Energy localization in the Φ^4 oscillator chain

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We study energy localization in a finite one-dimensional Φ^4 oscillator chain with initial energy in a single oscillator of the chain. We numerically calculate the effective number of degrees of freedom sharing the energy on the lattice as a function of time. We find that for energies smaller than a critical value, energy equipartition among the oscillators is reached in a relatively short time. On the other hand, above the critical energy, a decreasing number of particles sharing the energy is observed. We give an estimate of the effective number of degrees of freedom as a function of the energy. Our results suggest that localization is due to the appearance, above threshold, of a breather-like structure. Analytic arguments are given, based on the averaging theory and the analysis of a discrete nonlinear Schrödinger equation approximating the dynamics, to support and explain the numerical results.

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I. INTRODUCTION

We study localized excitations in oscillator chains motivated by the need to understand phenomena occurring in DNA molecules (transcription, denaturation, etc.). Such phenomena involve the generation and propagation of localized excitations along the macromolecule [1], so that the analysis of existence, stability, and movability of periodic and almost-periodic localized structures in oscillator chains is of relevance. An important result is a theorem of MacKay and Aubry (MA) [2] on the existence and stability of time-periodic localized excitations in chain models satisfying suitable structural conditions. The MA theory [2] states that, for large enough initial energy placed on a single particle, the subsequent motion is close to the periodic motion that particle would have if it were isolated, its interaction with the nearby particles being the more negligible the higher the energy. In a subsequent proof given by Bambusi [3], it was shown that if one starts close enough to the exact breather solution, the corresponding orbit stays close to a breather solution for exponentially long times. For a review on discrete breathers, see Refs. [4,5]. Breathers represent particular solutions of the system, and as such, they correspond to suitably selected initial data. On the other hand, in the physical phenomenon of DNA transcription, the initial conditions are fixed by the problem and cannot be chosen arbitrarily. In such a case, a localized initial excitation might give rise to a motion that is far from a simple breather. Thus, a natural question is whether, in the physical case, energy spreads out to all degrees of freedom available, or if it stays localized on a few degrees of freedom, giving rise to a breather or some other localized structure (moving or at rest). In the present paper, we study the dynamics corresponding to the initial excitation of a single particle of a finite one-dimensional Φ^4 chain with periodic boundary conditions. We focus on the localization of energy in real space, i.e., we count the fraction of particles sharing the energy after some long (but fixed) time scale. The qualitative findings are as follows; there exists a threshold value of the energy, below which spatial equipartition of energy takes place. Above threshold, the larger the energy, the smaller the number of particles involved in the motion. The mechanism triggering energy localization just above the threshold seems to be the formation of a breather centered at the initially excited site. Such a breather becomes narrower and narrower as the energy increases, eventually approaching, at very high values of energy, the single-site breather corresponding to the (zeroth-order) anticontinuum limit solution of Aubry [5].

It is interesting to contrast our present results to the usual phenomenology of the Fermi-Pasta-Ulam problem (FPU) [6,7]. Our results are somewhat complementary to the usual FPU phenomenology in real space: instead of a single mode, we excite a single particle, and we observe the lack of equipartition at high energy instead of at low energy. Moreover, we find that breathers play the same significant role played by solitons in the standard FPU problem. In particular, as energy increases, soliton formation in the standard FPU problem is responsible for the limitation of the number of modes sharing the energy (see, e.g., [8]), while we find that breather formation is responsible for the decrease in the number of particles taking part in the motion. It is of interest to mention a recent paper by Flach *et al.* [9], in which the

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concept of a q breather in the standard FPU problem has been introduced. This paper is organized as follows: In Sec. II, we describe the numerical results, and Sec. III is devoted to the analytic arguments, while in Sec. IV we have the conclusions and discussion.

II. NUMERICS AND RESULTS

A. General setting

The Hamiltonian equations of motion of a Φ^4 oscillator chain with N degrees of freedom and periodic boundary conditions are

$$\ddot{x}_n = x_{n+1} + x_{n-1} - (2+m^2)x_n - \lambda x_n^3, \quad n = -\frac{N}{2}, \ldots, \frac{N}{2}, \tag{1}$$

$$x_{-N/2} = x_{N/2}, \quad \dot{x}_{-N/2} = \dot{x}_{N/2}. \tag{2}$$

The nonlinear coupling constants λ and m are positive parameters defining the model. These equations of motion were integrated numerically using a 10th-order Runge-Kutta-Nystrom integrator [10]. The initial energy E is always placed at the central particle located at the site $n=0$, i.e.,

$$x_n(0) = a\,\delta_{n,0}, \quad \dot{x}_n(0) = b\,\delta_{n,0}, \tag{3}$$

where $\delta_{n,0}$ denotes the Kronecker delta and the constants a and b are related to the energy E by

$$E = \frac{b^2}{2} + \frac{(m^2+2)a^2}{2} + \frac{\lambda a^4}{4}. \tag{4}$$

In the numerical calculations, values of m ranging from $m=\sqrt{3}$ to $m=10$ have been used, for a chain of $N=500$ particles. Without loss of generality, we chose to fix $\lambda=1$. Indeed, for other values of λ the rescaled initial condition $b=\tilde{b}/\sqrt{\lambda}$ and $a=\tilde{a}/\sqrt{\lambda}$ in Eq. (4) corresponds to the rescaled energy $\lambda E=\tilde{b}^2/2+(m^2+2)\tilde{a}^2/2+\tilde{a}^4/4$, so that the dynamics depends on the single control parameter λE. For what concerns the choice of a and b, we realized that localization takes place at a lower energy when the initial excitation is defined by the following kick-like excitation $a=0$ and $E=b^2/2$. The results reported refer to this special case, which does not require varying the initial conditions for a fixed energy. Note that because of a symmetry of Eq. (1), one obtains the same dynamics both for positive and for negative values of b. The reason for the special role played by kick-like excitations will be explained below.

In order to measure the degree of localization on the lattice, we use a time-dependent measure of the effective number of degrees of freedom sharing the energy at time t, as first introduced in Refs. [11,6] and explained in the following. We define the normalized instantaneous energy of particle n by

$$\varepsilon_n \equiv \frac{1}{E}\left[\frac{\dot{x}_n^2}{2} + \frac{m^2 x_n^2}{2} + \frac{(x_{n+1}-x_n)^2}{4} + \frac{(x_n - x_{n-1})^2}{4} + \frac{\lambda x_n^4}{4}\right], \tag{5}$$

where at the exceptional end point $n=-N/2$ we apply Eq. (5) with $x_{n-1}=x_{N/2}-1$, as the ends are identified by the periodic boundary condition. Because of this identification of the end points, the chain has effectively N degrees of freedom only, and not $N+1$. It can be shown that $\Sigma_{N/2-1}^{N/2}\varepsilon_n(t)=1$ if E in Eq. (5) is taken as the energy constant of motion. From the instantaneous ε_n defined in Eq. (5), we construct the effective number of degrees sharing the energy, $N_{eff}(t)$, as

$$N_{eff}(t) \equiv \exp\left(-\sum_{n=-N/2}^{N/2-1} \varepsilon_n \ln \varepsilon_n\right). \tag{6}$$

Note that, in principle, N_{eff} reaches its maximum at equipartition, i.e., $\varepsilon_n=1/N$ and $N_{eff}=N$. Any other distribution of the ε_n's, which necessarily implies some degree of energy localization, yields a lower value of N_{eff}. The limit case is $\varepsilon_{n_*}=1$ and $\varepsilon_n=0$ for $n\neq n_*$, for which one has $N_{eff}=1$, i.e., extreme localization. In fact, with our particular choice of kick-like initial condition, we start with the system in such a state, with energy concentrated in the site $n=0$. In actual computations, the argument of the exponential in Eq. (6) is averaged over a suitable time window, in order to avoid fluctuations on short time scales. In numerical simulations, the absolute maximum equipartition value $N_{eff}=N$ is never observed. The actual value of N_{eff} corresponding to equipartition is instead the lower value

$$\nu \equiv \left(\frac{N_{eff}}{N}\right)_{\text{equip.}} \simeq 0.7, \tag{7}$$

which is due to fluctuations of the ε_n's, as explained from the phase-space arguments in [7,12,13]. In the present numerical experiments, with $N=500$ and $\nu\simeq 0.7$, the equipartition value of N_{eff} is $N\nu\simeq 350$.

B. Numerical results

In the numerical integrations, we fix a maximum integration time T_m; and the results shown refer to $T_m=5\times 10^3$. Longer runs have been made to confirm the validity of the present conclusions. The plots of N_{eff} vs time for a given energy E show the following qualitative behavior. There is a critical energy E_c such that if $E<E_c$, then $N_{eff}(t;E)$ starts from its initial value $N_{eff}(0;E)=1$ and reaches the equipartition value $N_{eff}(T_m;E)\simeq \nu N$ in a short time scale, that is maintained up to T_m for any $E<E_c$. On the other hand, if $E>E_c$, then N_{eff} saturates at a level that is lower than the equipartition value, so that $N_{eff}(T_m;E)<\nu N$, and $N_{eff}(T_m;E)$ turns out to be a decreasing function of the energy E, i.e., energy tends to localize in space. More precisely, we get the following empirical law:

$$\frac{1}{N_{eff}(T_m;E)} \simeq \frac{1}{\nu N}, \quad E<E_c,$$

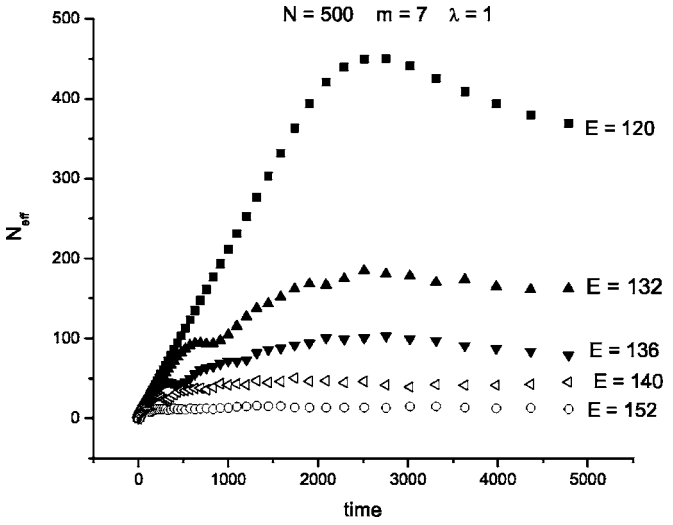

FIG. 1. N_{eff} vs time for $m=7$, at different values of the energy E. Equipartition level at $N=500$ is $\nu N=350$ and $E_c=130$.

$$\frac{1}{N_{eff}(T_m;E)} \simeq \frac{1}{\nu N} + \alpha \ln(\lambda E/m^2) + \beta, \quad E \gg E_c, \qquad (8)$$

where $E_c \simeq \frac{8m^2}{3\lambda}$. We note that if m is large enough, the coefficients α and β in Eq. (8) turn out to be independent of the parameters entering the model. More precisely, fitting the numerical data yields $\alpha \in (1.5, 2)$ and $\beta \in (0.5, 0.9)$. Note also that in the limit $N \to \infty$ the first contribution on the right-hand side of Eq. (8) tends to zero. As we discuss below, the numerical laws of Eq. (8) represent a clear signature of energy localization due to the formation of breathers in the system.

In Figs. 1 and 2 we plot $N_{eff}(t;E)$ vs time up to the time T_m for different values of the energy E and for $m=7$ and $m=10$. In Fig. 3, we plot $\ln(E)$ vs $1/N_{eff}(T_m;E)$ for four different values of m, namely, $m=\sqrt{3}$, $m=\sqrt{10}$, $m=7$, and $m=10$. Note that above some critical energy depending on m,

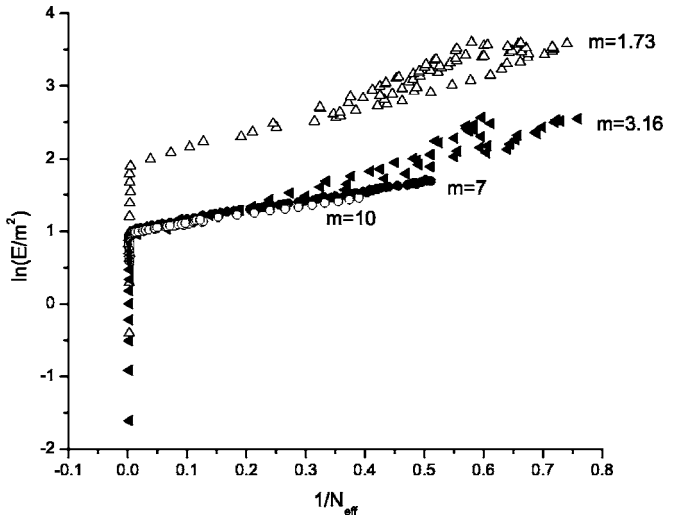

FIG. 2. N_{eff} vs time for $m=100$, at different values of the energy E. Equipartition level at $N=500$ is $\nu N=350$ and $E_c=266$.

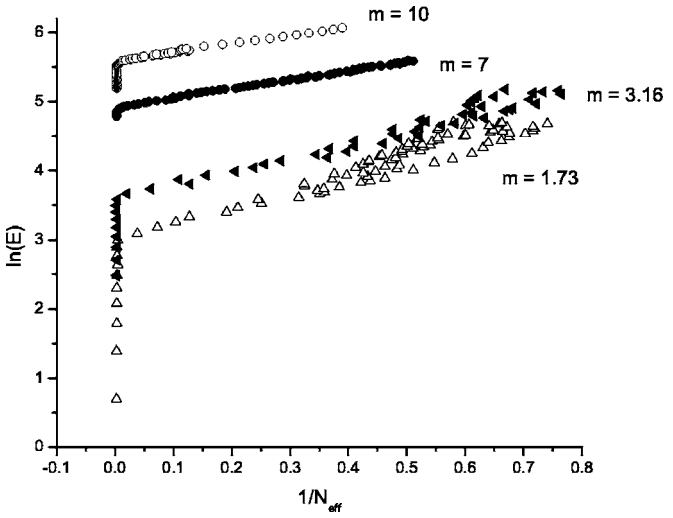

FIG. 3. Logarithm of the energy E vs $1/N_{eff}(T_m,E)$ for four different values of m. Note that the slope of all curves look the same but for the curve at $m=1.73$.

the profiles become almost rectilinear, especially for $m=7$ and $m=10$. In Fig. 4, we plot instead $\ln(E/m^2)$ vs $1/N_{eff}(T_m;E)$. Now the curves corresponding to $m=\sqrt{10}$, 7, and 10 appear almost superposed, while the curve corresponding to $m=\sqrt{3}$ is clearly detached. As we explain below, when m is large, we expect one parameter only ruling energy localization in the system, and such a parameter turns out to be proportional to E/m^2 (recall that we set $\lambda=1$). Clearly, we can deduce from Figs. 3 and 4 that in the case $m=1.73$, the phenomenology of localization is similar to that of the other cases, but the two parameters ruling it, E and m^2, do not merge in a simple combination.

In Ref. [11], a plot similar to Fig. 3 is reported for the double-well Φ^4 model, consisting of the same equations of motion (1) with a minus sign in front of the m^2 term. Apart from the fact that the model is different from the model

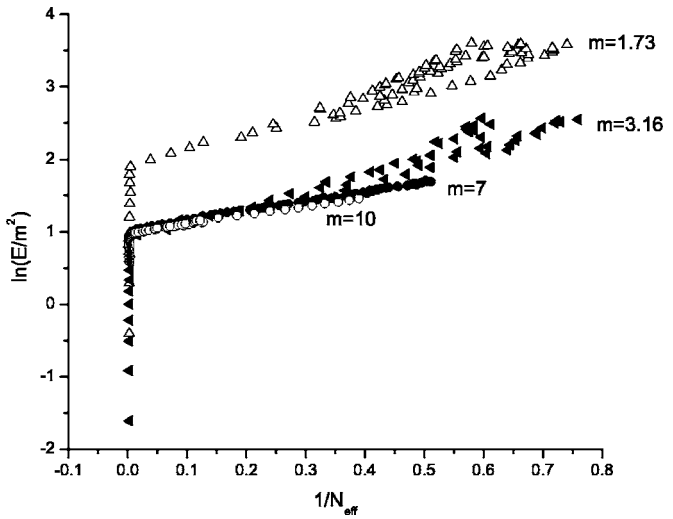

FIG. 4. Logarithm of the ratio E/m^2 vs $1/N_{eff}(T_m,E)$ for the same four different values of m of Fig. 3. Note that all curves are superposed but the curve at $m=1.73$.

considered, we emphasize that in Ref. [11] the authors plotted the normalized logarithm of N_{eff} (the so-called spectral entropy) vs the energy, from which no simple law immediately appears. Our present choice of graphs follows the lead given in Ref. [3], where it was pointed out that a logarithmic dependence of the form of Eq. (8) should be expected.

III. THEORETICAL ANALYSIS

A. Averaging

We introduce three suitable quantities defined in terms of the parameters m and λ of the Φ^4 model, and of the parameters a, b, and E defining the initial data [see Eqs. (3) and (4)], namely,

$$\mathcal{E} \equiv \frac{b^2 + m^2 a^2}{2} = E - a^2 - \frac{\lambda a^4}{4}, \tag{9}$$

$$e^{i\theta} \equiv \frac{ma + ib}{\sqrt{2\mathcal{E}}}, \tag{10}$$

$$g \equiv \frac{3\lambda \mathcal{E}}{4m^2}. \tag{11}$$

They represent, respectively, part of the energy initially placed at site $n=0$, the phase of the initial datum ($i=\sqrt{-1}$), and what turns out to be the only fundamental parameter of the theory after averaging (see below). Using the complex change of variables $(x,\dot{x})(t) \mapsto (\psi,\psi^*)(\tau)$ defined by

$$\psi_n = e^{imt} e^{-i\theta} \frac{m x_n + i \dot{x}_n}{\sqrt{2\mathcal{E}}}, \tag{12}$$

$$t \equiv m\tau, \tag{13}$$

into the equations of motion (1), we obtain

$$i\frac{d\psi_n}{d\tau} = -\frac{1}{2}(\psi_{n+1} + \psi_{n-1} - 2\psi_n) + g|\psi_n|^2 \psi_n + R_n(\psi,\psi^*,\tau), \tag{14}$$

where the remainder R_n is

$$R_n(\psi,\psi^*,\tau) \equiv -\frac{1}{2}(\psi^*_{n+1} + \psi^*_{n-1} - 2\psi^*_n) e^{2i(m^2\tau-\theta)} + g\left[|\psi_n|^2 \psi^*_n e^{2i(m^2\tau-\theta)} + \frac{1}{3}\psi_n^3 e^{-2i(m^2\tau-\theta)} + \frac{1}{3}(\psi^*_n)^3 e^{4i(m^2\tau-\theta)} \right]. \tag{15}$$

The periodic boundary conditions (2) simply imply that $\psi_{-N/2} = \psi_{N/2}$, while for what concerns the initial data (3), by use of Eqs. (9) and (12), we obtain $\psi_n(\tau=0) = \delta_{n,0}$. The reformulation of the problem in terms of the complex variables ψ_n is, up to this stage, exact. Now, we observe that

$$\langle R_n \rangle \equiv \frac{m^2}{\pi} \int_0^{\pi/m^2} R_n(\psi,\psi^*,\tau)|_{\psi=\text{const.}} d\tau = 0, \tag{16}$$

i.e., the average of R_n over one period of the fast oscillation, π/m^2, at constant ψ, is zero. This means that R_n is expected to give small contributions to the dynamics and can be neglected in a first approximation, which is an application of the averaging technique; see for example, Ref. [14]. Thus, we are left with the simplified problem:

$$i\frac{d\psi_n}{d\tau} = -\frac{1}{2}(\psi_{n+1} + \psi_{n-1} - 2\psi_n) + g|\psi_n|^2 \psi_n, \tag{17}$$

$$\psi_n(0) = \delta_{n,0}, \tag{18}$$

$$\psi_{-N/2}(\tau) = \psi_{N/2}(\tau). \tag{19}$$

.

Note that, as an effect of averaging, the only relevant parameter entering the theory is now the constant g defined in Eq. (11). Equation (17) is a discrete nonlinear Schrödinger equation (DNLS) [15]. In the theoretical analysis below, we will work, for convenience, in the limit $N \to \infty$, which is however consistent with the initial datum (18) and the periodic boundary condition (19). In what follows, we study Eq. (17) as a good approximation to Eq. (1). In this respect, a few fundamental remarks are in order. (i) In the range of values of m where Eq. (17) is valid, any critical behavior in the dynamics of the system must correspond to the crossing of some critical value of the parameter g. This explains why we found, for m large enough, the universal law (8), and a critical energy $E_c \simeq \frac{8m^2}{3\lambda}$. (ii) For what concerns the critical energy E_c, note that $g \propto \lambda \mathcal{E}/m^2$, so that $g=g_c$ implies $\mathcal{E}_c \propto m^2/\lambda$; since $\mathcal{E}=E-a^2-\lambda a^4/4$, one gets that the minimum of E_c over all the possible initial conditions is reached at $a=0$, namely, for kick-like initial data. (iii) The averaging performed above is expected to be valid if m is large enough, so that the oscillations at frequency m are much faster than the drift described by Eq. (17). Thus, as the value of m increases, a better and better agreement with what is predicted by Eq. (17) is expected. Figures 3 and 4 suggest that $m=1.73$ has to be considered too low, in the sense that, for that value, Eq. (17) does not represent a good approximation.

B. DNLS analysis I: Asymptotic linear map

A simple way to understand our numerical law is as follows. First of all, let us suppose that $N \to \infty$ and that a time-periodic, strongly localized solution of Eq. (17) exists for some g. Its frequency is determined, in a first approximation, by neglecting the coupling of the initially excited sites to the neighboring ones (the so-called anticontinuum limit of Aubry). Rescaling time as $t \to \tau/g$ one can rewrite Eq. (17) as follows:

$$i\frac{d\psi_n}{d\tau} = -\epsilon(\psi_{n+1} + \psi_{n-1} - 2\psi_n) + |\psi_n|^2 \psi_n, \tag{20}$$

where $\epsilon \equiv 1/(2g)$. Both approaches in Refs. [2,3] start, at order zero, by putting $\epsilon=0$, which is equivalent to neglecting

the discrete Laplacian on the right-hand side of Eq. (17). In Ref. [3], it was observed that a breather solution of Eq. (20) is expected to be exponentially localized in space, with a profile decreasing like $e^{-k(\epsilon)n}$, and an asymptotics $k(\epsilon)\sim\ln(1/\epsilon)$ was guessed on the basis of Nekhoroshev's theorem. This is our starting point. However, we go on to refer, for consistency, to Eq. (17). Neglecting the discrete Laplacian yields $\psi_n(\tau)\simeq e^{-ig|\psi_n(0)|^2\tau}$, which, when matched to the initial datum (18), yields $\psi_n(\tau)=\delta_{n,0}e^{-ig\tau}$. This is valid if g is large enough [which, in the equivalent formulation pointed out above, corresponds to $\epsilon=1/(2g)$ small enough]. The frequency of the zero-order, single-site breather is thus g. Now, following [4], if the motion of the chain is really localized around the site $n=0$, at site $n\gg 0$ nonlinearity can be neglected, and thus, we are led to look for an asymptotic $(n\to\infty)$ solution of the linearized DNLS equation (17) in the form $\psi_n(\tau)=u_n e^{-ig\tau}$. Thus we obtain the linear map

$$\begin{pmatrix} u_{n+1} \\ u_n \end{pmatrix} = \begin{pmatrix} 2(1-g) & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} u_n \\ u_{n-1} \end{pmatrix}. \tag{21}$$

Suppose we start at a site $n_0\gg 0$ and iterate the map to the right. If $\mu_\pm$ denote the two eigenvalues, and $V_\pm$ denotes the corresponding eigenvectors of matrix M, and if $U_{n_0}=c_+V_+ + c_-V_-$, the result of the iteration is

$$U_{n_0+n} = M^n U_{n_0} = c_+(\mu_+)^n V_+ + c_-(\mu_-)^n V_-. \tag{22}$$

The only way to have $U_{n_0+n}\to 0$ as $n\to+\infty$, is that $c_-=0$ (a condition on U_{n_0}) and $g>2$ so that $\mu_-<-1<\mu_+<0$. In such a case, we have $\mu_+=1-g+\sqrt{(1-g)^2-1}$, and

$$U_{n_0+n}\sim(-1)^n|\mu_+|^n=(-1)^n e^{-n\,\ln(1/|\mu_+|)}. \tag{23}$$

Thus, if a localized excitation persists on the lattice, it asymptotically decreases, on the right, as e^{-kn}. The rate of decrease k can be obviously identified with the inverse of the number of particles taking part in the motion of the chain. One has, for $g\gg 2$,

$$\frac{1}{N_{eff}}\propto k=\ln\left[\frac{1}{(g-1)-\sqrt{(g-1)^2-1}}\right]\sim\ln(2g). \tag{24}$$

Now, recalling the definition of g given in Eq. (11), one finds that the threshold condition $g\gg 2$ reads

$$\mathcal{E}=E-a^2-\lambda a^4/4\gg\frac{8m^2}{3\lambda}. \tag{25}$$

In terms of the energy E, the threshold has a minimum approximately at $a=0$, which explains the special role played by the kick-like initial excitations, as follows. These excitations minimize the energy threshold for breather formation on the lattice. Condition (25) for $a=0$ yields the critical energy (8). The expression of $1/N_{eff}$ given by Eq. (24) for $g\gg 2$, in the case $a=0$ (i.e., $g\propto E$), explains the numerical law (8), namely,

$$1/N_{eff}\sim\ln\left(\frac{\lambda E}{m^2}\right),\quad E\gg E_c=\frac{8m^2}{3\lambda}. \tag{26}$$

Note that it follows from Eq. (24) that when $g\to 2^+$, $1/N_{eff}\to 0$, and for $g<2$, the eigenvalues $\mu_\pm$ have both unitary modulus, which implies that no localized state is possible. This is in qualitative agreement with law (8) for the case $E<E_c$ (recall that, for the sake of simplicity, it was assumed $N\to\infty$). Last, we note that the no correct asymptotics can be deduced from (24) in the limit $g\to 2^+$: indeed, at the beginning we made the zero-order hypothesis of single-site breather, i.e., of a strongly localized excitation, which means that $1/N_{eff}\propto k(g)$ must be very large.

C. DNLS analysis II: Radiation and solitons

In this section, we analyze in some detail the dynamics of the DNLS equation, Eq. (17), in order to understand the case when g is small $(g<2)$. We start by seeking a solution of Eq. (17) in the form

$$\psi_n(\tau)=e^{-ig\tau}[\delta_{n,0}+\phi_n(\tau)], \tag{27}$$

and we linearize the resulting equations of motion for the ϕ_n's. Consistency with the initial datum (18) imposes that $\phi_n(0)=0$ for any n. Note that $e^{-ig\tau}\delta_{n,0}$ is not an exact solution of the DNLS equation (17), but, if the ϕ_n's remain small, in the linear approximation, it can be guessed that the real solution is close to it. Because of the symmetry of Eqs. (17)–(19), its solutions satisfy $\psi_{-n}(\tau)=\psi_n(\tau)$, which because of Eq. (27) implies $\phi_{-n}(\tau)=\phi_n(\tau)$.

For $n\geq 1$, the linearized equations of motion for the ϕ_n's are

$$i\dot{\phi}_n=-\frac{1}{2}\delta_{n,1}-\frac{1}{2}(\phi_{n+1}+\phi_{n-1}-2\phi_n)-g\phi_n, \tag{28}$$

where the dot denotes the derivative with respect to τ. Equation (28) can easily be analyzed by means of the Fourier transform. Substituting

$$\phi_n(\tau)=\frac{1}{2\pi}\int_{-\pi}^{\pi}\Phi_q(\tau)e^{inq}dq, \tag{29}$$

into Eq. (28) and using $\delta_{n,1}=\int_0^{2\pi}e^{i(n-1)q}dq/(2\pi)$ yields

$$\frac{d\Phi_q}{d\tau}=i[g-2\sin^2(q)]\Phi_q+\frac{i}{2}e^{-iq}. \tag{30}$$

The solution of the latter equation, corresponding to the initial condition $\Phi_q(0)=0$ (recall that $\phi_n(0)=0$), is

$$\Phi_q(\tau)=e^{-iq}\frac{e^{i[g-2\sin^2(q)]\tau}-1}{2[g-2\sin^2(q)]}. \tag{31}$$

Now, if $g<2$, there exist two values of $q\in[-\pi,\pi]$, say $q_\pm$, symmetrically located with respect to $q=0$, such that $g-2\sin^2(q_\pm)=0$. In such a case, it follows from Eq. (31) that if $\delta q=q-q_\pm$ is small enough, then

$$|\Phi_{q_\pm \delta q}| \simeq \left| \frac{\sin[\delta q \sin(q_\pm)\tau]}{\delta q \sin(q_\pm)} \right|, \quad (32)$$

i.e., modes very close to $q_\pm$ tend to grow almost linearly in time, which in turn implies that all the ϕ_n's grow. On the other hand, if $g>2$ there is no singularity (i.e., resonance) in the denominator of Eq. (31), and the ϕ_n's are bounded (and small if g is large). Of course, the resonance at $g<2$ and the growth of the modes $q_\pm$ implies that the linear approximation made above breaks down in a finite time, and one has to attack the problem taking into account the effect of the nonlinearity.

The presence of two dominant (resonant) modes only suggests that the dynamics of the system for $g<2$, after a transient time, can be understood in the narrow packet approximation. To fix ideas, and for the sake of simplicity, we treat the case of one mode only, say q_+. More precisely, we search for a solution of Eq. (17) in the form

$$\psi_n(\tau) = e^{i(q_+ n - g\tau)} \Psi(x=n,\tau), \quad (33)$$

where $\Psi(x,\tau)$ is a slowly varying function of x. By substituting Eq. (33) into (17), formally expanding the finite differences up to second order one gets

$$i\Psi_\tau = -i\sqrt{1-(1-g)^2}\Psi_x + \frac{g-1}{2}\Psi_{xx} + g|\Psi|^2\Psi. \quad (34)$$

In deriving the above nonlinear Schrödinger equation (NLS), we repeatedly used $2\sin^2(q_+)=1-\cos(q_+)=g$. As is well known, the NLS equation (34) may have soliton solutions, depending on the initial data, only if the coefficients of the dispersive and nonlinear terms (the second and third term on the right-hand side, respectively) have the same sign, which in this case means $g>1$ or, in terms of the critical energy $E>E_c/2=4m^2/(3\lambda)$.

If we had considered mode q_-, we would have obtained an equation identical to Eq. (34) up to the sign in front of the translation term ($\propto\Psi_x$) (actually, this is the technical fact that allows one to treat the two modes separately).

The qualitative scenario for energy localization emerging from the above analysis is the following. At low energies, $0<E<E_c/2$, one has the resonant radiation of two Fourier modes $q_\pm$, which gives rise to equipartition in real space. If $E_c/2<E<E_c$, the resonant modes are expected to have slowly modulated amplitude; in this range, energy can start to localize inside NLS-like solitons, which move both on the right and on the left (by the symmetry of the problem). When E approaches E_c from below, the velocity of propagation of the solitons tends to zero, the resonant modes $q_\pm$ both approach the value $q=\pi$, and the band-edge mode is known to bifurcate to the breather [4]. Finally, above E_c, a breather centered at the initial site ($n=0$) appears, becoming narrower and narrower as the energy increases. However, from the numerical results we obtained, we must conclude that the effect of localization due to solitons, if any, must be much weaker than the localization due to breathers. Indeed, no prelocalization at $E_c/2$ was observed, and laws (8) are not compatible with NLS solitons.

IV. DISCUSSION AND CONCLUSIONS

We have studied a complementary FPU problem in real space (for the Φ^4 chain), showing that breather formation is the mechanism triggering energy localization on the lattice, thus preventing spatial equipartition of energy if the total energy is large enough [16]. With respect to the standard FPU problem and the possible relevance of the present results to the dynamics of biomolecules, we make the following concluding remarks.

(i) The energy threshold $E_c \simeq 8m^2/3\lambda$ seems to be independent of the number N of degrees of freedom (in varying N from 100 to 500, we did not observe any significant variation). This means that energy localization in real space might take place at zero temperature: $E_c/N \to 0$ as $N \to \infty$ (we identify temperature with specific energy). This would imply that such FPU phenomenology in real space could be relevant at any temperature. However, one should investigate what happens for a more general initial condition, involving, for example, a large number of particles.

(ii) According to the theorem of Ref. [3] and also pointed out in Ref. [17], the lifetime of the breather is expected to be finite but very long, a stretched exponential of the inverse of the small parameter of the theory. With reference to our Figs. 1 and 2, this means that waiting for a longer time should make the value of $N_{eff}(t;E)$ reach the equipartition value $N\nu$. We did not investigate this fact. However, in light of the previous remark, it would be interesting to study the dependence of the Nekhoroshev lifetime found by Bambusi in Ref. [3] on the energy and on the number of degrees of freedom of the system. If such a lifetime depends only on the energy E, then it is not relevant in the thermodynamic limit ($E \propto N \to \infty$). On the contrary, if this lifetime depends on the specific energy E/N, then it is significant below some small but finite temperature. Only in this latter case could the breather be relevant in the real physics of biomolecules.

(iii) The excitation of a single particle corresponds to the excitation of all normal modes of the system in a special combination. In the standard FPU problem, this amounts to start with an almost-equipartited state. The absence of equipartition in real space would imply that the FPU phenomenology (freezing of degrees of freedom, lack of equipartition, etc.) might be generic, i.e., observable for generic initial data.

(iv) The present results, as with any FPU phenomenology, is relevant to the dynamics of biomolecules only if it is robust with respect to inhomogeneities in the chain oscillators [18]. We started to investigate the case of the Φ^4 model with random $\lambda's$. A few experiments with random models seem to indicate that the phenomenology is robust.

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