# Energy localization in a nonlinear discrete system

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We show that, in the weak amplitude and slow time limits, the discrete equations describing the dynamics of a one-dimensional lattice can be reduced to a modified Ablowitz-Ladik equation. The stability of a continuous wave solution is then investigated without and with periodic boundary conditions. Energy localization via modulational instability is predicted. Our numerical simulations, performed on a cyclic system of six oscillators, agree with our theoretical predictions. [S1063-651X(96)08105-6]

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## I. INTRODUCTION

Localization phenomena are of great physical importance as well as of applicability in various domains of science, such as molecular physics, polarons in ionic crystals or proton solitons [1], etc. Although vibrational localization in linear lattices with defects has been well understood for a long time [2], the study of localization in nonlinear lattices without impurities was developed only recently [3]. The socalled intrinsic nonlinear localized excitations have been since then the subject of remarkable interest [4-11]. Following the pioneering work of Fermi, Pasta, and Ulam [12], who demonstrated that a system of coupled nonlinear oscillators does not result in energy equipartition, most of the investigations have been devoted to simple one-dimensional lattices, with one degree of freedom per unit cell and nearest neighbor interaction [13,14]. Other studies were developed by considering an external substrate potential or systems with a small number of particles separated by a heavy one [15,16].

In fact, in nonlinear physical systems, the interplay between nonlinear and dispersion effects can lead to a selfinduced modulation of the steady state. This Benjamin-Feir or modulational instability (MI), first studied in hydrodynamics [17], is also well known in nonlinear optics [18], electrical transmission lines [19], etc. MI appears in continuous models, but also in discrete systems, which are modeled by a set of coupled ordinary differential equations, such as integrable or nonintegrable discrete nonlinear Schrödinger equations (IN-DNLS) [20–23]. For these models, MI was proved to be responsible for energy localization mechanisms [24].

In this paper we first discuss, in the weak amplitude and slow time limits, the existence of MI in an infinite onedimensional lattice model with a specific nonlinear coupling potential. Although this potential can be regarded only as a good approximation of the Morse one, it allows one to reduce the theoretical study to a modified Ablowitz-Ladik equation. This equation is known to be analytically tractable for MI investigation [22]. Moreover, we focus on lattices with periodic boundary conditions, that are equivalent to cyclic systems. We show that, above an energy threshold, some modes are unstable, leading to energy localization inside the system. The validity of this study is finally checked by numerical simulations on the dynamics of a model corresponding to a cyclic system of six identical oscillators.

## **II. THEORETICAL STUDY**

For the sake of clarity, we first consider the dynamics of an infinite chain made of oscillators of mass m separated by a lattice spacing a. The Hamiltonian of our model is

$$H = \sum \frac{m\omega_0^2}{2} [u_n]^2 + \sum \frac{m}{2} \left(\frac{du_n}{dt}\right)^2 + \sum V(u_{n+1} - u_n),$$
(2.1)

where  $u_n(t)$  denotes the displacement of oscillator *n*. According to (2.1), each oscillator is submitted to a harmonic on-site potential with characteristic frequency  $\omega_0$ , and is an-harmonically coupled to its nearest neighbors, via the potential  $V(r_n)$ ,

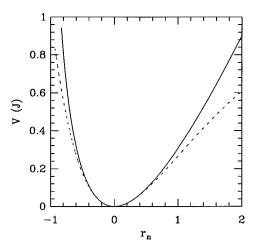


FIG. 1. Dependence of the coupling potential  $V(r_n)$  according to Eq. (2.2) (solid line) and of the Morse potential (dashed line) vs the relative dimensionless displacement  $r_n$ . The parameters A, B, and a are chosen to be equal to unity.

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$$V(r_n) = Ar_n - BLn\left(1 + \frac{A}{B}r_n\right).$$
(2.2)

Here,  $r_n(t) = (u_{n+1} - u_n)/a$  is the relative dimensionless displacement of oscillators n+1 and n, while A and B are positive parameters. Note that for  $r_n=0$ , the oscillators n and n+1 are separated by the equilibrium distance a. As shown in Fig. 1, where A and B have been taken equal to unity, for  $|r_n| < 0.5$ , the potential (2.2) (solid line) is a good approximation of the Morse potential

$$U(r_n) = \frac{9B}{8} \left[ \exp\left(\frac{2Ar_n}{3B}\right) - 1 \right]^2$$

(dashed line). From (2.1) and (2.2), the absolute motion of oscillator n is given by the equation

$$\frac{d^2 u_n}{dt^2} = -\omega_0^2 u_n + u_0^2 \left(\frac{u_{n+1} - u_n}{1 + \gamma(u_{n+1} - u_n)/a} - \frac{u_n - u_{n-1}}{1 + \gamma(u_n - u_{n-1})/a}\right),$$
(2.3)

where  $u_0^2 = A^2/mBa^2$  is the coupling constant and  $\gamma = A/B$  is a nonlinear dimensionless coefficient. Consequently, we get for the relative motion of the oscillators

$$\frac{d^2 r_n}{dt^2} = -\omega_0^2 r_n + u_0^2 \left( \frac{r_{n+1}}{1 + \gamma r_{n+1}} + \frac{r_{n-1}}{1 + \gamma r_{n-1}} - 2 \frac{r_n}{1 + \gamma r_n} \right).$$
(2.4)

Equation (2.4) is then transformed into

$$\left(\frac{d^{2}r_{n}}{dt^{2}} + \omega_{0}^{2}r_{n}\right)\left[1 + \gamma(r_{n+1} + r_{n-1} + r_{n}) + \gamma^{2}(r_{n+1}r_{n-1} + r_{n}r_{n-1} + r_{n}r_{n+1}) + \gamma^{3}r_{n+1}r_{n}r_{n-1}\right]$$
  
$$= u_{0}^{2}\left[r_{n+1}r_{n-1} - 2r_{n} + \gamma(2r_{n+1}r_{n-1} - r_{n+1}r_{n} - r_{n}r_{n-1})\right].$$
 (2.5)

Linear oscillations of frequency  $\omega$  and wave number k are described by the dispersion relation

$$\omega^2 = \omega_0^2 + 4u_0^2 \sin^2 \frac{ka}{2}.$$
 (2.6)

which shows that the linear spectrum has a gap  $\omega_0$  and is limited by the cutoff frequency  $\omega_{\max} = (\omega_0^2 + 4u_0^2)^{1/2}$ . Here,  $\omega_0$ is assumed to be large with respect to the coupling constant  $u_0$  that is, the discreteness effects are strong. It is important to stress that the specific choice of  $V(r_n)$  given by (2.2), completed by the assumption  $u_0 \ll \omega_0$ , allows one to make the analytical calculations further than a Taylor expansion of a standard Hamiltonian, for example. The present study can also model a physical system as an atomic chain lying on a strong harmonic substrate, while the potential  $V(r_n)$  weakly couples each atom to its neighbors [15].

As a first consequence, the assumption  $u_0 \ll \omega_0$  involves that, for any wave with frequency  $\omega$  in the spectrum width  $[\omega_0, \omega_{\text{max}}]$ , all harmonics lie above  $\omega_{\text{max}}$  and can therefore be neglected in a first approximation [19]. Restricting moreover our study to weak amplitude and slow temporal variations of the wave envelope, and setting  $T = \epsilon^2 t$ , where  $\epsilon$  is a small parameter, we look for a solution in the form

$$r_n(t) = \epsilon \varphi_n(T) \exp(-i\omega t) + \epsilon \varphi_n^*(T) \exp(i\omega t). \quad (2.7)$$

Inserting (2.7) in (2.5), and restricting ourselves to the third order in  $\epsilon$ , yields first the dc terms:

$$\varphi_{n+1}\varphi_{n-1}^{*} + \varphi_{n+1}^{*}\varphi_{n-1} + \frac{\omega^{2} - \omega_{0}^{2} - u_{0}^{2}}{2u_{0}^{2}} \left[\varphi_{n}(\varphi_{n+1}^{*} + \varphi_{n-1}^{*}) + \varphi_{n}^{*}(\varphi_{n+1} + \varphi_{n-1})\right] + \frac{\omega^{2} - \omega_{0}^{2}}{u_{0}^{2}} |\varphi_{n}|^{2} = 0.$$
(2.8)

Next, for the terms in  $\exp(-i\omega t)$ , after having used (2.8), we get

$$2i\omega \frac{d\varphi_n}{dT} + u_0^2(\varphi_{n+1} + \varphi_{n-1}) + \varphi_n(\omega^2 - \omega_0^2 - 2u_0^2)$$
  
$$-\gamma^2 |\varphi_n|^2 \varphi_n \frac{(\omega^2 - \omega_0^2)^2}{u_0^2} + \gamma^2 \frac{\omega^2 - \omega_0^2}{2u_0^2}$$
  
$$\times [(5u_0^2 + \omega_0^2 - \omega^2) |\varphi_n|^2 (\varphi_{n+1} + \varphi_{n-1})]$$
  
$$+ (3u_0^2 + \omega_0^2 - \omega^2) \varphi_n^2 (\varphi_{n+1}^* + \varphi_{n-1}^*)]$$
  
$$+ \gamma^2 (\omega^2 - \omega_0^2) \varphi_n^* \varphi_{n+1} \varphi_{n-1} = 0.$$
(2.9)

Setting  $T = (2\omega/u_0^2)\tau$ , and  $\varphi_n = \psi_n \exp i\{[(\omega^2 - \omega_0^2)/u_0^2]\tau\}$ , we finally get a modified Ablowitz-Ladik equation,

$$i \frac{d\psi_n}{d\tau} + \psi_{n+1} + \psi_{n-1} + \mu |\psi_n|^2 (\psi_{n+1} + \psi_{n-1}) + 2\nu |\psi_n|^2 \psi_n + \mu' \psi_n^2 (\psi_{n+1}^* + \psi_{n-1}^*) + 2\nu' \psi_n^* \psi_{n+1} \psi_{n-1} = 0.$$
(2.10)

with the nonlinear coefficients

$$\mu = \gamma^{2} \frac{(\omega^{2} - \omega_{0}^{2})(5u_{0}^{2} + \omega_{0}^{2} - \omega^{2})}{2u_{0}^{4}},$$

$$\mu' = \gamma^{2} \frac{(\omega^{2} - \omega_{0}^{2})(3u_{0}^{2} + \omega_{0}^{2} - \omega^{2})}{2u_{0}^{4}},$$

$$\nu = -\gamma^{2} \frac{(\omega^{2} - \omega_{0}^{2})^{2}}{2u_{0}^{4}}, \text{ and } \nu' = \gamma^{2} \frac{(\omega^{2} - \omega_{0}^{2})}{2u_{0}^{2}}.$$
(2.11)

Next, looking for uniform plane wave solutions of (2.10), that is,  $\psi_n(\tau) = \psi_0 \exp i [kna - \Delta \omega \tau + \theta_0]$ , we obtain the nonlinear dispersion relation  $\Delta \omega = -2 \cos(ka)$   $-2\psi_0^2[\nu+\nu'+(\mu+\mu')\cos(ka)]$ . The modulational instability being indicative [22] of the occurrence of localized states in the chain, we now turn our attention to the linear stability of these plane wave solutions by considering small real amplitude and phase perturbations,  $b_n$  and  $c_n$ , respectively, with frequency  $\Omega$  and wave number K. Thus we consider  $\psi_n(\tau)$  of the form

$$\psi_n(\tau) = (\psi_0 + b_n + ic_n) \exp i[kna - \Delta \omega \tau + \theta_0].$$
(2.12)

Inserting (2.12) in (2.10) yields a set of two linear equations in  $b_n$  and  $c_n$  whose determinant must be zero, that is,

$$\begin{aligned} \Omega &-2 \sin(ka)\sin(Ka)[1 + (\mu - \mu')\psi_0^2] & 4 \cos(ka)\psi_0^2[\mu \cos^2(Ka/2) + \mu \sin^2(Ka/2)] \\ &-8\nu'\psi_0^2 \sin^2(Ka/2) - 4 \cos(ka)\sin^2(Ka/2) \\ &+4\nu\psi_0^2 - 4 \cos(ka)\sin^2(Ka/2) & \Omega - 2 \sin(ka)\sin(Ka)[1 + (\mu + \mu')\psi_0^2] \end{aligned} = 0.$$
(2.13)

Solving this condition with respect to the frequency  $\Omega$ , we get imaginary solutions, when

$$\sin^{2}(ka)\sin^{2}(Ka)\mu'^{2}\psi_{0}^{4}+4\{\cos(ka)\psi_{0}^{2}[\mu\cos^{2}(Ka/2)+\mu'\sin^{2}(Ka/2)]-2\nu'\psi_{0}^{2}\sin^{2}(Ka/2)-\cos(ka)\sin^{2}(Ka/2)\} \times \{\cos(ka)\psi_{0}^{2}[(\mu+\mu')\cos^{2}(Ka/2)+\nu'\cos(Ka)]+\nu\psi_{0}^{2}-\cos(ka)\sin^{2}(Ka/2)\} < 0.$$
(2.14)

Therefore, substituting  $\mu$ ,  $\mu'$ ,  $\nu$ , and  $\nu'$  in (2.14) by means of (2.6) and (2.11), we find that MI occurs when the amplitude  $\psi_0$  exceeds a threshold  $\psi_{0t}$  and when the wave numbers k and K lie in definite domains (MI regions), as represented in Fig. 2, with the relevant amplitude threshold. Note that we have truncated the amplitude threshold axis at 0.5 because, above this value,  $|r_n| < 1$  is not satisfied, and the potential (2.2) is no longer realistic.

Figure 2 shows that for  $k = \pi/2a$  and for k about  $\pi/3a$ , the plane waves are always stable. Everywhere else, when  $k < \pi/2a$ , the plane waves are modulationally unstable only for small K and when the amplitude exceeds a threshold. This threshold increases very fast with K, such that no MI finally occurs if K is sufficiently large. Let us note here that the presence of  $\mu' \neq 0$  and  $\nu' \neq 0$  in (2.10) drastically modifies the MI conditions, compared to the IN-DNLS case [22] where  $\mu'=0$  and  $\nu'=0$ . In fact, MI windows exist here for  $k < \pi/2a$ . As a comparison, in electrical transmission networks [25], where the theoretical study yields an IN-DNLS equation, plane waves with  $k < \pi/2a$  were found to be stable.

Let us consider now the case  $k > \pi/2a$  in Fig. 2. The waves are always stable in a small region near  $k = \pi/2a$  and for large *K*. Elsewhere, MI occurs with an amplitude threshold which increases with the perturbation wave number *K*. Specifically, setting  $k = \pi/a$  in (2.14), that is, when the neighboring particles oscillate out of phase, the threshold can be explicitly calculated with respect to *K*:

$$\gamma^2 \psi_{0t}^2 = \frac{\tan^2(Ka/2)}{10 + 6\tan^2(Ka/2)}$$
(2.15)

The above results were derived for an infinite lattice, but can be straightforwardly extended to lattices with periodic boundary conditions,  $r_n(t) = r_{n+N}(t)$ , that corresponds to a cyclic chain. This implies that both main wave number k and perturbation wave number K must be of the form  $2p\pi/Na$ , where the integer p is 0,  $\pm 1$ ,  $\pm 2$ ,...,  $\pm (N-2)/2$ , or +N/2, if N is even, and 0,  $\pm 1$ ,  $\pm 2$ ,..., or  $\pm (N-1)/2$  if N is odd. Replacing k and K by these expressions in (2.14) or in Fig. 2 allows us to determine if the cyclic chain is modulationally stable or unstable for each of the N possible modes, and in the latter case, to calculate the theoretical amplitude threshold required for MI. For example, if the chain is composed of N=6 oscillators (see Table I), no MI is predicted for k=0 or  $k = \pm \pi/3a$ . Note that the mode p = 0 (k = 0) corresponds to the oscillations of the center of mass and is necessarily stable because the external potential in (2.1) is harmonic. Thus we will not consider it in the following. On the other hand, MI is expected when  $|k| > \pi/2a$ . In this case, the amplitude threshold is minimal for  $K = \pm \pi/3a$ . Namely, for this value of K, the MI threshold is  $\gamma \psi_{0t} = 0.144$  for  $k = \pm 2 \pi/3a$  and is 0.167 for  $k = \pi/a$ . Note that with these amplitudes, the potential (2.2) remains very close to the Morse potential (see Fig. 1).

### **III. NUMERICAL STUDY**

In order to check the validity of our analytical approach and to determine the evolution of plane wave oscillations and energy localization of the cyclic system under small perturbations, we have performed numerical simulations with the

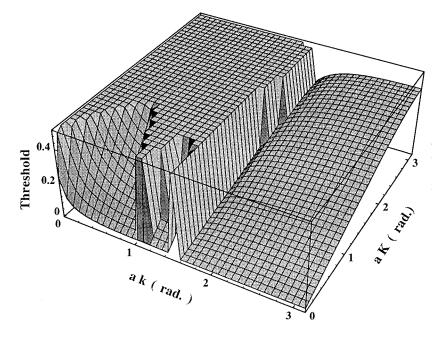


FIG. 2. MI regions numerically depicted vs ak and aK, a being the lattice spacing, k the carrier wave number, and K the perturbation wave number. The MI amplitude threshold is represented vertically when it is smaller than 0.5 (dimensionless units). Otherwise, the carrier wave is always modulationally stable.

set of differential equations (2.3), describing the system evolution before any approximation. We have used a fourth order Runge-Kutta method, with a time step chosen to preserve the Hamiltonian to an accuracy better than  $10^{-5}$  over a complete numerical experiment. The parameters of the chain are a=1,m=1,A=1,B=1, that is,  $u_0^2 = \gamma = 1$ . The lower gap frequency corresponds to  $\omega_0^2 = 100$ , so that the condition  $\omega_0 \gg u_0$  is satisfied.

The initial condition is a plane wave, whose amplitude is slightly modulated,

$$u_n(t=0) = 2\phi_0[1+0.01\cos(Kna)]\cos(kna).$$
 (3.1)

Here, the amplitude parameter  $\phi_0$  of the absolute displacement is straightforwardly related to  $\psi_0$  involved in (2.12) by

$$\psi_0 = 2\,\phi_0\,\sin\frac{ka}{2}.$$
(3.2)

As a specific example, we consider a chain of N=6 oscillators, with periodic boundary conditions, that is, the wave numbers k and K are both 0,  $\pm \pi/3a$ ,  $\pm 2\pi/3a$ , or  $+\pi/a$ , while  $\omega$  is deduced from (2.6).

TABLE I. Comparison between the theoretical predictions and numerical results, concerning the MI occurrence for a plane wave with amplitude  $\psi_0$  and wave number k, slightly modulated at wave number  $K = \pi/3a$ , propagating in a chain with periodic boundary conditions (N=6). As specified in the text,  $a = m = A = B = u_0^2 = 1$ , while  $\omega_0^2 = 100$ .

Carrier wave number	$k = \pm \pi/3a$	$k = \pm 2 \pi/3a$	$k = + \pi/a$
Theoretical predictions	stable	unstable	unstable
		$\psi_{0t} = 0.144$	$\psi_{0t} = 0.167$
Numerical results	stable	unstable	unstable
	[see Fig. 3(a)]	$\psi_{0t} = 0.183$	$\psi_{0t} = 0.210$
			[see Fig. 3(b)]

For  $k = \pm \pi/3a$ , no instability is detected for all the six possible values of K. For instance, Fig. 3(a) shows the time evolution of the spatial Fourier components  $S_p$ , when k=K $= \pi/3a$  and  $\psi_0 = \phi_0 = 0.35$ . The carrier wave  $(p = \pm 1)$  is stable over about 800 periods, and the oscillations of the sideband  $(p = \pm 2)$  cannot be detected. Note that the last spatial Fourier component (p=3) remains negligible, as supposed in the preceding section.

For  $k = \pm 2\pi/3a$ , MI develops for wave number  $K = \pi/3a$ 3*a*, when the amplitude  $\psi_0$  exceeds of 0.183 (see Table I). We also obtain MI for  $k = \pi/a$ , and  $K = \pi/3a$ , with a threshold value at 0.210. This agrees rather well with theoretical predictions of Table I, in spite of the approximations made in Sec. II. We have represented in Fig. 3(b) the spatial Fourier components  $S_p$  versus the time for  $k = \pi/a$ ,  $K = \pi/3a$ , and  $\psi_0 = 0.26$ , that is,  $\phi_0 = 0.13$ . The sidebands  $k \pm K(p = \pm 2)$ quickly increase and become rather large with respect to the carrier level (p=3). Note that the bands  $k \pm 2K$  (that is, p= $\pm 1$ ), not considered in the theoretical section, also increase versus time, but seem to play a negligible role. All these sidebands oscillate in time, and as time evolves (until 10 000 time units, not represented in this paper), these oscillations present a recurrence behavior. The averaged period of this recurrence is about 80 time units.

For the previous numerical experiment [see Fig. 3(b)], we have also represented in Figs. 4(a) and 4(b), for each particle, the evolution versus time of its energy, defined from (2.1) by

$$H_{n} = \frac{m\omega_{0}^{2}}{2} [u_{n}]^{2} + \frac{m}{2} \left(\frac{du_{n}}{dt}\right)^{2} + \frac{1}{2} [V(u_{n+1} - u_{n}) + V(u_{n} - u_{n-1})], \qquad (3.3)$$

where the potential  $V(r_n)$  is uniformly distributed between particles *n* and *n*+1. Each energy  $H_n$  starts at about *H*/6. Due to MI and since the total energy *H* of the cyclic chain is conserved, 60% of the energy is confined in the vibration of the sixth particle at *t*=120 units, 21% in the vibration of the

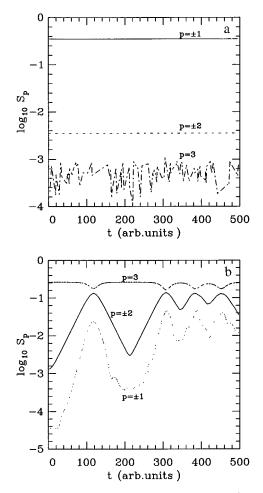


FIG. 3. Time evolution of the Fourier components  $(p = \pm 1, \pm 2, and 3)$ , with a logarithmic scale, for a wave with amplitude  $\psi_0 = 0.35$  and wave number  $k = \pi/3a$  slightly modulated with wave number  $K = \pi/3a$ , and propagating in a chain with periodic boundary conditions (N=6). As specified in the text,  $a=m=A=B=u_0^2=1$ , while  $\omega_0^2=100$ . (b) The same, but for  $\psi_0=0.26$ ,  $k=\pi/a$ , and  $K=\pi/3a$ .

first and fifth ones, while the three others have almost no energy. Next, the energy is located only in particles 1 and 2 (at t=310 units), and later, in particles 3 and 4 (at t=390units), and so on. At t=460 units, the energy localizes again in particle 6, that is, the chain presents a recurrence behavior. Carrying on the numerical simulation for 10 000 time units, we get an average value for the recurrence period of about 160 time units, twice the recurrence time observed for the spatial Fourier sidebands  $k\pm K$ . Thus each oscillator takes alternatively most of the total energy every 160 time units, i.e., every 260 carrier oscillations, while energy returns to a uniform distribution twice during this time. This recurrence time depends not only on k and K, but also on the difference between the amplitude and the amplitude threshold, as suggested by the theoretical study of Sec. II.

In conclusion, we have shown that the physics of a onedimensional lattice, with a specific coupling nonlinear potential, can be described, in the weak amplitude and slow time limits, by a modified Ablowitz-Ladik equation. We have next considered a lattice with periodic boundary conditions, that corresponds to a cyclic system. The stability of the cw modes has been investigated. Some of these modes, espe-

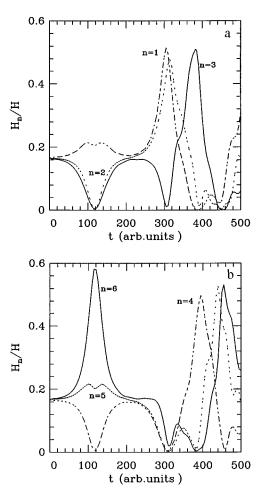


FIG. 4. Time evolution of the relative energy of particles 1-3, showing spatial localization, the parameters being fixed as for Fig. 3(b). (b) The same for particles 4-6.

cially the mode  $k = \pi/a$  where the particles oscillate out of phase, are found to be unstable under small perturbation, when the amplitude exceeds a certain threshold. The instabilities are related to energy localization, that is, the energy concentrates then periodically in the vibrations of each particle. This prediction is numerically checked for a simple model of six particles, and the numerical amplitude thresholds for MI agree rather well with the theoretical ones, in spite of the approximations. For these amplitude values, the considered potential is very close to the Morse potential, which is often used in different physical domains. Our results suggest that the present analysis could be applied to physical systems of coupled nonlinear oscillators, with a rather small number of particles, and also to cyclic molecules, such as benzene C6H6 or silane SiH4, where some signatures of energy localization in specific bonds have been observed [26]. In such molecules, the substrate potential may be considered, to a first approximation, as an interaction between the heavy part of the system and the hydrogen atoms, while the nonlinear potential V(r) couples each hydrogen atom with its neighbors.

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