, the product $|\lambda_t N^2|$ decreases with N, as in the π-mode and converges asymptotically to the value $2\pi^2/3$; for $\beta<0$ the same product increases with N toward the same value.

The theoretical analysis of the stability of the $N/4$ mode is much more complicated than that of the $N/2$ mode. The study of the stability of the $N/2$ mode is simpler because the different components of the perturbation in modal space are all decoupled, are described by an equation of the Hill type, and can be studied separately. On the contrary, the analysis of the stability of the $N/4$ mode implies the study of a system of coupled linear differential equations with periodic coefficients. In this paper we give an analytical explanation of the numerical results by means of the Floquet analysis of the stability of the mode.

II. ONE-MODE SOLUTIONS

Calling q_i and p_i the coordinates and the momenta of the oscillators, the Hamiltonian for the FPU-β system is

$$H=\frac{1}{2}\sum_{i=1}^{N}p_i^2+\frac{1}{2}\sum_{i=1}^{N}(q_{i+1}-q_i)^2+\frac{\beta}{4}\sum_{i=1}^{N}(q_{i+1}-q_i)^4 \tag{2}$$

with $q_{N+1}=q_1$. All quantities in Eq. (2) are dimensionless.

If we introduce the normal coordinates Q_i and P_i of the normal modes through the relations:

$$Q_i = \sum_{j=1}^{N} S_{ij} q_j, \tag{3}$$

$$P_i = \sum_{j=1}^{N} S_{ij} p_j, \tag{4}$$

$$S_{ij} = \frac{1}{\sqrt{N}}\left(\sin\frac{2\pi ij}{N} + \cos\frac{2\pi ij}{N}\right),$$

the harmonic energy of mode i is

$$E_i = \frac{1}{2}(P_i^2 + \omega_i^2 Q_i^2)$$

where, for periodic boundary conditions,

$$\omega_i^2 = 4\sin^2\frac{\pi i}{N}. \tag{5}$$

For $\beta=0$, all normal modes oscillate independently and their energies E_i are constants of motion. In the anharmonic case ($\beta \neq 0$), the normal modes are instead coupled and the variables Q_i do not have simple sinusoidal oscillations.

The nonlinear OMSs correspond to the values of n reported in Eq. (1). Consider now the case $n=N/4$. Let us put $Q=Q_{N/4}$ and $P=P_{N/4}$. The equation of motion for the OMS amplitude Q is [8]

$$\ddot{Q} = -2Q - 8\frac{\beta}{N}Q^3. \tag{6}$$

We recall that the dynamical properties of the FPU-β system depend only on the product $\lambda=\varepsilon\beta$. In all the numerical experiments we fix the value of β and we change the value of the energy density $\varepsilon=E/N$, which is our control parameter, where

$$E = \frac{1}{2}\left(P^2 + 2Q^2 + 4\frac{\beta}{N}Q^4\right)$$

is the energy of the nonlinear $N/4$ mode. We excite this mode at $t=0$ always putting $Q\neq 0$ and $P=\dot{Q}=0$. Then, initially, all the energy is the potential energy V, associated to Eq. (6), given by

$$V = Q^2\left(1 + 2\frac{\beta}{N}Q^2\right).$$

We remark that, unlike the case $\beta>0$, with $\beta<0$ the choice of the energy of the system does not determine unequivocally the initial value Q_0 of Q. For $\beta<0$, the extremal values of the potential V are $Q=0$, which is a minimum, and $Q=\pm\sqrt{\frac{N}{4|\beta|}}$ which are maxima, where $V=\frac{N}{8|\beta|}$. For a given value of the energy density $0<\varepsilon<\frac{1}{8|\beta|}$, we have four possible initial values of Q, namely:

$$Q_0 = \pm\sqrt{\frac{N}{4|\beta|}(1 \pm \sqrt{1-8\varepsilon|\beta|})}.$$

Only the "internal" solutions (minus sign under the square root), as initial conditions for the Eq. (6), give bounded solutions. For $\varepsilon=\frac{1}{8|\beta|}$ the "external" values of Q_0 coincide with the internal ones and one has only two solutions.

The external values of Q_0 correspond to unbounded solutions.

For $\beta>0$ the solution of Eq. (6), with initial conditions $Q(0)=Q_0$ and $\dot{Q}(0)=0$, is

$$Q(t) = Q_0\,\mathrm{cn}(\Omega t; k_n^2), \tag{7}$$

where cn is the periodic Jacobi elliptic function with period $T=4K(k)/\Omega$, $K(k)$ is the complete elliptic integral of the first kind and, in terms of energy density

$$Q_0^2 = \frac{N}{4\beta}(\sqrt{1+8\varepsilon\beta} - 1), \tag{8}$$

$$k^2 = \frac{1}{2}\frac{\sqrt{1+8\varepsilon\beta}-1}{\sqrt{1+8\varepsilon\beta}}, \tag{9}$$

and

$$\Omega^2 = \frac{2}{1-2k^2}. \tag{10}$$

We remark that the same formulas hold for $n=3N/4$, so the modes $n=N/4$ and $n=3N/4$ have the same behavior. For $\beta<0$ and energy density in the interval $0<\varepsilon<\frac{1}{8|\beta|}$, the solution of Eq. (6), with initial conditions $Q(0)=Q_0$ and $\dot{Q}(0)=0$, is

$$Q(t) = Q_0\,\mathrm{sn}(\Omega t + K; k^2), \tag{11}$$

where sn is the Jacoby elliptic sine and, in terms of energy density,

$$Q_0^2 = \frac{N}{4|\beta|}(1 - \sqrt{1-8\varepsilon|\beta|}), \tag{12}$$

$$k^2 = \frac{1-\sqrt{1-8\varepsilon|\beta|}}{1+\sqrt{1-8\varepsilon|\beta|}}, \tag{13}$$

and

$$\Omega^2 = \frac{2}{1+k^2}. \tag{14}$$

Also in this case, the modes $n=N/4$ and $n=3\ N/4$ have the same behavior.

III. EQUATIONS FOR THE PERTURBED MODES

Let us consider the bounded OMS, given by Eq. (7) when $\beta>0$ and by Eq. (11) when $\beta<0$, found in the previous section.

To study the stability of these OMSs, we recall that in the Fermi-Pasta-Ulam β-system with periodic boundary conditions, the differential equation for the rth mode is [8]

$$\ddot{Q}_r = -\omega_r^2 Q_r - \frac{\beta\omega_r}{2N}\sum_{i,l,j=1}^{N-1}\omega_i\omega_j\omega_l C_{rijl}Q_iQ_jQ_l, \qquad (15)$$

where $r=1,2,\ldots,N-1$, ω_r is given by Eq. (5), and

$$C_{rijl} = -\Delta_{r+i+j+l} + \Delta_{r+i-j-l} + \Delta_{r-i+j-l} + \Delta_{r-i-j+l}$$

with

$$\Delta_k = \begin{cases} (-1)^m & \text{if } k=mN \text{ with } m\in Z \\ 0 & \text{otherwise} \end{cases}.$$

The coefficients C_{rijl} are invariant under any permutation of the i, j, and l indexes.

Now, let us suppose that only a mode n is excited. If ΔQ_r is the error on the mode Q_r, from Eq. (15) one obtains:

$$\Delta\ddot{Q}_r = -\omega_r^2\Delta Q_r - \frac{3\beta\omega_r}{2N}\omega_n^2Q_n^2\sum_{l=1}^{N-1}\omega_l C_{rnnl}\Delta Q_l, \qquad (16)$$

where

$$C_{rnnl} = -\Delta_{r+2n+l} + 2\delta_{r,l} + \Delta_{r-2n+l}$$

and $\delta_{r,l}$ is the Kronecker delta. For $n=N/4$ one has

$$\Delta_{r+N/2+l} = -\theta\left(\frac{N}{2}-r-1\right)\delta_{l,N/2-r} + \theta\left(r-\frac{N}{2}-1\right)\delta_{l,3N/2-r},$$

$$\Delta_{r-N/2+l} = \theta\left(\frac{N}{2}-r-1\right)\delta_{l,N/2-r} - \theta\left(r-\frac{N}{2}-1\right)\delta_{l,3N/2-r},$$

where

$$\theta(x) = \begin{cases} 0 & \text{if } x<0 \\ 1 & \text{if } x\geq 0 \end{cases}$$

is the Heaviside function. Since $\omega_{N/2-r}=2\cos\pi r/N$ and $\omega_{3N/2-r}=-2\cos\pi r/N$, Eq. (16) can be written as

$$\Delta\ddot{Q}_r = -\left(1+\frac{6\beta}{N}Q^2\right)\omega_r^2\Delta Q_r - \frac{12\beta}{N}Q^2\sin\frac{2\pi r}{N}\left\{\theta\left(\frac{N}{2}-r-1\right)\Delta Q_{\frac{N}{2}-r} + \theta\left(r-\frac{N}{2}-1\right)\Delta Q_{\frac{3N}{2}-r}\right\}, \qquad (17)$$

where $Q=Q_{N/4}$ is given by Eq. (7) for $\beta>0$ and by Eq. (11) for $\beta<0$. We remark that in Eq. (17) the off-diagonal terms vanish only for $r=\frac{N}{4}$, $\frac{N}{2}$, and $\frac{3N}{4}$. For these values of r one has:

$$\Delta\ddot{Q}_{N/2} = -4\left(1+6\beta\frac{Q^2}{N}\right)\Delta Q_{N/2},$$

$$\Delta\ddot{Q} = \Delta\ddot{Q}_{N/4} = -2\left(1+12\beta\frac{Q^2}{N}\right)\Delta Q_{N/4},$$

$$\Delta\ddot{Q}_{3N/4} = -2\Delta Q_{3N/4}.$$

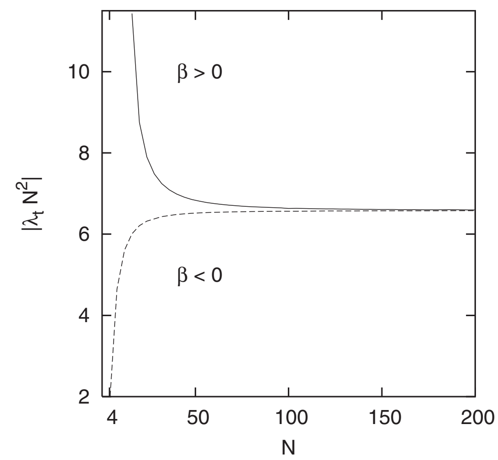

FIG. 1. Numerical results for $n=N/4$: $|\lambda_t N^2|$ vs N for $\beta>0$ and $\beta<0$.

IV. STABILITY OF THE $\frac{N}{4}$ MODE SOLUTION

A recent numerical study of the stability of the one-mode solutions for the α and β models is reported in [14]. By means of the Floquet method, the instability of a given set of modes is recognized when there are eigenvalues of the corresponding monodromy matrix with modulus exceeding 1 by 10^{-5}. No explicit analytical results on the dependence on N of the energy density threshold are given in general and for the $N/4$ mode in particular.

In this paper we present first the numerical results, then we expose the method of analysis of the stability of the equations of perturbed modes and the analytical results obtained. Explicit dependence on N of the threshold value λ_t will be given, for large values of N, both for $\beta>0$ and $\beta<0$.

A. Numerical results

To study numerically the stability of the $N/4$ mode, we utilize the same method used in Ref. [17], where we tested the stability of the $N/2$ mode with $\beta>0$, against the errors introduced by the algorithm of numerical integration. The equations of motion in the variables q_i, p_i are integrated by means of a bilateral symplectic algorithm [19]. In all the numerical experiments we fix the value of β (1 or -1) and we change the value of the energy density $\varepsilon=E/N$. We excite the OMS at $t=0$ always putting $Q\neq 0$ and $P=0$. From the inverse transformations of Eqs. (3) and (4), the initial values of $q_i(0)$ and $p_i(0)$ are obtained.

A preliminary numerical study of the stability of the $N/4$ mode, for $\beta>0$, was reported in Ref. [17], where a dependence of threshold value λ_t on N^{-2}, for large values of N, was found. In this paper we present the results of a numerical analysis extended to larger values of N both for $\beta>0$ and $\beta<0$. This analysis confirms that for large values of N and $\beta>0$ the product $\lambda_t N^2$, as a function of N, decreases and converges to the asymptotic value $(2/3)\pi^2$, double of the asymptotic value of the case $N/2$.

For $\beta<0$, the product $|\lambda_t N^2|$ increases with N and converges toward the same asymptotic value. Figure 1 shows this behavior of the product $|\lambda_t N^2|$ as a function of N for $\beta>0$ and $\beta<0$.

B. Analytical results for $\beta > 0$

With reference to Eq. (17), the stability of the system can be studied considering separately the case $r \leq N/2-1$ and $r \geq N/2+1$. We have verified that in both cases one obtains the same final results. Then, let us consider the case $r \leq N/2-1$. From Eq. (17) the equation for the rth perturbed mode is

$$\Delta\ddot{Q}_r = -\left(1 + 6\frac{\beta}{N}Q^2\right)\omega_r^2 \Delta Q_r - 12\frac{\beta}{N}Q^2 \sin 2\pi\frac{r}{N}\Delta Q_{N/2-r}. \tag{18}$$

From numerical results, we know that λ_t is very small for large values of N so, from Eq. (9), we can suppose $k^2 \ll 1$. If we now consider the expansion of the elliptic function cn in terms of trigonometric function [20] and we perform the change of variable $\tau = (\pi\Omega/2K)t$, taking into account Eqs. (8) and (10), from Eq. (18), we obtain, up to k^6 terms,

$$\begin{aligned}\Delta\ddot{Q}_r(\tau) = &-\frac{1}{2}\left[1 - \frac{q^2}{6} - \frac{2}{9}q^3 + \left(2q + \frac{4}{3}q^2 + \frac{85}{72}q^3\right)\cos 2\tau \right.\\ &\left. + \left(\frac{q^2}{3} + \frac{4}{9}q^3\right)\cos 4\tau + \frac{1}{24}q^3 \cos 6\tau\right]\omega_r^2 \Delta Q_r \\ &- \left[2q + q^2 + \frac{7}{9}q^3 + \left(2q + \frac{4}{3}q^2 + \frac{85}{72}q^3\right)\cos 2\tau \right.\\ &\left. + \left(\frac{1}{3}q^2 + \frac{4}{9}q^3\right)\cos 4\tau + \frac{1}{24}q^3 \cos 6\tau\right] \\ &\times \sin 2\pi\frac{r}{N}\Delta Q_{\frac{N}{2}-r},\end{aligned} \tag{19}$$

$$\begin{aligned}\Delta\ddot{Q}_{N/2-r}(\tau) = &-\frac{1}{2}\left[1 - \frac{q^2}{6} - \frac{2}{9}q^3 + \left(2q + \frac{4}{3}q^2 + \frac{85}{72}q^3\right)\cos 2\tau \right.\\ &\left. + \left(\frac{q^2}{3} + \frac{4}{9}q^3\right)\cos 4\tau + \frac{1}{24}q^3 \cos 6\tau\right] \\ &\times \omega_{N/2-r}^2 \Delta Q_{N/2-r} - \left[2q + q^2 + \frac{7}{9}q^3 \right.\\ &+ \left(2q + \frac{4}{3}q^2 + \frac{85}{72}q^3\right)\cos 2\tau \\ &\left. + \left(\frac{1}{3}q^2 + \frac{4}{9}q^3\right)\cos 4\tau + \frac{1}{24}q^3 \cos 6\tau\right] \\ &\times \sin 2\pi\frac{r}{N}\Delta Q_r,\end{aligned} \tag{20}$$

where

$$q = \frac{3}{4}k^2. \tag{21}$$

The system of differential Eqs. (19) and (20) is of Hill type and the stability of the OMS corresponding to $n=N/4$ can be analyzed by studying the stability of the coupled modes r and $N/2-r$, for each value of $r \leq N/2-1$. The threshold value λ_t for the mode $N/4$ is the smallest between the values of λ_t of these couples of equations.

Let $X(\tau)$ be the (4×4) fundamental matrix of the system of Eqs. (19) and (20) that satisfies the initial condition $X(0)=\mathbf{I}$, where $\mathbf{I}$ is the (4×4) identity matrix. Then the system is equivalent to the following matrix equation:

$$\frac{d}{d\tau}X(\tau) = AX(\tau) + qB(\tau)X(\tau) + q^2C(\tau)X(\tau) + q^3D(\tau)X(\tau), \tag{22}$$

where

$$A = \begin{pmatrix} 0 & 1 & 0 & 0 \\ -a_1^2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & -a_2^2 & 0 \end{pmatrix}$$

with $a_1^2 = \omega_r^2/2$ and $a_2^2 = \omega_{N/2-r}^2/2$;

$$B = \begin{pmatrix} 0 & 0 & 0 & 0 \\ -2a_1^2 \cos 2\tau & 0 & -2b(1+\cos 2\tau) & 0 \\ 0 & 0 & 0 & 0 \\ -2b(1+\cos 2\tau) & 0 & -2a_2^2 \cos 2\tau & 0 \end{pmatrix}$$

with $b = \sin(2\pi r/N)$ and C and D are matrices whose elements that differ from zero are

$$c_{21} = \left(\frac{1}{6} - \frac{4}{3}\cos 2\tau - \frac{1}{3}\cos 4\tau\right)a_1^2,$$

$$c_{23} = -\left(1 + \frac{4}{3}\cos 2\tau + \frac{1}{3}\cos 4\tau\right)b,$$

$$c_{41} = c_{23},$$

$$c_{43} = \frac{c_{21}}{a_1^2}a_2^2,$$

and

$$d_{21} = -\left(-\frac{2}{9} + \frac{85}{72}\cos 2\tau + \frac{4}{9}\cos 4\tau + \frac{1}{24}\cos 6\tau\right)a_1^2,$$

$$d_{23} = -\left(\frac{7}{9} + \frac{85}{72}\cos 2\tau + \frac{4}{9}\cos 4\tau + \frac{1}{24}\cos 6\tau\right)b,$$

$$d_{41} = d_{23},$$

$$d_{43} = \frac{d_{21}}{a_1^2}a_2^2,$$

respectively.

We look for solutions of Eq. (22) having the form:

$$X(\tau) = \sum_{0}^{\infty} q^n X_n(\tau), \tag{23}$$

with all $X_n(\tau)$ of class C^∞. We assume that the series $\Sigma_{n=0}^{\infty} q^n[X_n(\tau)]_{jk}$ are all uniformly convergent with respect to τ. This guarantees the derivation term to term with respect to τ.

Inserting Eq. (23) in Eq. (22), we obtain

$$\frac{d}{d\tau}X_0(\tau) = AX_0(\tau) \tag{24}$$

with $X_0(0)=\mathbf{I}$;

$$\frac{d}{d\tau}X_1(\tau) = AX_1(\tau) + B(\tau)X_0(\tau) \tag{25}$$

with $X_1(0)=\mathbf{0}$;

$$\frac{d}{d\tau}X_2(\tau) = AX_2(\tau) + B(\tau)X_1(\tau) + C(\tau)X_0(\tau)$$

with $X_2(0)=\mathbf{0}$ and, for $n\geq 3$, the recurrence relation

$$\frac{d}{d\tau}X_n(\tau) = AX_n(\tau) + B(\tau)X_{n-1}(\tau) + C(\tau)X_{n-2}(\tau) + D(\tau)X_{n-3}(\tau)$$

with $X_n(0)=\mathbf{0}$.

From Eq. (24) one obtains:

$$X_0(\tau) = e^{A\tau}X_0(0) = e^{A\tau}$$

or, in matrix form:

$$X_0(\tau) = \begin{pmatrix} \cos a_1\tau & \dfrac{\sin a_1\tau}{a_1} & 0 & 0 \\ -a_1 \sin a_1\tau & \cos a_1\tau & 0 & 0 \\ 0 & 0 & \cos a_2\tau & \dfrac{\sin a_2\tau}{a_2} \\ 0 & 0 & -a_2 \sin a_2\tau & \cos a_2\tau \end{pmatrix}.$$

Equation (25) gives

$$X_1(\tau) = \int_0^\tau e^{A(\tau-\tau_1)}B(\tau_1)e^{A(\tau_1)}d\tau_1$$
$$= \int_0^\tau X_0(\tau-\tau_1)B(\tau_1)X_0(\tau_1)d\tau_1.$$

In the same way, for $n=2$ and $n=3$, one obtains

$$X_2(\tau) = \int_0^\tau X_0(\tau-\tau_1)B(\tau_1)X_1(\tau_1)d\tau_1 + \int_0^\tau X_0(\tau-\tau_1)C(\tau_1)X_0(\tau_1)d\tau_1,$$

$$X_3(\tau) = \int_0^\tau X_0(\tau-\tau_1)B(\tau_1)X_2(\tau_1)d\tau_1 + \int_0^\tau X_0(\tau-\tau_1)C(\tau_1)X_1(\tau_1)d\tau_1 + \int_0^\tau X_0(\tau-\tau_1)D(\tau_1)X_0(\tau_1)d\tau_1,$$

and in general:

$$X_n(\tau) = \int_0^\tau X_0(\tau-\tau_1)B(\tau_1)X_{n-1}(\tau_1)d\tau_1 + \int_0^\tau X_0(\tau-\tau_1)C(\tau_1)X_{n-2}(\tau_1)d\tau_1 + \int_0^\tau X_0(\tau-\tau_1)D(\tau_1)X_{n-3}(\tau_1)d\tau_1.$$

Since the trace of the matrix $A+qB(\tau)+q^2C(\tau)+q^3D(\tau)$ is equal to zero, from Eq. (22) one has that the determinant of $X(\tau)$ satisfies the relation

$$\det X(\tau) = \det X(0) = \det \mathbf{I} = 1.$$

In particular, for $\tau=\pi$, the period of matrices B, C, and D, the characteristic numbers λ of the system described by Eq. (22), which are also eigenvalues of matrix $X(\pi)$, satisfy the relation

$$\lambda_1\lambda_2\lambda_3\lambda_4 = \det X(\pi) = 1. \tag{26}$$

Thus we can have four real eigenvalues, two real and two complex conjugate eigenvalues or two couples of complex conjugate eigenvalues.

If all the eigenvalues are real and distinct, the system is stable if their values are in the interval $(-1,1)$. Since their product must be equal to one, there is always an eigenvalue λ_i such that $|\lambda_i|>1$, so the system is unstable in this case.

If λ_1 and λ_2 are real, $\lambda_3=\gamma_3+i\delta_3$ and $\lambda_4=\gamma_3-i\delta_3$, one has

$$\lambda_1\lambda_2(\gamma_3^2+\delta_3^2) = 1$$

and the system is unstable also in this case.

The existence of the stability threshold, that we observe numerically by increasing the energy density, must then be associated with the third case, that corresponds to four complex values of the eigenvalue λ. If we put

$$\lambda_1 = \alpha_1 + i\beta_1,$$

$$\lambda_2 = \alpha_2 + i\beta_2,$$

$$\lambda_3 = \bar{\lambda}_1,$$

$$\lambda_4 = \bar{\lambda}_2,$$

and we suppose the stability of the system, we have, from relation (26):

$$\alpha_2^2 + \beta_2^2 = 1,$$

$$\alpha_2^2 + \beta_2^2 = 1, \tag{27}$$

and

$$\mathrm{Tr}\, X(\pi) = 2\alpha_1 + 2\alpha_2.$$

Furthermore, since the relation is valid:

$$\lambda_1^2 + \lambda_2^2 + \lambda_3^2 + \lambda_4^2 = \mathrm{Tr}[X(\pi)]^2,$$

which, from Eq. (27), can be written as $4(\alpha_1^2 + \alpha_2^2 - 1) = \mathrm{Tr}[X(\pi)]^2$, we have

$$\alpha_1 + \alpha_2 = \frac{\mathrm{Tr}\, X(\pi)}{2},$$

$$\alpha_1^2 + \alpha_2^2 = \frac{\mathrm{Tr}[X(\pi)]^2}{4} + 1.$$

Then we can obtain α_1 and α_2 as solutions of an algebraic equation of second degree, namely

$$\alpha_{1,2} = \frac{\frac{\mathrm{Tr}\, X(\pi)}{2} \pm \sqrt{\frac{\mathrm{Tr}[X(\pi)]^2}{2} + 2 - \frac{[\mathrm{Tr}\, X(\pi)]^2}{4}}}{2}, \tag{28}$$

with the stability condition that $\alpha_{1/2}$ should be real and in the interval $(-1,1)$. Let us calculate $\mathrm{Tr}\, X(\pi)$ and $\mathrm{Tr}[X(\pi)]^2$ by assuming $0 < q \ll 1$ and

$$X(\pi) = X_0(\pi) + qX_1(\pi) + q^2X_2(\pi) + q^3X_3(\pi) + 0(q^4). \tag{29}$$

Hereafter we omit the argument π. It is easy to show that $\mathrm{Tr}\, X_1 = \mathrm{Tr}[X_0X_1] = 0$ and that, up to q^3 terms, the argument Δ of the square root in Eq. (28) can be written as

$$\Delta = F_0 + q^2F_2 + q^3F_3, \tag{30}$$

where

$$F_0 = \frac{\mathrm{Tr}[X_0]^2}{2} - \frac{[\mathrm{Tr}\, X_0]^2}{4} + 2,$$

$$F_2 = \frac{\mathrm{Tr}[X_1]^2}{2} + \mathrm{Tr}[X_0X_2] - \frac{\mathrm{Tr}[X_0]\mathrm{Tr}[X_2]}{2},$$

and

$$F_3 = \mathrm{Tr}[X_0X_3] + \mathrm{Tr}[X_1X_2] - \frac{1}{2}\mathrm{Tr}[X_0]\mathrm{Tr}[X_3].$$

The stability analysis of the system of Eqs. (19) and (20) should be made for each value of r; here we can limit ourselves to the study of the coupled modes $r = N/4 - 1$ and $r = N/4 + 1$. This choice, made for the sake of clarity, is clear if one considers Fig. 2, where the values of mode energies, normalized to the initial value of energy of the $N/4$ mode, are shown for $N = 100$; the mode $N/4$ is initially excited with a value of λ slightly greater than the threshold value. The mode energies are calculated after an integration time equal to that used to study numerically the stability of the mode $N/4$. From the figure it is evident that the first modes that

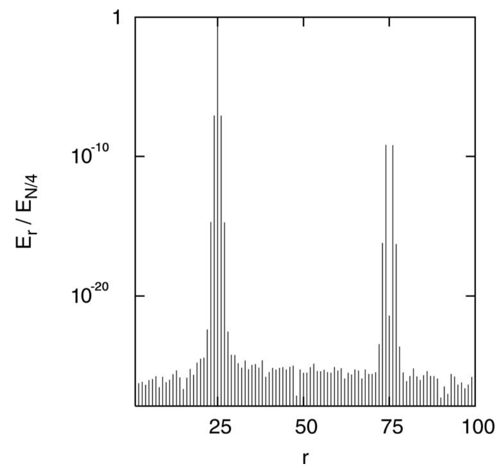

FIG. 2. Normalized mode energy vs mode number r for $N = 100$ and $\beta > 0$. The mode $N/4$ is initially excited with a value of λ slightly greater than the threshold value λ_t.

become unstable are the modes $N/4 \pm 1$ and $3N/4 \pm 1$. This justifies our approach. However, as will be clear in the final discussion, we can analytically prove this fact.

Hereafter we put $r = N/4 - 1$. We obtain:

$$\mathrm{Tr}\, X_0 = 2(\cos a_1\pi + \cos a_2\pi),$$

$$\mathrm{Tr}[X_0]^2 = 4(\cos^2 a_1\pi + \cos^2 a_2\pi - 1),$$

and

$$F_0 = (\cos a_1\pi - \cos a_2\pi)^2.$$

The calculation of the other traces are much more complicated, but they can be evaluated by utilizing the package of the computer system for symbolic calculations MATHEMATICA [21]. The result is that the right-hand term of relation (28) can be exactly calculated.

Starting from $q = 0$, the argument Δ of the square root in Eq. (28), which is positive, decreases with rising q and we have two real solutions for $\alpha_{1,2}$ in the interval $(-1,1)$ as long as $\Delta = 0$ for some value q_t of q. For values of $q > q_t$ we have two complex conjugate solutions, the initial hypothesis that $\alpha_{1,2}$ should be real is not satisfied and the system becomes unstable. Then the threshold value q_t for the instability is given by Eq. (30) when $\Delta = 0$, namely when

$$F_0 + q_t^2F_2 + q_t^3F_3 = 0. \tag{31}$$

This formula allows us to calculate the threshold value of q, and then of k^2, not only asymptotically, but also for any value of N for which q is sufficiently small. For very large values of N, we obtain

$$F_0 = \pi^{10}\frac{1}{N^6} - \frac{1}{6}\pi^{12}(3 + 2\pi^2)\frac{1}{N^8} + 0\left(\frac{1}{N^{10}}\right),$$

$$F_2 = -\pi^6\frac{1}{N^2} + \frac{1}{6}\pi^8(43 + 2\pi^2)\frac{1}{N^4} + 0\left(\frac{1}{N^6}\right),$$

$$F_3 = \frac{11}{3}\pi^6\frac{1}{N^2} - \pi^8\left(\frac{211}{36} + \frac{11}{9}\pi^2\right)\frac{1}{N^4} + 0\left(\frac{1}{N^6}\right),$$

and from Eq. (31):

$$q_t = \frac{\pi^2}{N^2} + \frac{31}{6}\frac{\pi^4}{N^4} + 0\left(\frac{1}{N^6}\right). \quad (32)$$

Since from relation (9)

$$\lambda \approx \frac{k^2}{2} + \frac{10}{3}k^4 = \frac{2}{3}q + \frac{8}{3}q^2,$$

formula (32) implies for the threshold value λ_t of λ

$$\lambda_t N^2 = \frac{2}{3}\pi^2 + \frac{56}{9}\frac{\pi^4}{N^2} + 0\left(\frac{1}{N^4}\right). \quad (33)$$

Then, we obtain the result, found numerically by direct integration of motion equations that, for large values of N, the product $\lambda_t N^2$ decreases toward the constant value $\frac{2}{3}\pi^2$.

The case $r \geq N/2+1$ can be studied in the same way. In this case, the modes analyzed are the modes $3N/4 \pm 1$ which, together the modes $N/4 \pm 1$, are the first modes that become unstable. We find that the threshold value λ_t is given again by formula (33).

To give an idea of the degree of approximation of formula (33), let us compare the analytical with the numerical results. For example, for $N=100$, the numerical integration of motion equations gives $\lambda_t N^2 = 6.641\,00$, to compare with the value $\lambda_t N^2 = 6.640\,35$, given by formula (33); the difference is 0.01%.

C. Analytical results for $\beta < 0$

For $\beta < 0$, we can follow the same procedure used for $\beta > 0$. The starting equation is the Eq. (17) with function Q given by formula (11) and Q_0^2, k^2, and Ω^2 given, respectively, by Eqs. (12)–(14). We have a system of equations similar to Eqs. (19) and (20) with the same link [Eq. (21)] between q and k. Also in this case, the first modes that become unstable are the modes $N/4 \pm 1$ and $3N/4 \pm 1$, so the study of the stability can be limited to the coupled modes $N/4-1$ and $N/4+1$. If we introduce matrices A and B, we see that matrix A has the same elements of the matrix A of the case $\beta > 0$, whereas the elements of matrix B change sign. As a consequence, for $\beta < 0$, X_0 and X_1^2 remain the same, X_1 changes sign and we have again $\mathrm{Tr}[X_1] = \mathrm{Tr}[X_0 X_1] = 0$. As concerns the matrices C and D, their elements different from zero are

$$c_{21} = -a_1^2\left[-\frac{1}{6} - \frac{4}{3}\cos 2\tau + \frac{1}{3}\cos 4\tau\right],$$

$$c_{23} = b\left[\frac{5}{3} + \frac{4}{3}\cos 2\tau - \frac{1}{3}\cos 4\tau\right],$$

$$c_{41} = c_{23},$$

$$c_{43} = c_{21}\frac{a_2^2}{a_1^2},$$

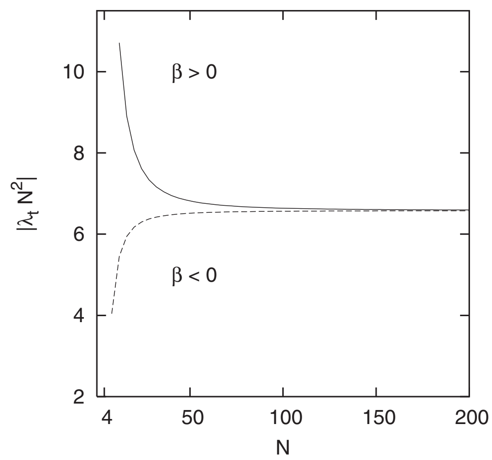

FIG. 3. Analytical results for $n=N/4$: $|\lambda_t N^2|$ vs N for $\beta > 0$ and $\beta < 0$.

$$d_{21} = a_1^2\left[\frac{2}{9} + \frac{85}{72}\cos 2\tau - \frac{4}{9}\cos 4\tau + \frac{1}{24}\cos 6\tau\right],$$

$$d_{23} = b\left[\frac{5}{3} + \frac{85}{72}\cos 2\tau - \frac{4}{9}\cos 4\tau + \frac{1}{24}\cos 6\tau\right],$$

$$d_{41} = d_{23},$$

$$d_{43} = d_{21}\frac{a_2^2}{a_1^2}.$$

Following the same procedure used for the case $\beta > 0$, one finds that $\mathrm{Tr}[X2]$ and $\mathrm{Tr}[X_0 X_2]$ assume the same values they assume for $\beta > 0$. Then also F_0 and F_2 do not change. The difference between the two cases is given by the coefficient F_3 of q^3 which for $\beta < 0$ is

$$F_3 = -\frac{19}{3}\frac{\pi^6}{N^2} + \frac{899}{36}\frac{\pi^8}{N^4} + \frac{19}{9}\frac{\pi^{10}}{N^4} + 0\left(\frac{1}{N^6}\right)$$

and by the different link between λ and q given, from relation (13), by

$$|\lambda| \approx \frac{k^2}{2} - k^4 = \frac{2}{3}q - \frac{16}{9}q^2.$$

The final result is

$$|\lambda_t N^2| = \frac{2}{3}\pi^2 - \frac{5}{3}\frac{\pi^4}{N^2} + 0\left(\frac{1}{N^4}\right). \quad (34)$$

The product $|\lambda_t N^2|$ is therefore an increasing function of N and converges asymptotically toward the same limit $2\pi^2/3$ as in the case $\beta > 0$. In Fig. 3 $|\lambda_t N^2|$, given by Eqs. (33) and (34), is shown as a function of N. To remark the excellent agreement with the numerical results shown in Fig. 1, in Fig. 4 numerical and analytical results are compared for N between 80 and 100: the irregular curves refer to numerical results.

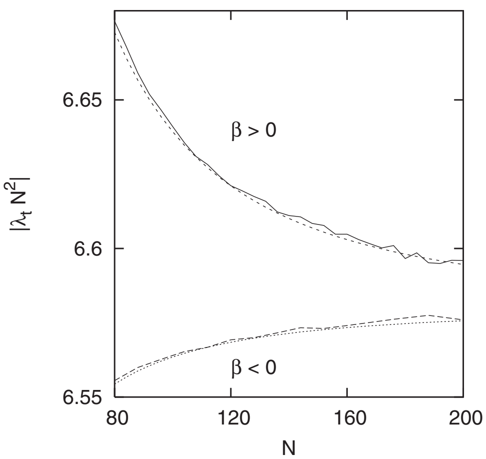

FIG. 4. Comparison between numerical and analytical results: irregular curves refer to numerical results.

V. DISCUSSION

In this paper we have studied the stability of the $N/4$ ($\pi/2$-mode) one-mode nonlinear solution of the Fermi-Pasta-Ulam-β system, both for positive and negative values of the nonlinearity parameter β. The numerical results, obtained through the numerical integration of motion equations, have been explained, at least asymptotically, by a detailed Floquet analysis of the system of differential equations which describe the perturbed modes. The analytical results, formulas (33) and (34), have been obtained by an application of the Floquet method. We want to remark on some aspects concerning the necessity of considering expansion up to terms q^3 in Eqs. (19), (20), and (29). If one considers only q-terms in the first two equations and formally look for solutions of the form $X(t)=X_0(t)+qX_1(t)+q^2X_2(t)$, one finds the correct asymptotic value $\lambda_t N^2=2\pi^2/3$, but one observes that the product $\lambda_t N^2$ is a decreasing function of N both for $\beta>0$ and $\beta<0$; furthermore, also with the addition of q^2 terms in Eqs. (19) and (20) it is impossible to obtain the behavior shown in Fig. 1. One finds indeed that the correction of order $1/N^2$ to the leading term $2\pi^2/3$ is equal and positive in the two cases. Only the q^3 terms allow one to obtain the correct behavior.

Finally, we remark that our method can be utilized to evaluate the threshold value $|\lambda_t|$ for any value of index r in Eqs. (19) and (20). If one calculates the asymptotic value of $|\lambda_t N^2|$ for $r=N/4\pm j$ and $3N/4\pm j$, one finds the result

$$|\lambda_t N^2| = \frac{2}{3}\pi^2 j^2,$$

so the first modes that become unstable are the modes $N/4\pm 1$ and $(3N)/4\pm 1$, as suggested by Fig. 2 and as we have previously assumed.

This work was supported by MUR, Italy.

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