# Numerical analysis of the one-mode solutions in the Fermi-Pasta-Ulam system

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The stability of the one-mode nonlinear solutions of the Fermi-Pasta-Ulam $\beta$ system is numerically investigated. No external perturbation is considered for the one-mode exact analytical solutions, the only perturbation being that introduced by computational errors in the numerical integration of motion equations. The threshold energy for the excitation of the other normal modes and the dynamics of this excitation are studied as a function of the parameter $\mu$ characterizing the nonlinearity, the energy density $\epsilon$ and the number $N$ of particles of the system. The results achieved confirm in part previous ones, obtained with a linear analysis of the problem of the stability, and clarify the dynamics by which a one-mode exchanges energy with the other modes with increasing energy density. In a range of energy density near the threshold value and for various values of the number of particles $N$, the nonlinear one-mode exchanges energy with the other linear modes for a very short time, immediately recovering all its initial energy. This sort of recurrence is very similar to Fermi recurrences, even if in the Fermi recurrences the energy of the initially excited mode changes continuously and only periodically recovers its initial value. A tentative explanation for this intermittent behavior, in terms of Floquet's theorem, is proposed. Preliminary results are also presented for the Fermi-Pasta-Ulam $\alpha$ system which show that there is a stability threshold, for large $N$, independent of $N$.

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## I. INTRODUCTION

Since the computer experiment of Fermi, Pasta, and Ulam (FPU) [1], many theoretical and numerical investigations followed to explain the unexpected results of the experiment [2–7]. What one expected according to a theorem of Poincarè [8] and a theorem proved by Fermi [9] himself in his youth, and what was instead observed, has been described in several papers (see, e.g., Ref. [10]) in which various aspects of the experiment have been analyzed in the framework of the KAM theorem [11], the ergodic problem [12], statistical mechanics, and the chaotic behavior of dynamical systems [13–15].

It is well known [16,17] that, for a periodic FPU $\beta$ chain with an even number of oscillators, an initial condition with only a set of excited modes, all having even (odd) indices only, cannot lead to the excitation of modes having odd (even) indices. This means that, if one considers the set of all modes partitioned in the two subsets of the even and odd modes, an initial excitation, completely contained in one of the two subsets, cannot propagate to the other.

There are also other partitions. For example, partitions exist for which a subset contains one mode only [18]. More specifically, for each of the modes

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

[of course when $N$ has the divisibility property required for $n$ in Eq. (1) to be an integer] one has that, if only one of these modes is initially excited, it remains excited without transferring energy to any other mode.

An important problem is obviously the stability of these one-mode solutions (OMSs), since it is reasonable to expect some relation between the loss of their stability and the onset of chaos in the system. In some sense, the destabilization of the nonlinear modes can provide an ''upper bound'' estimate for the onset of large scale chaos. The analysis of the stability of a generic OMS is very difficult from a mathematical point of view. Only for the case $n=N/2$ are there analytical results (see, for example, Refs. [18–21]) which estimate the threshold energy density for the mode to become unstable. In fact the mode $n=N/2$ is the simplest one, since the different components of the perturbation, in modal space, are all decoupled and are described by a single Lamé equation.

In this paper we numerically revisit the problem of the stability of OMSs. We make a numerical study of the stability of OMSs as a function of the number $N$ of particles and the product $\epsilon\mu$, where $\epsilon$ is the energy density and $\mu$ is the parameter of nonlinearity in the Hamiltonian of the system. The analysis, based on the numerical integration of the full nonlinear FPU model, is extensively made for the case $\mu>0$. Preliminary results are also presented for the case $\mu<0$. No external perturbation is considered for the OMS, the only perturbation being that introduced by computational errors in numerical integration of motion equations. This simple method works very well: our results confirm previous ones obtained with a linear analysis of the problem of the stability [18–21] and clarify the dynamics by which a nonlinear one-mode exchanges energy with the other linear modes, with increasing energy densities. We find that, in a large range of initial excitation energy density, the energy of the OMSs remains constant for very long intervals of time, and for short intervals there is partial transfer to other linear modes; furthermore the OMSs corresponding to the two values $n=N/4$ and $n=\frac{3}{4}N$ and the OMSs corresponding to $n=N/3$ and $n=\frac{2}{3}N$ have the same stability properties.

As regards the FPU $\alpha$ system, we find that the OMS $N/2$ is not always instable for very large values of $N$, independent of the sign of the nonlinearity parameter $\mu$. Our results are in disagreement with those of Ref. [19] and in agreement with those of Ref. [21].

 

## II. FPU SYSTEM

The FPU system is a one-dimensional chain of oscillators (with unit mass), with a weakly nonlinear nearest-neighbor interaction. Calling $q_n$ and $p_n$ the coordinates and the momenta of the oscillators, we have the Hamiltonian

$$H=\frac{1}{2}\sum_{k=1}^{N} p_k^2+\frac{1}{2}\sum_{k=1}^{N}(q_{k+1}-q_k)^2+\frac{\mu}{r}\sum_{k=1}^{N}(q_{k+1}-q_k)^r, \tag{2}$$

with $r=3$ for the FPU $\alpha$ system, $r=4$ for the FPU $\beta$ system, and $q_{N+1}=q_1$ in both cases. We remark that all quantities in Eq. (2) are dimensionless.

If we introduce the normal coordinates $Q_k$ and $P_k$ of the normal modes through the relations

$$Q_k=\sum_{j=1}^{N} S_{kj}q_j, \tag{3}$$

$$P_k=\sum_{j=1}^{N} S_{kj}p_j, \tag{4}$$

$$S_{kj}=\frac{1}{\sqrt{N}}\left(\sin\frac{2\pi kj}{N}+\cos\frac{2\pi kj}{N}\right), \tag{5}$$

the harmonic energy of mode $k$ is

$$E_k=\frac{1}{2}(P_k^2+\omega_k^2Q_k^2), \tag{6}$$

where, in the case of periodic boundary conditions,

$$\omega^2{}_k=4\sin^2\frac{\pi k}{N}. \tag{7}$$

Since $\omega_k=\omega_{N-k}$, there are only $N/2$ different frequencies (if we assume $N$ even, for simplicity).

From Eq. (2), the Hamilton equations are obtained in the variables $q_k$ and $p_k$, which, integrated by standard methods, allow one to calculate the normal modes and the energy of each mode.

## III. ONE-MODE SOLUTIONS

From now on we refer only to the FPU $\beta$ system. For $\mu=0$, all normal modes oscillate independently and their energies $E_k$ are constants of motion. In the anharmonic case ($\mu\neq 0$), the normal modes are instead coupled and the variables $Q_k$ do not have simple sinusoidal oscillations. The differential equation for the $k$th mode is [18]

$$\ddot{Q}_k=-\omega_k^2Q_k-\frac{\mu\omega_k}{2N}\sum_{i,j,l}^{N-1}\omega_i\omega_j\omega_l C_{kijl}Q_iQ_jQ_l$$

$$(k=1,\ldots,N-1), \tag{8}$$

where

$$C_{ijkl}=-\triangle_{i+j+k+l}+\triangle_{i+j-k-l}+\triangle_{i-j+k-l}+\triangle_{i-j-k+l}, \tag{9}$$

being $\triangle_k=(-1)^m$ for $k=mN$, if $m$ is a positive integer, and $\triangle_k=0$ otherwise.

The nonlinear OMSs correspond to the values of $n$ reported in Eq. (1). From Eqs. (8) and (9), one deduces [18] that, if only one of these modes is initially excited, it remains excited without transferring energy to any other mode. In this case, the equation of motion for the excited mode amplitude $Q_n$ is

$$\ddot{Q}_n=-\omega_n^2Q_n-\frac{\mu\omega_n^4C_{nnnn}}{2N}Q_n^3. \tag{10}$$

If we assume that at time $t=0$ $Q_n\neq 0$ and $P_n=0$, the solution of Eq. (10) is

$$Q_n(t)=A\,\mathrm{cn}(\Omega_n t,k), \tag{11}$$

where $\Omega_n$ and the modulus $k$ of the Jacobi elliptic function cn both depend on $A$:

$$\Omega_n=\omega_n\sqrt{1+\delta_nA^2}, \tag{12}$$

$$k=\sqrt{\frac{\delta_nA^2}{2(1+\delta_nA^2)}}, \tag{13}$$

with $\delta_n=\mu\omega_n^2C_{nnnn}/2N$.

Solution (11) is periodic with period $T_n=4K(k)/\Omega_n$ where $K(k)$ is the complete elliptic integral of the first kind. The energy of the mode is

$$E_n=\frac{1}{2}\left(P_n^2+\omega_n^2Q_n^2+\mu\frac{\omega_n^4Q_n^4C_{nnnn}}{4N}\right). \tag{14}$$

The stability properties of the nonlinear mode $N/2$ was studied analytically some years ago. In Ref. [19], the stability analysis of this mode starts from the equations of motion for the variables $q_k$. From Eq. (3) and the properties of $S_{kj}$ one has, if the only excited mode is the mode $N/2$:

$$q_k=\frac{1}{\sqrt{N}}(-1)^k\ Q_{N/2},\quad k=1,2,\ldots,N. \tag{15}$$

These relations imply that the equations of motion reduce to a single equation, describing the anharmonic oscillations of each particle, whose solution is the Jacobi elliptic cosine function. Perturbing this solution, and passing to normal modes variables $Q_k$ one obtains a Lamé equation. The stability of the solutions of this equation, which is an example of Hill's equation, and then the stability of the mode $N/2$, is studied with the Floquet theory. A numerical analysis shows that the first modes which are excited, as the energy density increases, are the modes $k=N/2-1$ and $N/2+1$. A simple approximate formula, valid for large $N$ and $\mu=1$, and derived approximating Hill's matrix with a $3\times 3$ matrix, gives, for the threshold energy density,

$$\epsilon_t = \frac{E_t}{N} = \frac{3.226}{N^2} + 0(N^{-4}). \tag{16}$$

The problem of stability of the mode $N/2$ was also tackled in Ref. [20]. In the limit of large $N$, the formula

$$\epsilon_t = \frac{E_t}{N} = \frac{\pi^2}{3N^2} \approx \frac{3.29}{N^2} \tag{17}$$

was derived for the threshold energy density. This result is slightly different from Eq. (16) and the small difference is probably due to the rough estimate of the eigenvalue spectrum of the Hill's matrix in Ref. [19].

The problem of stability of an OMS was reconsidered subsequently in Ref. [18] with a detailed analysis of the mode $N/2$. This is the simplest case, because, as we have seen, the different components of the perturbation, in modal space, are all decoupled and can be reduced to the single Lamé equation

$$\ddot{x}_r = -\omega_r^2 \left[ 1 + \frac{12\mu A^2 cn^2(\Omega_{N/2}t;k)}{N} \right] x_r, \quad r = 1, \ldots, N-1. \tag{18}$$

To obtain this equation in a very simple way, we observe that, from Eq. (2), with $r=4$, one has

$$\dot{p}_k = q_{k+1} + q_{k-1} - 2q_k + \mu[(q_{k+1}-q_k)^3 - (q_k - q_{k-1})^3].$$

If the coordinates $q_k$ are affected by some error, then the error on the $\dot{p}_k$, $\triangle \dot{p}_k$, will be

$$\triangle \dot{p}_k = \triangle q_{k+1} + \triangle q_{k-1} - 2\triangle q_k + 3\mu[(q_{k+1}-q_k)^2 \times (\triangle q_{k+1} - \triangle q_k) - (q_k - q_{k-1})^2 (\triangle q_k - \triangle q_{k-1})],$$

and then from Eq. (15) we have

$$\triangle \dot{p}_k = \triangle q_{k+1} + \triangle q_{k-1} - 2\triangle q_k + \frac{12\mu}{N} Q^2{}_{N/2} \times [\triangle q_{k+1} + \triangle q_{k-1} - 2\triangle q_k].$$

Since $\triangle \dot{q}_k = \triangle p_k$, the last equation reads:

$$\triangle \ddot{q}_k = \left[ 1 + \frac{12\mu}{N} Q^2{}_{N/2} \right] [\triangle q_{k+1} - 2\triangle q_k + \triangle q_{k-1}].$$

Passing to modal variables $Q_k$, we finally have

$$\triangle \ddot{Q}_k = -\omega^2{}_k \left[ 1 + \frac{12\mu}{N} Q^2{}_{N/2} \right] \triangle Q_k, \tag{19}$$

which is Eq. (18).

Let $\beta = \epsilon\mu$. As it is well known, this parameter is invariant under the scale transformation: $p_k \to \lambda N^{-1} p_k$, $q_k \to \lambda N^{-1} q_k$ and $\mu \to \lambda^{-2} N^2 \mu$, where $\lambda$ is the scale parameter. So the dynamics of the FPU $\beta$ system depends only on the control parameter $\beta = \epsilon\mu$.

Let us introduce the quantity

$$\rho = \sin^2(\pi r/N), \tag{20}$$

where $r$ is the mode number. The main results of the stability analysis reported in Ref. [18] are as follows.

(a) For each mode having $\rho > 1/3$, there is a threshold value $\beta_t$ of $\beta$ above which the nonlinear mode $n = N/2$ presents an instability, causing the growth of the mode corresponding to $\rho$, through parametric resonance.

(b) Conversely, modes with $\rho < 1/3$ (i.e., $r/N < 0.196$) are always stable in the linear approximation for any energy density of mode $n = N/2$, so that perturbations of this mode involving only modes with $\rho < 1/3$ never lead to instability. These modes, as well as modes with $\rho > 1/3$, when $\beta < \beta_t$, can grow only if they are triggered by the interaction with other modes which are unstable.

(c) For $N \geqslant 4$ there are always modes with $\rho > 1/3$, so that the mode $N/2$ can never be stable for all energy densities. Since $\beta_t$ is a decreasing function of $\rho$, the first modes to go unstable, when $\beta$ is increased from zero, are the modes $r = N/2 - 1$ and $r = N/2 + 1$, for which $\rho = \cos^2(\pi/N)$. Therefore, for each (even) number $N$ of particles, there is a nonzero value of $\beta_t$, a function of $N$, below which the nonlinear mode $N/2$ is stable. This value tends to zero for $N \to \infty$, namely, $\rho \to 1$.

(d) Using a power series expansion, one obtains, for $\beta_t$ the formula,

$$\beta_t = \frac{\pi^2}{3N^2} + 0(N^{-4}), \tag{21}$$

which confirms the $N^{-2}$ dependence found in Refs. [19] and [20] and the numerical value $\pi^2/3$ of the coefficient of $1/N^2$ in Ref. [20].

## IV. NUMERICAL RESULTS FOR THE CASE *N*/2

In this section, we present the results of our numerical analysis of the stability of the OMS corresponding to $n = N/2$, as a function of $\beta$ and of the number $N$ of particles, based on the numerical integration of the full nonlinear FPU model directly in variables $q_k$ and $p_k$. More precisely, we integrate the equations of motion in the variables $q_k$ and $p_k$ by means of a bilinear symplectic algorithm of the third order, adapted from an algorithm employed previously by Casetti [22]. Initial conditions for the variables $q_k$ and $p_k$ are obtained in the following way. We excite the OMS, at $t = 0$, always putting $Q_{N/2} \neq 0$ and $P_{N/2} = 0$. In all numerical experiments we fix $\mu = 0.1$ and change the value of the energy density $\epsilon = E_{N/2}/N$, where

$$E_{N/2} = \frac{1}{2} \left( P^2_{N/2} + \omega^2_{N/2} Q^2_{N/2} + \mu \frac{\omega^4_{N/2} Q^4_{N/2}}{2N} \right) \tag{22}$$

is the energy of the nonlinear one-mode $N/2$. If we fix the initial value of $E_{N/2}$ (or equivalently $\epsilon$), the initial value of $Q_{N/2}$ is obtained from Eq. (22) with $P_{N/2} = 0$. Finally, from inverse transformations of Eqs. (3) and (4), the values of $q_k(0)$ and $p_k(0)$ are obtained.

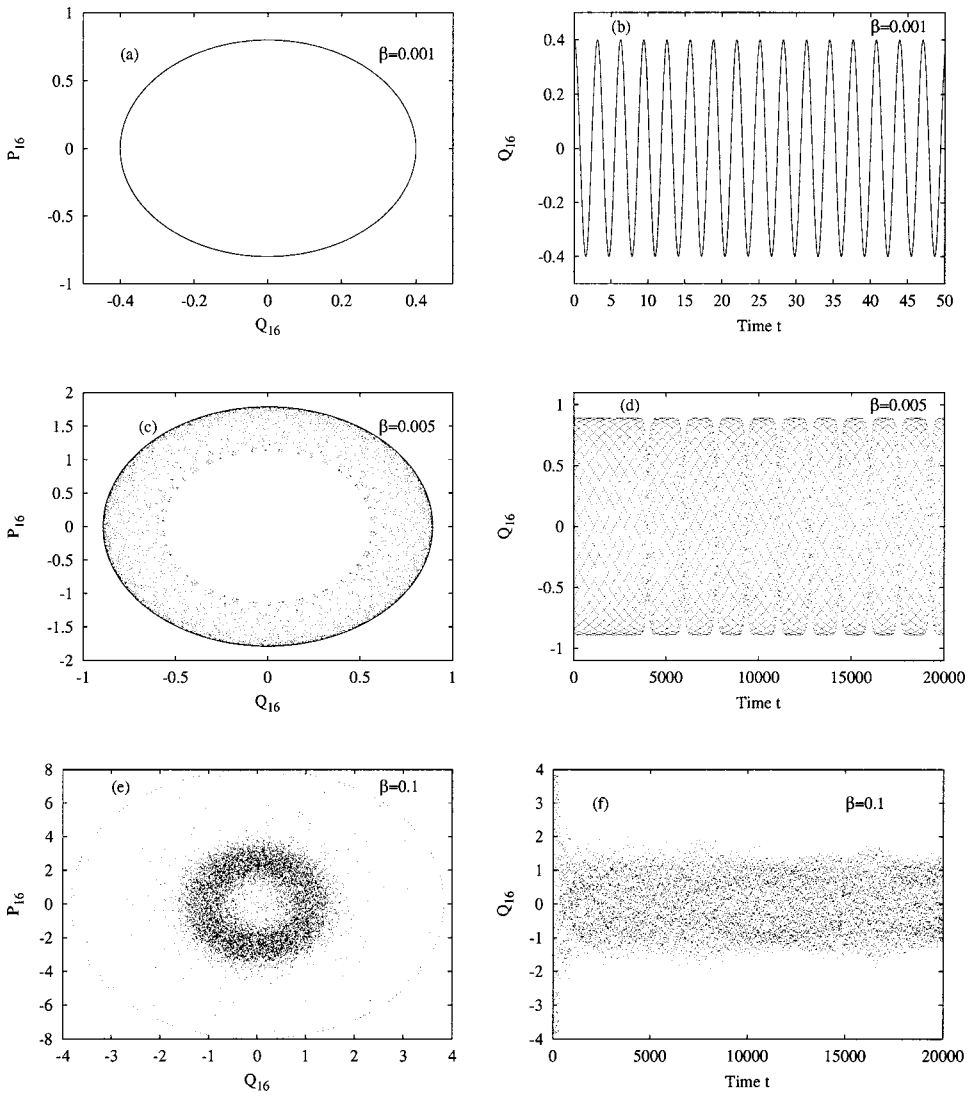


FIG. 1. $P_{16}$ vs $Q_{16}$ [(a), (c), (e)] and $Q_{16}$ vs $t$ [(b), (d), (f)] for three values of $\beta$.

The normal coordinates $Q_{N/2}$ and $P_{N/2}$ of the nonlinear one-mode and the normal coordinates $Q_k$ and $P_k$ of the other normal modes are calculated at fixed time intervals, multiples of the integration step. Then the study of the stability of the OMS is made through the analysis of both the time evolution of $Q_{N/2}$ and $P_{N/2}$ and the evolution of the other modes $Q_k$ and $P_k$ which are generated through computational errors.

For the numerical integration, we use an integration time step $\triangle t$ equal to 0.01. This value is approximately 1/300 of the smallest period of oscillation in the harmonic case and allows us to obtain a control of the total energy $E$ of the lattice, which ensures a relative error $\triangle E/E < 10^{-6}$.

To illustrate the various steps of our method of numerical analysis, let us consider the case $N=32$ and thus the OMS $N/2=16$. In this case $C_{nnnn}=2$, and we have formula (22) for the energy of the nonlinear mode. We take a value of the energy density $\epsilon$ and integrate the equations of motion for the variables $q_k$ and $p_k$. The integration time is fixed in such a way as to observe the instability of nonlinear mode, if the value of $\beta=\epsilon\mu$ is greater than the theoretical value $\beta_t$ [Eq. (21)]. Typical values of this time are of order $10^6\triangle t$.

For $N=32$, we have $\beta_t=\pi^2/3N^2=0.00321$. We consider three values of $\beta$: the first one, $\beta=0.001$, smaller than $\beta_t$, the second one, $\beta=0.005$, larger and the third, $\beta=0.1$, much larger than $\beta_t$. In Fig. 1, the behavior of the nonlinear mode in the plane $(Q_{16},P_{16})$ and $Q_{16}$ as a function of time, for these three values of $\beta$, are shown.

From an inspection of this figure, we observe that, for very small $\beta$, specifically well below the threshold value, the nonlinear OMS $N/2$ is stable and $Q_{16}$ is a periodic function with the same amplitude and same period of the analytical solution. For $\beta=0.005$, above the threshold, the situation is very different. The period of oscillation is equal to the period of the analytical solution and, for very long times, the representative point moves on a closed curve, in the plane $(Q_{16}, P_{16})$ as for values of very small $\beta$; but now, periodically and for short intervals of time, the amplitude of the oscillation varies, due to a decrease of the modal energy, and the representative point of the system moves on an open curve which tends periodically to shrink. For $\beta=0.1$, well above $\beta_t$, we observe a behavior which is probably chaotic. This behavior is also evident if we analyze the modal energy of the mode $N/2$ as a function of time for different values of the

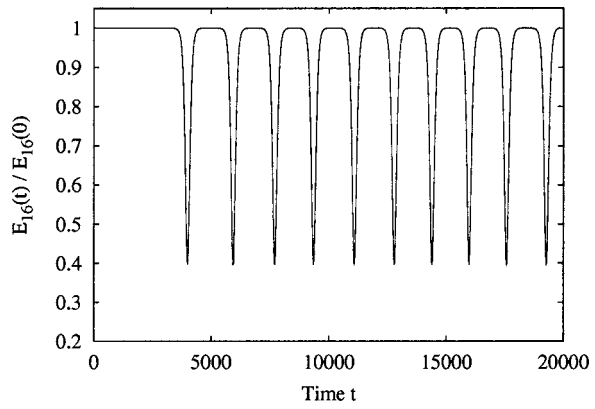


FIG. 2. Energy of mode 16 vs $t$ for $\beta=0.005$.

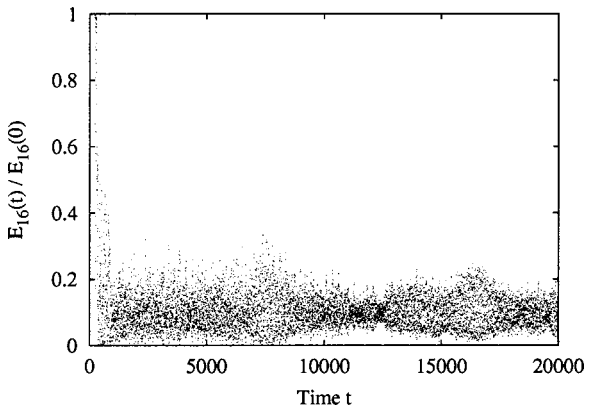


FIG. 3. Energy of mode 16 vs $t$ for $\beta=0.1$.

parameter $\beta$. For values of $\beta$ below the threshold for the excitation of the adjacent mode $N/2-1$, which is the first mode to be excited, the energy of the mode $N/2$ remains constant. For values of $\beta$ above the threshold, we have the behaviors shown in Figs. 2 and 3, which refer to the values $\beta=0.005$ and 0.1, respectively. In these figures, and in all the next figures which show the energy vs time, the energy is always normalized to the initial value of $E_{N/2}$. As can be seen from the last figures, the mode 16 exchanges energy with other modes. According to the theory developed in Refs. [18] and [19], for $\beta=0.005$, we are above the threshold for the excitation of the adjacent mode 15 and the excitation of this mode, due to nonlinear coupling, triggers other linear modes. In Fig. 4 the behavior of the adjacent mode 15 is shown. The contemporary excitation of the other modes, with smaller energy amplitudes, is also observed. We remark that the energy of the mode $N/2$ is calculated with formula (14), while, for the other modes, the usual formula (6) is utilized. Of course, formula (6) is only indicative for large excitation energy, when the variables $Q_k$ and $P_k$ lose their meaning of modal variables.

The initial time interval, necessary to excite, through computational errors, the other modes, depends obviously on the precision of numerical computations. All the previous numerical calculations have been performed in double precision. We have observed that, working in simple precision, the exchange of energy of the mode $N/2$ with the other modes occurs much earlier than in double precision. However, since the mechanism is primed, it repeats with the same properties either in double precision or in simple precision.

The instability of the OMS can also be seen from another point of view, by considering the Hamiltonian variables $q_k$. We recall that, if the OMS $Q_{N/2}$ were stable then, from Eq. (15), the sum $q_k+q_{k+1}$ would always be zero. In Fig. 5, as an example, we report the sum $q_{15}+q_{16}$ as a function of time. As can be seen from the figure, the instability (sum of the two coordinates different from zero) appears when mode 16 starts to exchange energy with the other modes.

In this context, and to obtain more insight into the behavior of an OMS, it is really very interesting to see what the positions of particles in the chain are, i.e. the spatial configuration of the chain, in correspondence with a well determined value of energy of the OMS. In Fig. 6, for $\beta=0.005$, the values of the coordinates of the 32 atoms, in correspondence with a particular value of the energy of mode 16, are shown. For clarity, the representative points of the particles are joined by segments. Figure 6 shows that the particle chain recovers its ''symmetrical form'' $(q_k+q_{k-1}=0)$ when the OMS recovers all its initial energy.

## V. CASE $N/2$ AS A FUNCTION OF $N$

In order to complete the analysis of the case $N/2$, in Fig. 7 we show the behavior of the energy of this mode as a function of time for various values of $N$, for $\beta=0.005$. From this figure it emerges that the mode $N/2$ tends to exchange all its energy, by increasing $N$. For $N=52$, this mode periodically loses and recovers almost all its energy. For $N>52$, the recovery is not complete, and moreover the curve of energy versus time becomes irregular. The irregularity and complexity of the curve increase with $N$ and, for $N$ very large, the system becomes probably chaotic.

Let us now consider formula (21), obtained analytically,

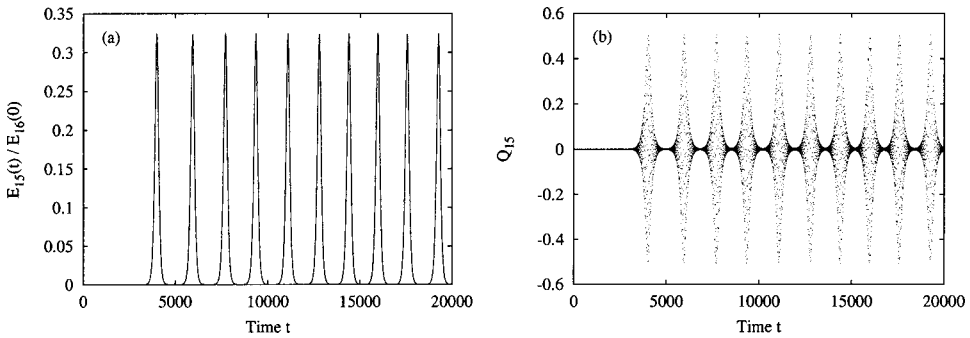


FIG. 4. Energy of mode 15 (a) and $Q_{15}$ (b) vs $t$ for $\beta=0.005$.

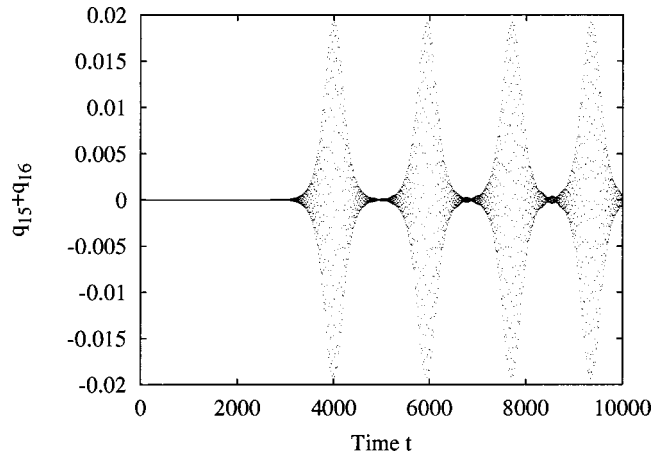


FIG. 5. $q_{15}+q_{16}$ vs $t$ for $\beta=0.005$ when mode 16 is initially excited.

and let us see how we can numerically obtain the dependence on $N$ of the threshold value $\beta_t$. From the analysis of the stability reported in Refs. [18] and [19], we know that the first modes excited, as the energy increases and the mode $N/2$ becomes unstable, are the modes $N/2-1$ and $N/2+1$. Then for a given value of $N$, starting from values of $\beta$ very small, and integrating the motion equations for fairly long times, we increase the value of $\beta$ until the first pulse in the energy of the mode $N/2-1$ or, equivalently, the first sudden change in the energy of the mode $N/2$, appears. We assume this value of $\beta$ as the threshold value $\beta_t$. In Fig. 8, the numerical value of the product $N^2\beta_t$, determined in this way, is compared with the theoretical value $\pi^2/3$ [formula (21)] for $N=6,8,\ldots,64$. A linear best fit of $\log\beta_t$ vs $\log N$, for large $N$, gives a slope of $-2.02$. We notice the good agreement of our results with Eq. (21).

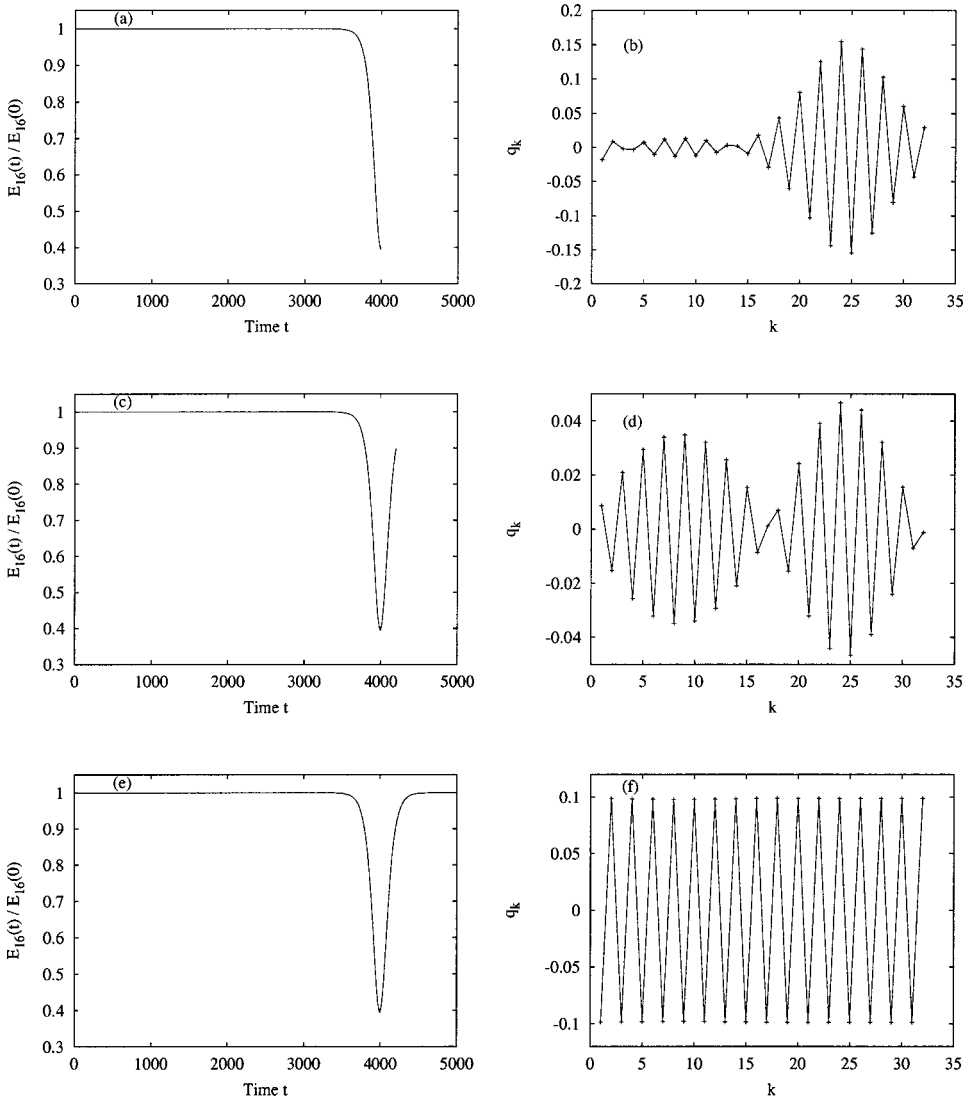


FIG. 6. Values of the displacements of atoms [(b), (d), (f)] in correspondence with the final value of the energy [(a), (c), (e)] for $N=32$ and $\beta=0.005$.

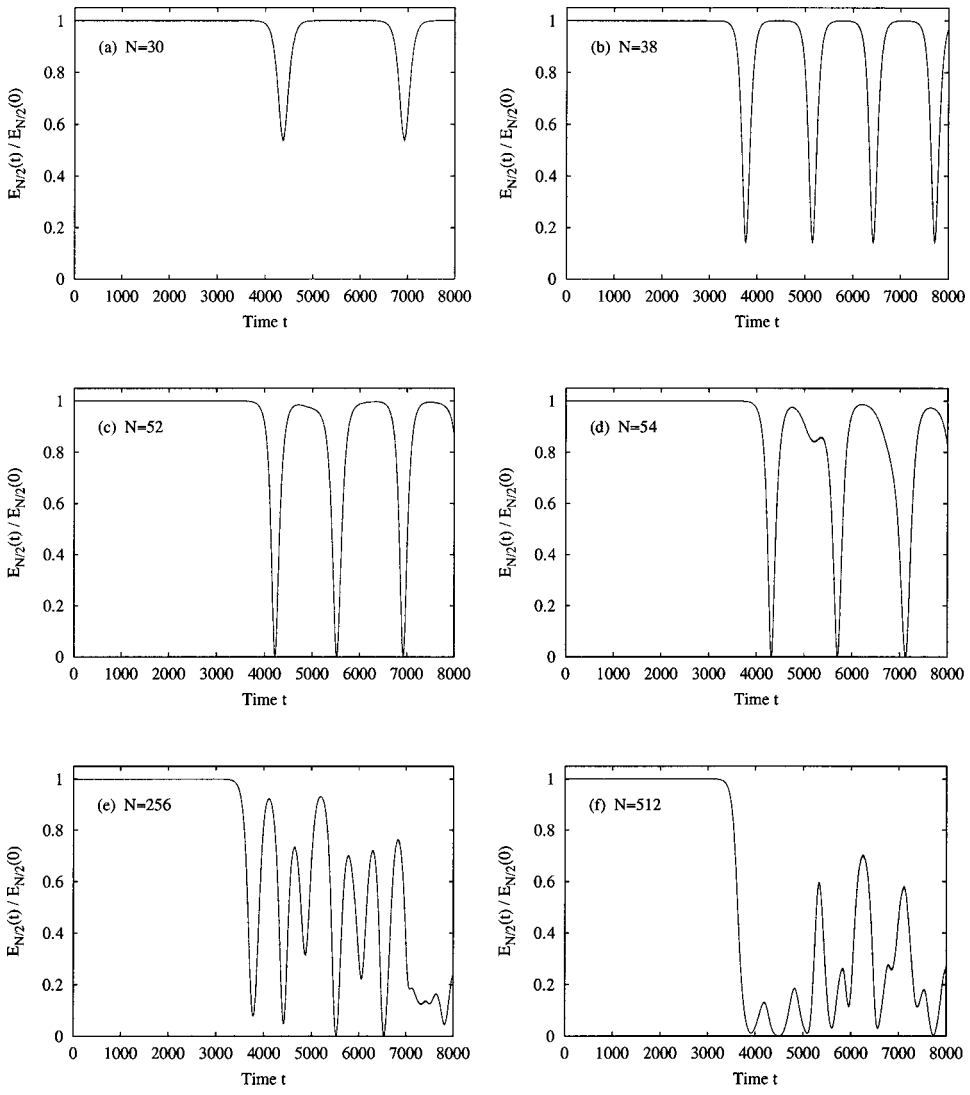


FIG. 7. Energy of the mode $N/2$ vs $t$ for $\beta=0.005$, for some values of $N$.

We have also analyzed the case $\mu<0$. We give here only preliminary results. We obtain the same result found in Ref. [19], namely, $|\beta_t|\to 0.214$ for large values of $N$. Moreover the instability properties of the OMS $N/2$ are very different from the case $\mu>0$: the OMSs diverge for $|\beta|>|\beta_t|$ and the other modes are not periodically excited.

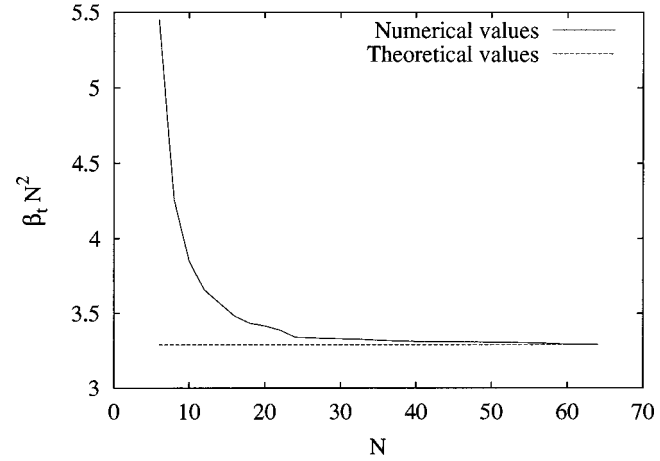


FIG. 8. $\beta_t N^2$ vs $N$ for the OMS $N/2$. The theoretical curve refers to formula (21).

## VI. CASES $\frac{N}{4}$, $\frac{3}{4}N$, $\frac{N}{3}$, AND $\frac{2}{3}N$

Following the same procedure used in the case $N/2$, we have calculated, numerically, the value of $\beta_t$ for the nonlinear OMSs $N/4$, $(3/4)N$, $N/3$, and $(2/3)N$ as functions of $N$. We have found that $\beta_t$ is the same for the cases $N/4$ and $(3/4)N$ and the cases $N/3$ and $(2/3)N$. This was foreseeable since the nonlinear modes $N/4$, $(3/4)N$, and $N/3$, $(2/3)N$ are symmetrical with respect to the mode $N/2$, and so are identical if the initial excitation energy is the same [see Eqs. (12)–(14)].

Figure 9 shows the behavior of the product $\beta_t N^2$ as a function of $N$, for the cases $N/2$, $N/3$, and $N/4$, and the theoretical estimate for the case $N/2$ given by formula (21). The numerical results suggest a dependence of $\beta_t$ on $N^{-2}$, for large values of $N$, also for the OMSs $N/3$ and $N/4$.

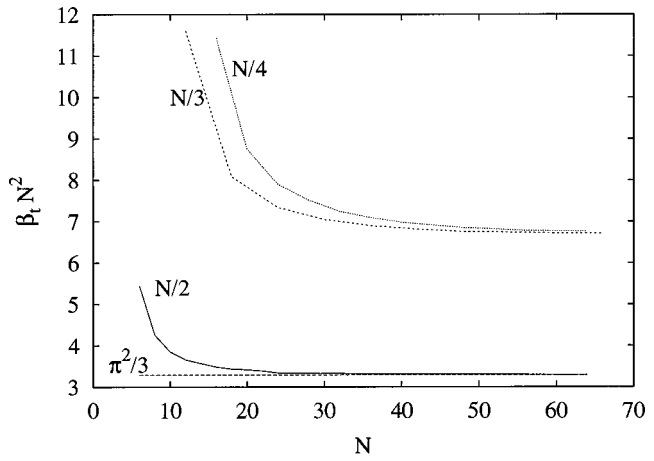


FIG. 9. $\beta_t N^2$ vs $N$ for the OMSs $N/2$, $N/3$, and $N/4$.

## VII. DISCUSSION

We have numerically analyzed the stability of the OMSs in the Fermi-Pasta-Ulam system. Previously, only for case $N/2$ were a theoretical analysis of the stability and approximate estimates of the stability threshold for large values of $N$ available. Our method is based on a numerical integration of full nonlinear differential equations of motion. The initial conditions for the Hamiltonian variables $q_k$ and $p_k$ are such that only a particular nonlinear one-mode solution is initially excited. No *a priori* initial perturbation of the analytical solution is introduced in the numerical algorithm, the only perturbation being that generated by computational errors in numerical integration. With this method we study the stability of the OMSs against the numerical errors introduced by the integration algorithm. We have accurately analyzed the case $N/2$, which in some sense works as a test, since, for this case, analytical results are available.

We remark that the OMSs are nonlinear analytical solutions of the complete Fermi-Pasta-Ulam system, with linear and nonlinear terms in the Hamiltonian, so their stability cannot be discussed in terms of the KAM theorem. The stability of linear modes and nonlinear OMSs, against computational errors, are completely disjoint in the sense that a linear mode, initially excited, is stable for very long integration times, if the parameter $\mu$ is set equal to zero in the Hamiltonian. Thus the linear modes, excited during the evolution of a nonlinear OMS, are triggered by the instability of this nonlinear mode and then only indirectly by the computational errors. This different behavior of the linear mode and of the nonlinear OMS is evident if we compare, for the same integration time, the orbits in the plane $(Q_{N/2}, P_{N/2})$ for the same value of $\epsilon = 0.5$ and two values of $\mu$: $\mu = 0$, for the linear case, and $\mu = 0.5$, in the nonlinear case, which corresponds to a value of $\beta$ very much larger than $\beta_t = 0.0033$. This different behavior is shown in Fig. 10.

Let us first consider the case $N/2$. From Figs. 1–3, as pointed out in Sec. IV, three regimes can be observed, varying the product $\beta = \epsilon\mu$. In the first regime, where $\beta < \beta_t$, the OMS is stable during the whole integration time.

As soon as $\beta$ exceeds $\beta_t$, after an initial time interval, depending on the precision of numerical calculations, during which the OMS is stable, the amplification of errors excites the first modes which become unstable, namely, the modes $N/2-1$ and $N/2+1$. Because of the nonlinear coupling between the modes, the excitation of these two modes triggers all the other linear modes. The characteristics of this second regime, when the parameter $\beta$ grows, are the increasing exchange of energy between the nonlinear mode and the other linear modes and the periodic recovery of energy of the nonlinear mode. This regime continues as long as the periodic exchange of energy is complete. A further increase of $\beta$ distorts the profile of the curve of energy of the nonlinear mode, as a function of time, and the behavior of the system always becomes more complex.

For large values of $N$, formula (21) gives a good estimate of the instability threshold, so we could try to explain the ''intermittent behavior'' of the second regime in the framework of the theory developed in Ref. [18]. As we have seen in Sec. III, modes with $\rho < 1/3$ are always stable in the linear approximation. For example, for the case $N = 32$ we have, from Eq. (20), that the modes with $r < 7$ are always stable, for any energy of mode $n = N/2 = 16$. These modes can grow only if they are triggered by the interaction with other unstable modes. As pointed out in Ref. [18], this kind of interaction is neglected in the linear approximation and comes into play only when unstable modes have grown and the linearized theory is no longer valid. This indirect triggering can be observed numerically if we compare, for example, the time evolution of modes 16 and 6: no triggering of mode 6 exists if $\beta < \beta_t$.

For $\beta > \beta_t$, in short time intervals, during which the nonlinear one-mode exchanges energy with the other modes, the time derivative of the energy of the OMS is not zero and Eq. (10) and formula (14) are no longer valid. During these time intervals, a strong coupling exists between mode $N/2$ and the

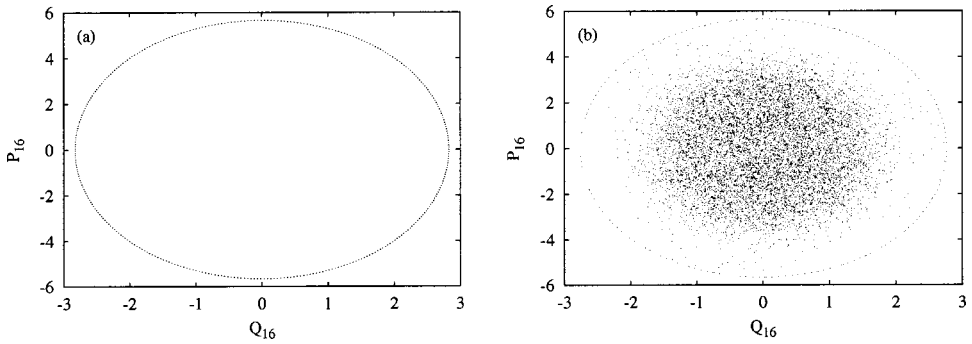


FIG. 10. Orbits in the plane $(Q_{16}, P_{16})$ for the linear case ($\mu = 0$) with $\epsilon = 0.5$ (a) and for the nonlinear case $\mu = 0.1$ with $\epsilon = 0.5$ (b).

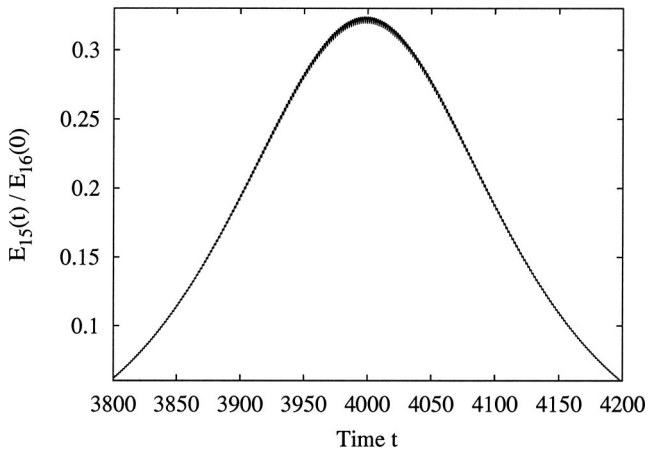


FIG. 11. Energy of mode 15 vs $t$ for $\beta=0.005$.

two adjacent modes and, indirectly, with all the other linear modes. However, the exact mechanism by which the nonlinear one-mode loses and recovers energy periodically is not clear. We now try to give an explanation of this mechanism in terms of Floquet's theorem for parametric oscillators [23,24]. Equation (19) is of the form

$$\frac{dx^2}{dt^2}+f(t)x=0, \tag{23}$$

where $f(t)$ is a periodic function of time with period $T$. Floquet's theorem means that the solution of Eq. (23) can be written as

$$x_r(t)=\lambda_r^{t/T}X_r(t), \tag{24}$$

where $r=1$ or 2, $\lambda_1\lambda_2=1$, and $X_r(t+T)=\pm X_r(t)$. The appropriate sign in front of $X_r(t)$ is determined by the particular form of $f(t)$. With the minus sign one has $X_r(t+2T)=X_r(t)$. Solution (24) also means that

$$x_r(t+T)=\lambda_r x_r(t). \tag{25}$$

Thus the values of $x_r(t)$, in successive cycles, depends on factor $\lambda_r$ when the time interval between the observations is

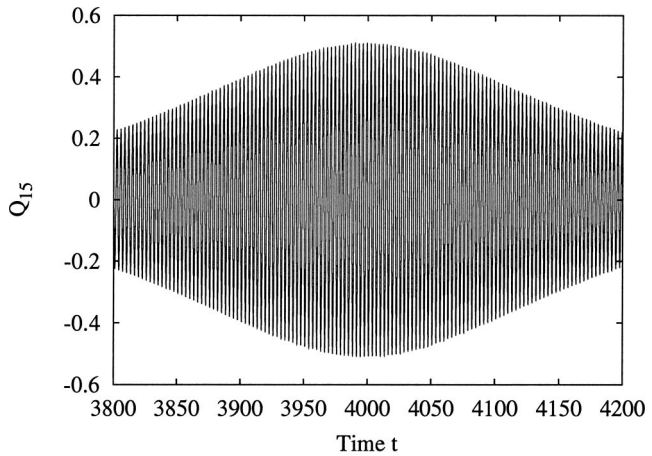


FIG. 12. $Q_{15}$ vs $t$ for $\beta=0.005$.

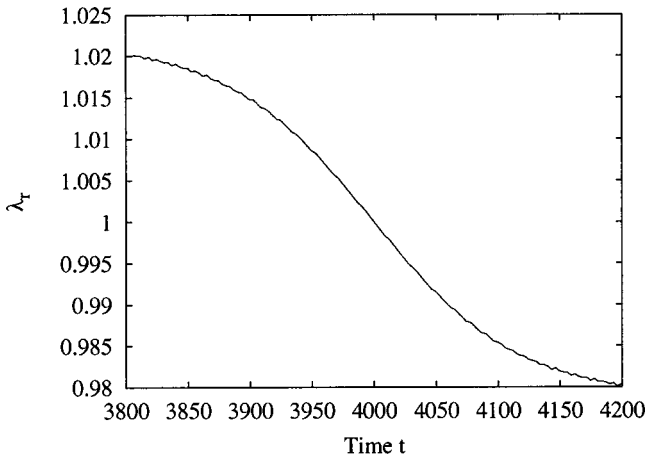


FIG. 13. $\mu$ vs $t$ for $Q_{15}$, $N=32$, and $\epsilon\mu=0.005$.

equal to the period of $f(t)$. Let us consider Figs. 11 and 12 which show, for $N/2=16$ and $\beta=0.005$, respectively the first energy pulse of mode 15 and the correspondent time variation of $Q_{15}$.

From numerical data we have verified that in the case of Eq. (18), we have $X_r(t+T)=-X_r(t)$ and so $X_r(t+2T)=X_r(t)$, where $T$ is the period of the Jacobian function $cn^2(\Omega_{N/2}t;k)$. For $\beta=0.005$, from Eqs. (12) and (13), we have $\Omega_{N/2}\approx\omega_{N/2}$ and $cn^2(\Omega_{N/2}t;k)\approx\cos^2\omega_{N/2}t$. Since $\omega_{N/2}=2$, the period of $\cos^2$ is $\pi/2$ and so $2T=\pi$. From Eq. (25), comparing the values of $Q_{15}$ each interval of $2T=\pi$, we can obtain the value of the parameter $\lambda_r$ which determines the stability or instability of the solution. The pulsed behavior of the energy of the nonlinear OMS and the consequent pulsed behavior of the linear modes, when $\beta>\beta_t$, can then be attributed to the time variation of $\lambda_r$ during the exchange of energy between the nonlinear one-mode and the other linear modes, when Eq. (18) is no longer exactly valid. If we suppose that the OMS $Q_{16}$ continues to oscillate with its normal frequency, but modulated in amplitude, during the energy exchange, the parameter $\lambda_r$ varies, causing the typical pulsed behavior for $\beta>\beta_t$. Furthermore, since the period of $Q_{15}^2$ is $T$, we have the small energy fluctuations of period $T=\pi/2$ in the energy pulse of mode 15 shown in Fig. 11. If $\beta$ is very large, many linear modes are involved, the exchange of energy is much greater and irreversible and the OMS does not recover all its initial energy.

In Fig. 13 the time behavior of the parameter $\lambda_r$ is shown for the solution $Q_{15}$, when the one-mode $Q_{N/2}$ is excited, for $N=32$ and $\beta=0.005$. With reference to Fig. 12, the values of $\lambda_r$ are obtained calculating the ratio between two consecutive maxima of $Q_{15}$. From Figs. 12 and 13 the link is clear between the exponential growth and the subsequent exponential decrease of $Q_{15}$ with the variation of the parameter $\lambda_r$ from values greater than 1 to smaller than 1.

We conclude this discussion, giving a short account of the FPU $\alpha$ system, which, as is well known, has very different features from the FPU $\beta$ system. In fact we remark that, for the $\alpha$ system, it is the quantity $\epsilon\mu^2$ (and not $\epsilon\mu$ as in the $\beta$ case) which is invariant under the symmetry (scale) transformation $q_k\rightarrow\lambda N^{-1}q_k$, $p_k\rightarrow\lambda N^{-1}p_k$, and $\mu\rightarrow\lambda^{-1}N\mu$,

where $\lambda$ is the scale parameter. Then the dynamical properties of the system are invariant for $\mu \rightarrow -\mu$. This implies that the stability of the OMSs does not depend on the sign of $\mu$. Here we give some preliminary results. Our numerical experiments show that, for $\mu = \pm 1$, the threshold energy density goes to the constant value 0.184 for large $N$. This result is in disagreement with that of Ref. [19], where for the threshold energy per particle, for $\mu = 1$, the relation $E_t/N \approx 0.8418/N$ was obtained, while it agrees with the result of Ref. [21]. The value 0.184 of the threshold energy density corresponds indeed to the value 0.303 of the parameter $\Lambda_3$ of Ref. [21].

## VIII. CONCLUSIONS

In this paper we have numerically studied the problem of stability of OMSs in the Fermi-Pasta-Ulam $\beta$ system. Although this problem has been tackled many times in the last few years, analytical results were available only for the case $N/2$, where $N$ is the number of particles in the chain. We have envisaged a simple numerical method, which tests the stability of solutions against the numerical errors introduced automatically by the numerical algorithm of integration of motion equations. The method reproduces the analytical results already known for case $N/2$, and allows one to obtain the threshold energy density, above which the OMS is unstable, in the other cases, namely, the cases $N/4$, $N/3$, $(2/3)N$, and $(4/3)N$.

We have found that, for each case, there is a characteristic value $\beta_t$ of the product $\epsilon\mu$, between the energy density $\epsilon$ and the nonlinearity parameter $\mu$, above which there is a large range of values of $\beta$ in which the OMS presents an intermittent behavior. For these values of $\beta$, the nonlinear mode keeps its initial excitation energy for long times and periodically, abruptly, loses and recovers a fraction of this energy. We have verified that, for the case $N/2$, the value of $\beta_t$ coincides, for large $N$, with the threshold value, above which the OMS is instable, given by Eq. (21). Then we have assumed this characteristic value as threshold value also in the other cases. We have also verified that, varying $N$, the cases $N/3$ and $\frac{2}{3}N$ and $N/4$ and $\frac{3}{4}N$ have the same threshold value $\beta_t$. A tentative explanation of the intermittent behavior, in terms of Floquet's theorem for parametric oscillators, has been given.

As concerns the FPU $\alpha$ system we have shown in particular that the dynamical properties are independent of the sign of the nonlinearity parameter $\mu$ and that, for large $N$, there is an energy density threshold constant, different from zero.


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