Application of the Bogoliubov-Krylov method of averaging to the Fermi-Pasta-Ulam system

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We apply the Bogoliubov-Krilov method of averaging to the study of the stability of the π-mode solution ($N/2$ one-mode nonlinear solution) of the Fermi-Pasta-Ulam-β system, with negative values of the nonlinearity parameter β in the Hamiltonian of the system. The analysis is made as a function of the number N of the particles and of the product $\lambda=\epsilon|\beta|$, where ϵ is the energy density. The results of this application are in excellent agreement with those obtained by the direct integration of motion equation.

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For a periodic Fermi-Pasta-Ulam (FPU)–β chain [1] with an even number N of oscillators and periodic conditions there are exact one-mode nonlinear solutions (OMSs) corresponding to the values of mode number n,

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

such that, if only one of these modes is initially excited, it evolves without transferring energy to any other mode [2]. An important problem is the stability of these OMSs against a generic perturbation; the study of the stability presents very interesting and intriguing aspects and it is in general connected with the problem of equipartition of energy and transition to chaos in dynamical systems.

In a recent paper [3] we have revisited the problem of stability of the OMSs. We made a numerical study of the stability of these nonlinear solutions as a function of the number N of particles and of the product $\lambda=\epsilon|\beta|$, where ϵ is the energy density and β is the nonlinearity parameter of the FPU Hamiltonian. In the numerical analysis, extensively made for $\beta>0$ and $n=N/2$, no external perturbation for the OMSs was considered, the only perturbation being that introduced by computational errors in the numerical integration of motion equations. This simple method confirms the previous result [2,4] on the energy-density threshold λ_t obtained with a Floquet analysis of the problem of stability that asymptotically $\lambda_t=\pi^2/(3N^2)$.

In this paper we apply the numerical method used in Ref. [3] in order to study the stability of the $N/2$ mode (π mode) with $\beta<0$ as a function of N and λ. Our numerical results confirm the previous result reported in Ref. [5] that there is an energy-density threshold independent of N for large values of N; in particular, we find that the value λ_t decreases with N and converges to the value 0.2140. We show that this behavior of λ_t, as a function of N, can be explained in a very simple and elegant way using the Bogoliubov-Krylov (BK) method of averaging [6,7].

The FPU-β system is a one-dimensional chain of N equal-mass oscillators, with weakly nonlinear nearest-neighbor interaction. Calling q_n and p_n the coordinates and the momenta of the oscillators, the Hamiltonian 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

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

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

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

the harmonic energy of mode i is

$$E_i=\tfrac{1}{2}(P_i^2+\omega_i^2Q_i^2), \tag{6}$$

where, for periodic boundary conditions,

$$\omega_i^2=4\sin^2\frac{\pi i}{N}. \tag{7}$$

The Hamiltonian equations in the variables q_i and p_i, obtained from Eq. (2) and integrated by standard methods, allow us to calculate the normal modes and the energy of each mode.

Consider now the case $n=N/2$. Let us put $Q=Q_{N/2}$, $P=P_{N/2}$, and $\omega=\omega_{N/2}$. The equation of motion for the excited OMS amplitude Q is [2]

$$\ddot{Q}=-\omega^2Q-\beta\frac{\omega^4}{N}Q^3. \tag{8}$$

We recall that the dynamical properties of the FPU-β system depend only on the product $\lambda=\epsilon|\beta|$. In all the numerical experiments, as we will see in the following, we fix the value of β and we change the value of the energy density $\epsilon=E/N$, where

$$E = \frac{1}{2}\left(P^2 + \omega^2 Q^2 + \beta\frac{\omega^4 Q^4}{2N}\right) \tag{9}$$

is the energy of the nonlinear one mode $N/2$. We will excite the $N/2$ 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. (8), given by

$$V = \frac{1}{2}\left(\omega^2 Q^2 + \beta\frac{\omega^4 Q^4}{2N}\right). \tag{10}$$

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. The extremal points of the potential V are the value $Q=0$, which is a minimum, and the points $Q=\pm\frac{1}{\omega}\sqrt{\frac{N}{|\beta|}}$, which are points of maximum, where $V=\frac{N}{4|\beta|}$. For a given value of the energy density in the interval $0<\epsilon<\frac{1}{4|\beta|}$, we have four possible initial values of Q, namely

$$Q_0 = \pm\sqrt{\frac{N}{\omega^2|\beta|}(1 \pm \sqrt{1-4\epsilon|\beta|})}. \tag{11}$$

Only the "internal" solutions (minus sign under the square root), as initial conditions for Eq. (8), give bounded solutions.

The solution of Eq. (8) with $\beta<0$ and initial conditions $Q(0)=Q_0$ and $\dot{Q}(0)=0$ is

$$Q(t) = Q_0\,\mathrm{sn}(\Omega t + K;k^2), \tag{12}$$

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

$$k^2 = \frac{1-\sqrt{1-4\epsilon|\beta|}}{1+\sqrt{1-4\epsilon|\beta|}} \tag{13}$$

and

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

Let us now suppose that only the mode $n=N/2$ is excited. If ΔQ_r is the error on the normal coordinate Q_r, the equation for the rth perturbed mode is [2]

$$\Delta\ddot{Q}_r = -\omega_r^2\left[1+\frac{12\beta}{N}Q_{N/2}^2\right]\Delta Q_r. \tag{15}$$

The stability properties of the $N/2$ mode can be obtained analytically, both with $\beta>0$ and $\beta<0$, by studying the stability of the solutions of Eq. (15), for all the perturbed linear modes. The case $\beta>0$ has been extensively studied in Refs. [2–5]. In this paper we investigate the case $\beta<0$. For the numerical analysis we utilize the same numerical method used in Ref. [3]; the equations of motion in the variables q_i, p_i are integrated by means of a bilateral symplectic algorithm [8]. Numerical integration introduces some errors in the values of the variables q_i and p_i; these errors can excite linear modes of the system, which can make unstable the OMS initially excited. We find that there is a threshold value for the product $\lambda=\epsilon|\beta|$, beyond which the OMS is unstable.

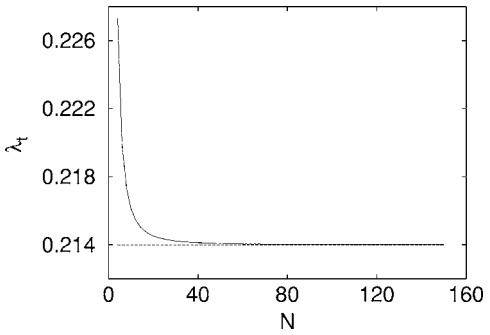

FIG. 1. λ_t vs N for $n=N/2$ and $\beta<0$; for clarity, the points are joined by segments.

In all the numerical experiments we put $\beta=-1$ and change the value of the energy density $\epsilon=E/N$. We excite the $N/2$ mode at $t=0$ always putting $Q\neq 0$ and $\dot{Q}=P=0$. From the inverse transformations of Eqs. (3) and (4), the initial values of $q_i(0)$ and $p_i(0)$ are obtained.

The behavior of λ_t as a function of N varying between 4 and 150 is shown in Fig. 1; for large values of N, the constant value $\lambda_t=0.2140$ is obtained. This means that, contrary to the case $\beta>0$, there always exists a stability range for the energy density.

The asymptotic value for very large values of N has been obtained theoretically in Ref. [5] using the Hill's determinant approach for the study of the Lamé's equations describing directly, in the variables q_i, p_i, the perturbed modes and considering up to 120 terms in the Fourier series expansion of elliptic functions.

Here we show a method that explains the behavior of λ_t for all values of N. Our approach is based on the BK method of averaging. First of all, we remark that with $\beta<0$, contrary to the case $\beta>0$, the term in square brackets in Eq. (15) can assume negative values by increasing energy, changing drastically the stability properties of the $N/2$ mode.

Let us write Eq. (15) in the form

$$\frac{dx^2}{dt^2} + \omega_r^2 f(t)x = 0, \tag{16}$$

with $f(t)$ periodic of period T. The BK method says that the Floquet's frequency of Eq. (16), given in first approximation by

$$\omega_{BK}^2 = \omega_r^2\langle f(t)\rangle, \tag{17}$$

where the average is calculated on one period T, is a significant parameter for the stability of Eq. (16), in the sense that the solution is unstable if ω_{BK}^2 is less than zero. In terms of β, ω, and ϵ, from Eqs. (11) and (12), $\langle f(t)\rangle$ is given by

$$\langle f(t)\rangle = 1 - \frac{12}{\omega^2}(1-\sqrt{1-4\epsilon|\beta|})\langle \mathrm{sn}^2(\Omega t + K;k^2)\rangle. \tag{18}$$

It changes from the value 1, for $\epsilon=0$, to the value $1-\frac{12}{\omega^2}\langle \mathrm{sn}^2(\Omega t+K;k^2)\rangle$, for $\epsilon=\frac{1}{4|\beta|}$. Since

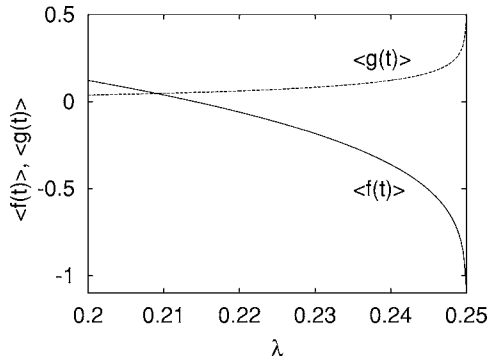

FIG. 2. $\langle f(t)\rangle$ and $\langle g(t)\rangle$ vs λ.

$$\langle \mathrm{sn}^2\rangle = \frac{1}{k^2}\left(1 - \frac{E(k)}{K(k)}\right), \tag{19}$$

where $E(k)$ is the complete elliptic integral of the second kind, one obtains

$$\langle f(t)\rangle = 1 - \frac{12}{\omega^2}(1 + \sqrt{1 - 4\epsilon|\beta|}) \quad \left(1 - \frac{E(k)}{K(k)}\right). \tag{20}$$

We remark that since Ω and k, which determine the values of E and K, don't depend on N, the value of the product $\lambda = \epsilon|\beta|$ at which $\langle f(t)\rangle = 0$ is the same for all values of N. This value is $\lambda_t = 0.2140$, just the threshold numerical value found for large N, by integrating the motion equations.

The behavior of λ_t as a function of N, shown in Fig. 1, can be found considering the next term in the expression of ω_{BK}^2 given by the BK method. Instead of Eq. (17) one has

$$\omega_{BK}^2 = \omega_r^2\{\langle f(t) + \omega_r^2 g(t)\rangle\}, \tag{21}$$

where

$$g(t) = \left[\int_0^t [f(t') - \langle f\rangle]dt'\right]^2. \tag{22}$$

The function $\langle g(t)\rangle$, as $\langle f(t)\rangle$, is independent of N. Figure 2 shows that $\langle f(t)\rangle$ and $\langle g(t)\rangle$ are a decreasing and an increasing function of λ, respectively. Starting from $\lambda = 0$, the zero of the function ω_{BK} given by Eq. (21) is obtained, for some value of λ, which now depends on r and thus on N, when

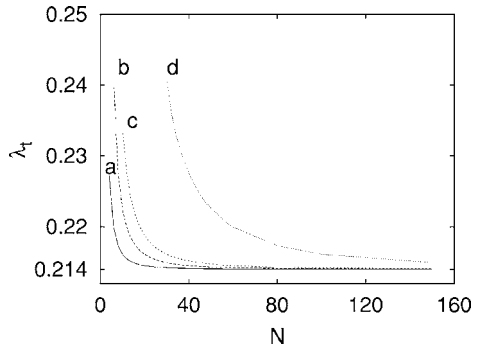

FIG. 3. λ_t vs N; curves a, b, c, and d refer to $\omega_r = \omega_1$, ω_2, ω_3, and ω_{10}, respectively.

$$\langle f(t) + \omega_r^2 g(t)\rangle = 0. \tag{23}$$

The smallest of these values of λ is the threshold value λ_t of the $N/2$ mode with $\beta < 0$. Since $\langle g(t)\rangle$ is a positive function, the smallest value of λ, at which Eq. (23) admits solution, occurs when ω_r assumes its minimum value different from zero, namely, when $r = 1$. Figure 3 shows the values of λ_t found with the BK method with $\omega_r = \omega_1$ and other values of ω_r, as a function of N (even) varying between 4 and 150. The curve a, corresponding to ω_1, reproduces exactly the curve shown in Fig. 1, obtained by the integration of motion equation: the values of λ_t, obtained with the two methods, differ on the fifth figure only. The curve b, corresponding to ω_2, starts from $N = 6$, since, for $N = 4$, Eq. (23) has no solution for this value of ω_r. For the same reason, the curve c starts from $N = 10$ and the curve d from $N = 30$.

As is clear from Figs. 1 and 3, the behavior of functions $\langle f(t)\rangle$ and $\langle g(t)\rangle$ are such that one has an excellent agreement between the numerical results and the results obtained with the BK method of averaging, with $\omega_r = \omega_1$. This shows that with $\beta < 0$ there are no other instability mechanisms that could lower the stability threshold and agrees with the fact that integration of motion equations shows clearly that, for $\lambda > \lambda_t$, the mode $r = 1$ is the first mode that becomes unstable, triggering the instability of the $N/2$ mode.

Finally we remark that our numerical and analytical results confirm that the π mode, in the termodynamic limit, is always stable, with $\beta < 0$, if $\epsilon < 0.214/|\beta|$, while for $\beta > 0$, it is always unstable.

[1] *Collected Papers of Enrico Fermi*, edited by E. Segré (University of Chicago Press, Chicago, 1965).
[2] P. Poggi and S. Ruffo, Physica D **103**, 251 (1997).
[3] A. Cafarella, M. Leo, and R. A. Leo, Phys. Rev. E **69**, 046604 (2004).
[4] S. Flach, Physica D **91**, 223 (1996).
[5] N. Budinsky and T. Bountis, Physica D **8**, 445 (1983).
[6] N. Krylov and N. N. Bogoliubov, *Introduction to Nonlinear Mechanics* (Princeton University Press, Princeton, N.J., 1947).
[7] N. N. Bogoliubov and Y. A. Mitropolsky, *Asymptotic Methods in the Theory of Non-linear Oscillations* (Gordon and Breach Science Publishers, Inc., New York, 1961).
[8] L. Casetti, Phys. Scr. **51**, 29 (1995).