An analytical estimate of stochasticity thresholds in Fermi-Pasta-Ulam and φ^4 models

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Abstract

We consider an infinitely extended Fermi-Pasta-Ulam model. We show that the slow modulating amplitude of a narrow wave packet asimptotically satisfies the nonlinear Schrödinger equation (NLS) on the real axis. Using well known results from Inverse Scattering theory we then show there exists a threshold on the energy of the central normal mode of the packet, with the following properties: below threshold the NLS equation presents a quasi-linear regime with no solitons in the solution of the equation, and the wave packet width remains narrow. Above threshold a generation of solitons is instead possible and the packet of normal modes can spread out. Analogous results are obtained for the φ^4 model. We also give an analytical estimate for such thresholds. Finally we make a comparison with the numerical results known to us and show they are in remarkable agreement with our estimates.

I. INTRODUCTION AND RESULTS

Since the pioneristic work of Fermi, Pasta and Ulam (FPU) [1] an incredible effort has been devoted to understanding classical many-body dynamical systems. It became clear from the beginning that a system as "simple" as the one described by the hamiltonian

$$H_N(\mathbf{q},\mathbf{p}) = \sum_{n=0}^{N} \frac{1}{2}p_n^2 + U(q_n) + V(r_n) \tag{1}$$

(where q_n is the position of the n-th particle on a one-dimensional lattice, p_n the corresponding conjugate momentum, $r_n \equiv q_{n+1} - q_n$, while U and V are given nonquadratic potentials, and some specific boundary conditions are assigned) gives rise, in general, to a complex dynamics, with a coexistence of ordered and chaotic motions, depending on the initial data, on the length of the integration time and on the number N of degrees of freedom. At present, a satisfactory understanding of this dependence is lacking. It has become customary to define suitable stochasticity thresholds, namely critical values of some control parameters such that below them one has somehow regular motions while above them the dynamics presents certain characters of irregularity or "chaoticity". Normal mode coordinates $\mathbf{Q},\mathbf{P}$ (normalizing the quadratic part of H_N) can be introduced in the familiar way, such that the hamiltonian (1) takes the form

$$H_N(\mathbf{Q},\mathbf{P}) = \frac{1}{2}\sum_k (P_k^2 + \omega_k^2 Q_k^2) + \mathcal{V}(\mathbf{Q}) \ , \tag{2}$$

where ω_k is the frequency of the k-th normal mode and $\mathcal{V}$ is a suitable perturbing term, producing mode-mode coupling. In the particular case of initial data corresponding to excitations of a packet of modes of nearby frequencies centered about a certain k_0, a suitable control parameter for a stochasticity threshold is the harmonic energy E of the initially excited packet; indeed, by increasing E, the energy sharing between normal modes due to $\mathcal{V}$ becomes the more and more effective, and the energy flows out of the initially excited packet, the motions becoming more irregular. A popular criterion to define a threshold in numerical simulations consists in checking whether equipartition is established within a fixed observation time (see [2] and [3]). Another one just requires that a certain fraction of the initial energy be given out by the initially excited packet, irrespective of the modes to which the energy flows [4] [5]. The available numerical results indicate that the energy threshold $E^c_{k_0}$, apart from the exceptional case of the so-called β model (see below), is an increasing function of ω_{k_0}.

As far as analytical estimates are concerned, the most famous one is due to Izrailev and Chirikov (IC) [6], who by the way were also the first ones to introduce the notion itself of a mode dependent threshold. The IC criterion is based on the concept of the so called overlapping of resonances, which is known to work rather well for very few degrees of freedom [7] [8]. By extending it to the limit of very many degrees of freedom and using the fact that in such a limit neighbouring normal mode frequencies become asimptotically resonant, the authors predicted that the threshold $E^c_{k_0}$ should be a decreasing function of ω_{k_0}, at least for the FPU β model. A completely different approach was introduced by Berman and Kolovskii [9], following the idea of approximating the equations of motion of the hamiltonian system by a well known integrable partial differential equation, namely the nonlinear Schrödinger equation (NLS). They showed that such an approximation should hold below a certain energy threshold, which they estimated to have the form $E^c_{k_0} \approx \frac{k_0}{N}\frac{1}{\beta}$.

In the present paper we too make reference to concepts involving the NLS equation, but exploit more consistently the notions of Inverse Scattering and Soliton Theory [10] [11]. This leads, in a way that will be described below, to a different analytical estimate for the threshold. This is worked out for two models. The first one is an infinitely extended FPU model, with hamiltonian

$$H(\mathbf{q},\mathbf{p}) = \sum_{n\in\mathbb{Z}} \frac{1}{2}p_n^2 + \frac{\Omega^2}{8}r_n^2 + \frac{\alpha}{3}r_n^3 + \frac{\beta}{4}r_n^4 \tag{3}$$

involving the real parameters Ω, α and β (with Ω, $\beta > 0$) for which the harmonic frequencies are known to be given by the dispersion relation $\omega(k) = \Omega\sin(k/2)$, $k \in (0,\pi]$; this includes the particular case $\alpha = 0$, which is known as the β model. For the threshold we find the estimate

$$\boxed{E^c_{FPU}(\omega) \approx \Omega^4 \frac{\omega^2}{8\alpha^2\left[1-(\omega/\Omega)^2\right] + 3\beta\omega^2}} \tag{4}$$

where ω is the frequency of the central normal mode of a narrow wave packet initially excited. The qualitative dynamical property characterizing the threshold is the following one: if at $t = 0$ one has $E(\omega) \ll E^c_{FPU}(\omega)$, the wave packet dynamics turns out to be dispersive and the width of the packet remains narrow, while for $E(\omega) \gg E^c_{FPU}(\omega)$ the width of the packet can increase because of the presence of solitons.

We then consider the so called φ^4 model, with hamiltonian

$$H(\mathbf{q},\mathbf{p}) = \sum_{n\in\mathbb{Z}} \frac{1}{2}p_n^2 + \frac{m^2}{2}q_n^2 + \frac{\epsilon}{2}r_n^2 + \frac{\lambda}{4}q_n^4 \tag{5}$$

involving the real parameters m, ϵ, λ (ϵ, $\lambda > 0$), and analogously obtain the estimate

$$\boxed{E^c_{\varphi^4}(\omega) \approx \frac{1}{\lambda}\left(\omega^4 - \omega_c^4\right)\theta(\omega - \omega_c)} \tag{6}$$

where $\omega_c \equiv \sqrt{m}\,(m^2 + 4\epsilon)^{1/4}$ while $\theta(\cdot)$ is the Heaviside step function. The sharp cutoff ω_c in the latter threshold is due to the special form of the dispersion relation of the linearized problem, namely $\omega(k) = \sqrt{m^2 + 4\epsilon\sin^2(k/2)}$.

It will be shown below that in both cases, namely for the FPU system and the φ^4 model, the thresholds given here are in remarkable agreement with the available numerical estimates.

Notice that, at variance with [6] and [9], who were considering finite chains of particles, we deal with infinitely extended chains. On the other hand, we consider initial data with packets having a finite amount of energy, namely with a vanishing energy per particle. This point will be discussed in the conclusive section.

The analytical treatment leading to the definition and the estimate of the threshold for the FPU model is given in section II, and the comparison with the available numerical estimates is given in section III. The analogous discussion for the φ^4 model is given in section IV, while some further comments are given in section V.

II. MULTIPLE-SCALE EXPANSION FOR THE FPU MODEL

In this section we study the hamiltonian (3). Inspired by [3], in analogy with the methods of fluid mechanics we introduce dimensionless variables and look for suitable dimensionless order parameters. Dimensionless variables τ, x_n and ρ_n are defined by $\tau = \frac{\Omega}{2}t$, $x_n = q_n/A$, $\rho_n = r_n/A$, where A is a parameter having the dimensions of a length and playing the role of a dimensional control parameter; indeed, for fixed x_n, by increasing A one increases the "actual" amplitudes $q_n = Ax_n$ and velocities $\dot{q}_n$ of the particles, and so also the energy of the excited modes. In terms of such dimensionless variables the equations of motion take the form

$$\begin{cases} \ddot{x}_n = (x_{n+1} + x_{n-1} - 2x_n)F(\rho_n, \rho_{n-1}; R, \mu) \\ \\ F = 1 + \sqrt{\mu R}\,(\rho_n + \rho_{n-1}) + R(\rho_n^2 + \rho_{n-1}^2 + \rho_n\rho_{n-1}) \end{cases} \tag{7}$$

(the dot denoting now derivative with respect to τ) where there just appear two dimensionless parameters, namely $R = 4\beta A^2/\Omega^2$ and $\mu = 4\alpha^2/(\beta\Omega^2)$; of these, R plays the role of a Reynolds number, while μ is independent of the "amplitude" A. In general, a realistic intermolecular potential has a form of the type $V(r_n) = V_0 f(r_n/\xi_0)$ with a suitable function f, where V_0 is a characteristic energy (measuring for example the depth of a well) and ξ_0 is a characteristic interaction length. A typical case is the Lennard-Jones (LJ) potential

$$V_{L-J}(r_n) = 4V_0 \left[\left(\frac{\xi_0}{r_n + 2^{1/6}\xi_0} \right)^{12} - \left(\frac{\xi_0}{r_n + 2^{1/6}\xi_0} \right)^{6} \right] + V_0 \ . \tag{8}$$

Truncating its Taylor expansion (about $r_n = 0$) to fourth order, one can approximate it by a FPU potential with the following coefficients: $\Omega^2/8 = 36V_0/(2^{1/3}\xi_0^2)$, $\alpha/3 = 252V_0/(\sqrt{2}\xi_0^3)$ and $\beta/4 = 1113V_0/(2^{2/3}\xi_0^4)$. It is easily shown that for all potentials of the above mentioned form the dimensionless parameter μ is independent of V_0 and ξ_0, depending only on the functional form of f; in particular, for the LJ potential one has $\mu \simeq 1.78$.

By the form of equations (7) it is natural to take $\sqrt{R}$ as the "small parameter" in a perturbative scheme. Following an approach familiar in the theory of wave propagation in nonlinear dispersive media, involving generation and modulation of higher harmonics of carrier waves, we introduce the *ansatz*:

$$x_n = \sum_{a\in\mathbb{Z}} e^{ia(qn-\omega_q\tau)} \psi^{(a)}(\zeta, \tau_1, \cdots, \tau_M; \sqrt{R}) \tag{9}$$

where $\zeta = R^{1/2}n$, $\tau_j = R^{j/2}\tau$ and $\omega_q = 2\,\mathrm{sen}\,(q/2)$ for a fixed wavevector $q \in (0, \pi)$, while $\tau_1, \cdots, \tau_M$ are the so-called *slow times*; fixing the number M of slow times takes the place of fixing the perturbative order in standard perturbation theory. The reality of x_n obviously implies $\psi^{(-a)} = \left(\psi^{(a)}\right)^*$. The ansatz (9) is known as a multiple-scale expansion (MSE) (see [12] and references therein).

It's easy to show that the MSE is nothing but a narrow packet approximation (NPA) [9] with a wave packet width $\delta k \approx \sqrt{R}$, provided some constraints are satisfied. Indeed, if the fundamental harmonic is the only one initially excited (i.e. $\psi^{(a)} = 0$ for $a \neq \pm 1$ at $\tau = 0$), the Fourier transform $\hat{x}_k$ of x_n turns out to be

$$\hat{x}_k = \sum_{a=\pm 1} \sum_n e^{-i(k-aq)n} \psi^{(a)} \left(\sqrt{R}\, n \right) \approx \frac{1}{\sqrt{R}} \sum_{a=\pm 1} \hat{\psi}^{(a)} \left(\frac{k - aq}{\sqrt{R}} \right) \ ; \tag{10}$$

in the last step the sum over n was converted into a Riemann integral using $R \ll 1$ as a lattice step, and the function $\hat{\psi}^{(a)}(\xi) = \int d\zeta e^{-i\xi\zeta} \psi^{(a)}(\zeta)$ was introduced. On the other hand, if we take initial data such that $\overline{\xi^2} \approx 1$, where

$$\overline{\xi^2} = \int d\xi \; \xi^2 |\hat{\psi}^{(\pm 1)}(\xi)|^2 \Big/ \int d\xi \; |\hat{\psi}^{(\pm 1)}(\xi)|^2 \; , \tag{11}$$

it follows that $\hat{x}_k(0) \neq 0$ only for $|k \pm q| \lesssim \sqrt{R}$, namely we are exciting a packet of normal modes centered about q with a width of size $\sqrt{R}$. Since we are taking $\sqrt{R} \ll 1$, this is a narrow (or quasi-monocromatic) wave packet.

Now, substituting the ansatz (9) into the equations of motion (7) and proceeding up to order $M = 2$ as sketched in the appendix, one finds that the zero-order amplitude of the fundamental harmonic $\psi \equiv \psi_0^{(1)} = \psi^{(1)}(\zeta - \frac{d\omega_q}{dq}\tau_1, \tau_2; 0)$ satisfies the nonlinear Schrödinger equation (NLS)

$$i\partial_{\tau_2}\psi - \frac{\omega_q}{8}\partial_\zeta^2\psi - \frac{\omega_q}{2}\left[8\mu\left(1 - \frac{\omega_q^2}{4}\right) + 3\omega_q^2\right]|\psi|^2\psi = 0 \; . \tag{12}$$

The function ψ turns out to be the dominant contribution to the approximate solution (9), because MSE calculations show that higher harmonics (with $|a| \geq 2$) are at most of order $\sqrt{R}$, i.e. negligible with respect to ψ, for $q \gg \sqrt{R}$, in the generic case in which $\mu \neq 0$. The fact that ψ dominates is instead always guaranteed in the special case $\mu = 0$ (or equivalently $\alpha = 0$).

The NLS equation (12) is an integrable one [13] [14]. From Inverse Scattering Transform (IST) it is known that, since the dispersion coefficient $-\frac{1}{8}\omega_q = \frac{1}{2}\frac{d^2\omega_q}{dq^2}$ and the coefficient of the nonlinear term $|\psi|^2\psi$ are both negative, equation (12) a priori admits *soliton* solutions in the class of initial data rapidly decreasing for $\zeta \to \pm\infty$ (this is indeed the class we choose to investigate here, corresponding to finite energy excitations in the lattice). The following theorem however holds [15] [11]:

If the initial datum satisfies the condition

$$\int_{\mathbb{R}} d\zeta |\psi(\zeta, \tau_2 = 0)| < \frac{\sigma}{\sqrt{2}}\left[8\mu\left(1 - \frac{\omega_q^2}{4}\right) + 3\omega_q^2\right]^{-1/2} \equiv \mathcal{S}_q \tag{13}$$

(where $\sigma = \ln(2 + \sqrt{3})$*), then equation* (12) *admits no soliton solutions.*

Condition (13) implies [10] that, for solutions $\psi(\zeta, \tau_2)$ of the NLS equation, the infinite time limit ($\tau_2 \to \infty$) and the low initial amplitude limit ($||\psi(0)||_1 \to 0$) commute; thus (13) guarantees that solutions of the NLS equation (12) present a purely dispersive dynamics and are analytical continuations of solutions of the linearized equation (corresponding to the quadratic part of the FPU hamiltonian). In other terms condition (13) guarantees that one is in a "regular" regime, with motions qualitatively similar to the unperturbed ones. An intense spreading of the energy out of the excited packet might instead occur only if condition (13) is violated. The reasons why this is actually expected are explained at the end of the present section. So we take the lowest energy violating condition (13) as our analytical estimate of the threshold.

We now formulate the threshold condition in terms of the harmonic energy of the central normal mode for a wave packet given by (9) at $\tau = 0$. To this end, we remark that by looking at the Fourier transform (10) one easily finds

$$E_q(\tau = 0; \sqrt{R}) \equiv \frac{1}{2}\left\{\left|\frac{d}{d\tau}\hat{x}_q\right|^2 + \omega_q^2|\hat{x}_q|^2\right\} = \frac{1}{R}e_q + o(1/R) \tag{14}$$

with a certain coefficient e_q whose expression is given below. Notice that the leading term of the R-expansion of E_q is singular because, as $R \to 0$, the equations of motion (7) become linear and the solution (9) represents a plane wave on an infinite lattice, thus having a diverging energy. A simple calculation shows that

$$e_q = \omega_q^2|\hat{\psi}(0,0)|^2 = \omega_q^2\left|\int d\zeta\ \psi(\zeta,0)\right|^2 \le \omega_q^2\left(\int d\zeta\ |\psi(\zeta,0)|\right)^2 . \tag{15}$$

Thus, if condition (13) holds, one necessarily has

$$E_q(0) \le \frac{1}{R}\omega_q^2\mathcal{S}_q^2 + o(1/R) = \frac{\sigma^2}{2R}\ \frac{\omega_q^2}{8\mu\left(1-\frac{\omega_q^2}{4}\right)+3\omega_q^2} + o(1/R) . \tag{16}$$

So we take as our estimate for the threshold the leading contribution to the r.h.s. of (16), namely $E_q^c = \omega_q^2\mathcal{S}_q^2/R$. Turning to physical (i.e. dimensional) variables, one has to multiply the latter expression by a factor $A^2\Omega^2/4 = R\Omega^4/(16\beta)$ and this produces the formula given in (4). In terms of $\mu = 4\alpha^2/(\beta\Omega^2)$ and ω/Ω it takes the form:

$$E_{FPU}^c(\omega) = \frac{\sigma^2\Omega^4}{96\beta}\frac{(\omega/\Omega)^2}{2\mu\left[1-(\omega/\Omega)^2\right]+3(\omega/\Omega)^2} . \tag{17}$$

We now illustrate why energy sharing is expected above threshold. Suppose we relax condition (13). As a consequence it might happen that $E_q(0) > E_q^c$ and also that the NLS equation (12) admits a general solution with both a radiative (i.e. dispersive) component and a multisoliton component [10]. In presence of solitons the two limits quoted above no longer commute, and qualitative differences with respect to the unperturbed case appear. A single soliton causes a wavevector shift $\delta k \approx \sqrt{R/\omega_q}$ and a frequency shift $\delta\omega \approx \sqrt{R/\omega_q}\ \frac{d\omega_q}{dq}$ in the fundamental harmonic component of the wave packet; the energy of the mode $q + \delta k$ turns out to be just $E_{q+\delta k}(\tau_2) \propto E_q^c$ (to leading order). This shows that solitons contribute to energy tranfer to normal modes initially not excited. When $E_q(0) \gg E_q^c$ we expect such a mechanism to become very efficient and a strong interaction between normal modes to take place, leading to an intense spreading of the wave packet.

III. COMPARISON WITH THE NUMERICAL RESULTS

We concentrate our attention on the numerical works [4] and [3]. In the latter one the β model (with $\alpha = 0$, i.e. $\mu = 0$) is studied, and results are found giving a threshold independent of frequency. This is in complete agreement with our estimate (17), where for $\mu = 0$ the dependence on ω is seen to completely disappear. Instead in the work [4] a Lennard-Jones model (i.e. with $\mu \simeq 1.78$) was studied, and a threshold increasing with ω more or less in a parabolic way was found. It seems non trivial that our analytical estimate (17) takes into account, at the same time, such two different results. This is illustrated in figure 1, where E^c (normalized to its maximum E^c_{max}) is plotted vs. ω for four different values of μ. The largest value of μ corresponds to the LJ potential (for which a parabolic-like behaviour is exhibited), while as $\mu \to 0$ the curves tend to the horizontal line $E^c/E^c_{max} = 1$.

A quantitative comparison between our estimate (17) and the numerical results found in [4] for the LJ potential is reported in figure 2. In the latter paper the threshold was defined in the following way. A packet of nearby frequencies, centered about a frequency ω, was initially given a certain energy E, and the dynamics was followed up to a certain observation time. A parameter p ($0 \leq p \leq 1$) was then introduced, representing the maximal fraction of the initial energy which was given out by the packet. The computations were repeated for increasing values of the initial energy E, and the value of p was found to be an increasing function of E. Having fixed a value of p, the critical energy $E^c(\omega; p)$ was then defined as the one required to produce the given value of p. It turns out that the "curves" E^c vs. ω (or vs. ω/Ω) thus defined, although depending parametrically on p, seem to collapse on a single curve if the ordinates are normalized through division by E^c_{max}. The fit with our theoretical formula, shown in figure 2, seems to be remarkable.

In passing, we point out that numerical results are also available for a two dimensional FPU system with L-J interaction; see [16].

IV. THE φ^4 MODEL

In this section we apply the MSE to the φ^4 model (5). Defining $x_n = q_n/A$ and $\tau = \frac{\Omega}{2}t$, the equations of motion in dimensionless form become

$$\ddot{x}_n = -\frac{4}{1+\eta}x_n + \frac{\eta}{1+\eta}(x_{n+1} + x_{n-1} - 2x_n) - Rx_n^3 \ . \tag{18}$$

Here, as usual, $\Omega = \sqrt{m^2 + 4\epsilon}$ is the maximum frquency in the dispersion relation $\omega(k) = \sqrt{m^2 + 4\epsilon \sin^2(k/2)}$; the dimensionless parameters $\eta = 4\epsilon/m^2$ and $R = 4\lambda A^2/\Omega^2$ (Reynolds number) were also introduced. Making the ansatz (9) and using exactly the same notations of the previous section, the slow modulating amplitude of the fundamental harmonic is easily shown to satisfy the NLS equation

$$i\partial_{\tau_2}\psi - \frac{(1+\eta)\omega_q^4 - 16}{2(1+\eta)\omega_q^3}\partial_\zeta^2\psi - \frac{3}{2\omega_q}|\psi|^2\psi = 0 \ , \tag{19}$$

where ω_q is the renormalized dispersion relation, namely $\omega_q = 2\omega(q)/\Omega = \frac{2}{\sqrt{1+\eta}}\sqrt{1 + \eta \,\mathrm{sen}^2(q/2)}$. Notice that the coefficient in front of the dispersive term $\partial_\zeta^2\psi$ is nothing but $\frac{1}{2}\frac{d^2}{dq^2}\omega_q$. For values of q such that $\omega_q < 2/(1+\eta)^{1/4}$ one has $\frac{d^2}{dq^2}\omega_q > 0$ and the NLS equation (19) becomes "defocusing" [14]. In such a case there can't be soliton solutions in the class of initial data $\{\psi(\zeta \to \pm\infty, 0) \to 0\}$ and, as a consequence, there is neither an upper bound on the L_1-norm of the initial data giving a criterion for a threshold, nor a clear-cut evidence of a quasi linear regime. For q such that $\omega_q \geq 2/(1+\eta)^{1/4}$ the theorem quoted in the previous section can instead be applied. The upper bound $\mathcal{S}_q$ to the L_1-norm of the initial datum is

$$\mathcal{S}_q = \sigma\sqrt{\frac{2}{3}}\frac{\sqrt{(1+\eta)\omega_q^4 - 16}}{\omega_q\sqrt{1+\eta}} \ , \quad \omega_q \geq \frac{2}{(1+\eta)^{1/4}} \tag{20}$$

and for the energy threshold $E_q^c \equiv \omega_q^2\mathcal{S}_q^2/R$ we then obtain

$$E_q^c = \frac{2\sigma^2}{3R}\frac{(1+\eta)\omega_q^4 - 16}{1+\eta} \quad , \quad \omega_q \geq \frac{2}{(1+\eta)^{1/4}} \quad . \tag{21}$$

Turning to physical variables this gives the result (6) quoted in the introduction. In terms of the dimensionless quantities η and ω/Ω it takes the form:

$$E_{\varphi^4}^c(\omega) = \begin{cases} \frac{2\sigma^2\Omega^4}{3\lambda}\left((\omega/\Omega)^4 - \frac{1}{1+\eta}\right) \ , \quad \omega \geq \omega_c \\ 0 \ , \quad \omega \leq \omega_c \end{cases} \ , \tag{22}$$

where $\omega_c = \Omega/(1+\eta)^{1/4}$. The energy threshold below the cutoff ω_c was set to zero for the reasons explained above. A plot of $E^c(\omega)/E_{max}^c$ for different values of $\eta = 4\epsilon/m^2$ is reported in figure 3.

A quantitative comparison with the numerical data of the work [5] is reported in figure 4. The numerical values of the parameters chosen in [5] were such that $\eta = 4\epsilon/m^2 = 40$. From figure 4 one sees that the agreement is very good for the high frequencies, while the situation concerning the low frequencies, below the cutoff ω_c, is not so clear. Further numerical investigations might clarify this point. In any case, the claim that some relevant role might be played by the cutoff frequency ω_c for the φ^4 model seems to be supported by the results of another numerical work, namely [17]. Actually, in such a paper, the attention was addressed not to the existence of energy thresholds in the sense discussed here, but rather to the "final" distribution of energy among the modes. However the results show that for the φ^4 model (at variance with the β FPU model) there exists a characteristic frequency, say ω^*, such that equipartition holds only for $\omega > \omega^*$, while the energy is lower for $\omega < \omega^*$ and tends to zero as ω tends to its minimum. Now, it turns out that the characteristic frequency ω^*, defined in such a way by numerical computations, agrees rather well with our frequency ω_c; a fact which seems hardly fortuitous.

V. FURTHER COMMENTS

We address here three points. The first one concerns the problem of the thermodynamic limit, namely the limit in which one deals with infinitely many particles and an infinite energy, with a finite energy per particle. This is a problem which plays an essential role in statistical mechanics, and was extensively studied in the frame of the FPU model (see [18], [19] and [20]). Now, it should be quite clear that the present work is not dealing at all (at least in a direct way) with the thermodynamic limit, because we are considering a system with infinitely many particles while exciting a narrow packet of modes with a finite amount of energy, so that our system has a vanishing energy per particle. We would like to stress however that the case considered here has a considerable physical interest. Indeed in nonlinear acoustics, for example, ultrasonic waves are used to study phonon-phonon interaction and in solid state physics a lot of phenomena can be produced by means of laser radiation; clearly in both such cases one is dealing with *coherent pulses* of finite energy (with a well defined frequency) in macroscopic systems. Anyway, it is not excluded a priori that the present results might turn out to shed some light on the problem of the thermodynamic limit itself. This is an interesting point which we plan to investigate in the future.

The second point concerns a comparison with the available analytical estimates for the energy thresholds, namely those of Izrailev and Chirikov [6] and of Berman and Kolovskii [9]. The estimate of Izrailev and Chirikov was concerned with the β model and gave a threshold decreasing with frequency, contrary to the flat behaviour of the numerical data of

[3], which agree very well with our formula (17). This seems to indicate that the approach based on the overlapping of resonances deserves further discussions in the case of infinitely many degrees of freedom.

Our results seem in any case to indicate that the methods of Inverse Scattering are appropriate when many degrees of freedom are involved, as was first suggested by Berman and Kolovskii. The problem then remains of understanding why did they find a different analytical estimate for the threshold. Our opinion is the following one. What we have in common is the idea of defining the threshold as corresponding to an intense spreading of the energy from the excited packet to other modes, in terms of properties of the NLS equation. At this point we make use of a deep analytical result known in the literature, giving a condition for the existence of solitons, which, at least in the models studied here, just turns out to constitute the mechanism for the energy sharing. Instead Berman and Kolovskii were using a criterion of self consistency for the validity of the narrow packet approximation. Our opinion is that the introduction of the latter criterion was indeed correct, and that the authors apparently just did not work it out in a completely satisfactory way. Indeed it can explicitly be shown that a more precise elaboration of their consistency criterion leads exactly to our formulas [21].

The third point is a short discussion on the meaning of the threshold introduced in the present paper. From the very definition given above, it should be quite clear that such a threshold is just an estimate “from below” ensuring, on the basis of a deep theoretical result of Soliton Theory, the existence of ordered motions with no effective energy spread out of an initially excited packet. What really occurs, or even might be expected, above threshold is an extremely interesting question. In particular, from the point of view considered here, one should extend the present result and understand the role solitons play in connection with Arnold’s diffusion along the so called stochastic web, i.e. understand the role of resonances within the multiple-scale approach. This would possibly allow one to produce also relevant information about the physically significant problem of the “final” distribution of energy among the modes. We hope to be able to come back to these very interesting problems in the future. The extremely good agreement of the present analytical estimate for the threshold with the numerical results seems to be promising.

APPENDIX: PERTURBATIVE METHOD

The "implementation" of the MPE is based on the following steps:

$$\begin{aligned}
x_{n\pm1} &= \sum_{a\in\mathbb{Z}} e^{\pm iaq} e^{ia(qn-\omega_q\tau)} \psi^{(a)} \left(\zeta \pm \sqrt{R}, \tau_1, \cdots, \tau_M; \sqrt{R}\right) = \\
&= \sum_{a\in\mathbb{Z}} e^{\pm iaq} e^{ia(qn-\omega_q\tau)} e^{\pm\sqrt{R}\ \partial_\zeta} \sum_{l\geq0} R^{l/2} \psi_l^{(a)} \left(\zeta, \tau_1, \cdots, \tau_M\right) \ ; \\
\frac{d^2}{d\tau^2} x_n &= \left(-ia\omega_q + \sum_{j\geq1} R^{j/2} \frac{\partial}{\partial\tau_j}\right)^2 x_n
\end{aligned}$$

Having made such $\sqrt{R}$-expansions, grouped together the terms of the same order and written down the equations of motion as power series, one has just to set to zero all of their coefficients, taking care that "secular" (i.e. time increasing) terms in the approximate solution (9) of the equations of motion are not generated in such a way. As usual in MSE applications [12], by "killing" a secular term at second order ($O(R)$ in our case) the NLS equation is obtained.

FIGURES

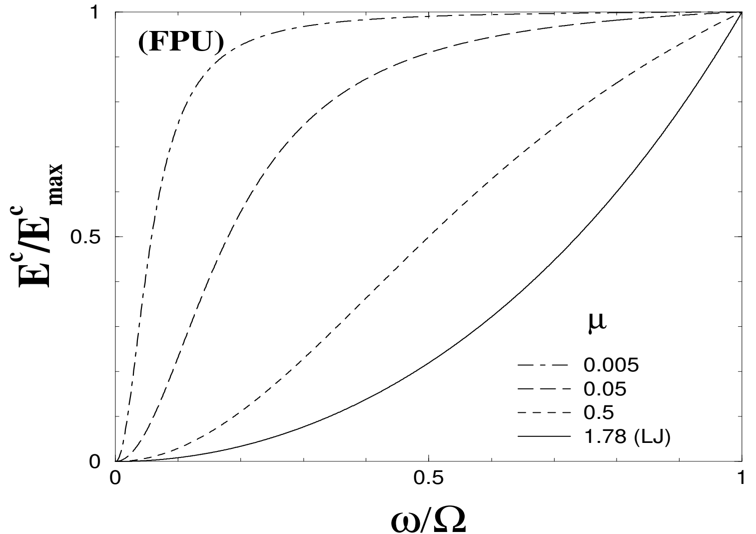

FIG. 1. FPU model; normalized energy threshold vs. ω/Ω for four different values of $\mu = 4\alpha^2/(\beta\Omega^2)$.

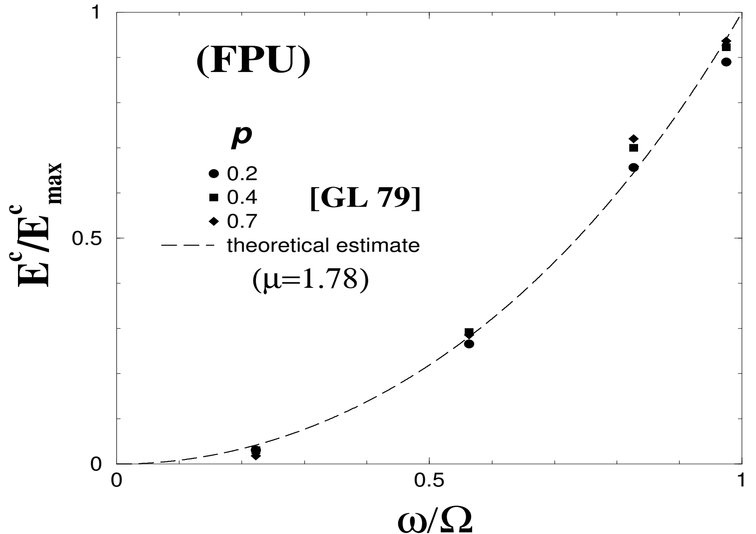

FIG. 2. FPU model; normalized energy threshold vs. ω/Ω; comparison between the theoretical estimate (for $\mu = 4\alpha^2/(\beta\Omega^2) = 1.78$) and the numerical data for a Lennard-Jones model. Different points, at a given frequency, correspond to different values of p, the parameter indicating the maximal fraction of initial energy given out by the excited packet.

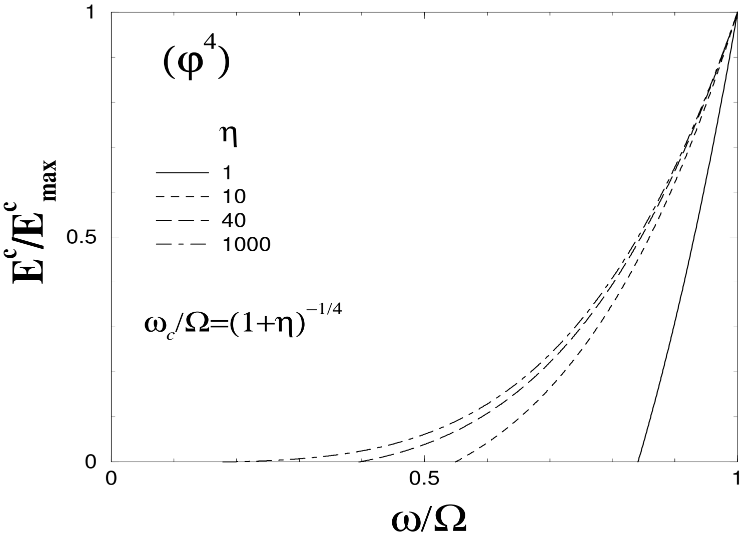

FIG. 3. φ^4 model; normalized energy threshold vs. ω/Ω for four different values of $\eta = 4\epsilon/m^2$.

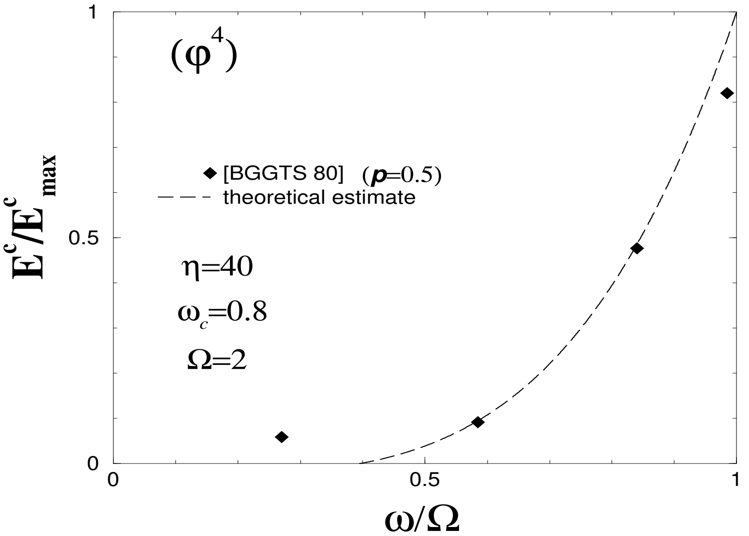

FIG. 4. φ^4 model; normalized energy threshold vs. ω/Ω; comparison between the theoretical estimate and the numerical data (corresponding to $p = 0.5$) for $\eta = 40$.

REFERENCES

[1] Fermi E., Pasta J., Ulam S.; in *Nonlinear wave motion*, Newell A. (ed.) (Lectures in Applied Mathematics, **15**, 1974, p. 143)

[2] Bocchieri P., Scotti A., Bearzi B., Loinger A.; Phys. Rev. A **2** (1970), 2013

[3] Livi R., Pettini M., Ruffo S., Sparpaglione M., Vulpiani A.; Phys. Rev. A **31** (1985), 1039

[4] Galgani L., Lo Vecchio G.; Nuovo Cimento B **52** (1979), 1

[5] Butera P., Galgani L., Giorgilli A., Tagliani A., Sabata H.; Nuovo Cimento B **59** (1980), 81

[6] Izrailev F.M., Chirikov B.V.; Sov.Phys.Dokl. **11** (1966), 30

[7] Chirikov B.V.; Phys. Rep. **52** (1979), 263

[8] Escande D.F.; Phys. Rep. **121** (1985), 165

[9] Bermann G.P., Kolovskii A.R.; Sov. Phys. JETP **60** (1984), 1116

[10] Ablowitz M.J., Segur H.; *Solitons and the Inverse Scattering Transform* (SIAM, Philadelphia, PA, 1981)

[11] Novikov S., Manakov S.V., Pitaevskii L.P., Zakharov V.E.; *Theory of Solitons* (Consultants Bureau, New York, 1984)

[12] Degasperis A., Manakov S.V., Santini P.M.; Physica D **100** (1997), 187

[13] Zakharov V.E., Shabat A.B.; Sov. Phys. JETP **34** (1972), 62

[14] Zakharov V.E., Shabat A.B.; Sov. Phys. JETP **37** (1973), 823

[15] Zakharov V.E., Manakov S.V.; Sov.Phys. JETP **44** (1976), 106

[16] Benettin G., Lo Vecchio G., Tenenbaum A.; Phys. Rev A **22** (1980), 1709

[17] Pettini M., Cerruti-Sola M.; Phys. Rev. A **44** (1991), 975

[18] Kantz H.; Physica D **39** (1989), 322

[19] Kantz H., Livi R., Ruffo S.; J. Stat. Phys **76** (1994), 627

[20] DeLuca J., Lichtenberg A.J., Ruffo S.; Phys. Rev. E **51** (1995), 2877

[21] Ponno A.; *Thesis* (1998), University of Rome "La Sapienza"