INTERACTION OF MOVING LOCALIZED OSCILLATIONS WITH A LOCAL INHOMOGENEITY IN NONLINEAR HAMILTONIAN KLEIN–GORDON LATTICES

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We study the interaction of moving localized oscillations with a local inhomogeneity in a discrete nonlinear Hamiltonian system. We conjecture that resonance with a static nonlinear localized oscillation centered at the local inhomogeneity is a necessary condition for observing the trapping phenomenon. Analytic calculations and numerical simulations agree well with our hypothesis.

Keywords: discrete breathers, mobile breathers, intrinsic localized modes, impurities, inhomogeneity

1. Introduction

The interaction of nonlinear localized oscillations with local inhomogeneities in a system is an important problem that has been studied in different frameworks: the scattering of kinks and envelope solitons on local inhomogeneities in one–dimensional atomic lattices with nonlinear interactions [1], the interaction between high-frequency continuous breathers and local inhomogeneities in the sine-Gordon model [2], [3], and the scattering of kinks in the continuous sine-Gordon and ϕ^4 models [4] and in the Frenkel–Kontorova model [5], [6]. Solitons that, depending on the velocity, can be reflected by the inhomogeneity or pass through it are described in [1], [5]. But in [2], [4], it was observed that solitons can also be trapped for intermediate velocities.

Much attention has recently been paid to localized oscillations in nonlinear discrete systems (discrete breathers). They can be obtained in Klein–Gordon lattices as exact solutions of dynamical equations [7]. In addition, these localized oscillations can move under certain conditions, and they are usually called *moving breathers* [8]–[12].

The interaction of a moving discrete breather with a local inhomogeneity in a Klein–Gordon chain was previously considered by Forinash et al. [13] in the weak nonlinearity approximation. They found three different behaviors: the moving breather passes through the inhomogeneity, it is reflected, or it is trapped, initiating a depository of energy. All these effects are related to resonances with a linear localized mode.

In this work, we study the features of the interaction of moving discrete breathers with a local inhomogeneity in a Hamiltonian Klein–Gordon chain of oscillators with nonweak nonlinearity. We conjecture that a necessary condition for the appearance of trapping is that there must exist a breather centered at the local inhomogeneity with a frequency close to that of the moving breather. This guarantees the existence of a wide range of parameters for which trapping is possible. Nevertheless, this condition is not sufficient, because the trapping phenomenon does not occur when the tails of this breather and the linear localized mode have different vibration patterns. We propose the hypothesis that both tails must have the same vibration pattern for the trapping to occur.

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2. Model

To study the effects of a local inhomogeneity on the movement of breathers, we consider a simple model in which moving breathers can be generated, i.e., a Klein–Gordon chain with nearest-neighbor attractive interactions [8], [9]. Its Hamiltonian is given by

$$H = \sum_{n=1}^{N} \left(\frac{m_n}{2} \dot{u}_n^2 + V_n(u_n) + W_n(u_n, u_{n-1}, u_{n+1}) \right), \tag{1}$$

where u_n is the displacement of the nth particle with respect to its equilibrium position, W_n is the coupling potential, and $V_n(u_n)$ is the substrate potential at the nth site. If we introduce a local inhomogeneity, the dynamical equations have two kinds of solutions: linear ones, which correspond to oscillations of small amplitude, and nonlinear ones, which correspond to intrinsic localized modes or discrete breathers.

2.1. Soft substrate potential. As the first case, we consider a soft on-site potential. We choose V as the Morse potential, i.e., $V_n(u) = D_n(e^{-u} - 1)^2$, where D_n is the well depth at the nth site. We also consider a linear coupling term $W_n(u_n, u_{n-1}, u_{n+1}) = C_n(2u_n - u_{n+1} - u_{n-1})$ and introduce the inhomogeneity by assuming a different well depth at only one site, i.e., $D_n = D_o(1 + \alpha\delta_{n,0})$, or, similarly, varying the coupling constant $C_n = C_0(1 + \beta\delta_{o,n})$ $(C > 0)$ or the mass of a particle $m_n = m_0(1 + \gamma\delta_{o,n})$. We then call the particle located at $n = 0$ a local inhomogeneity with the magnitude controlled by the parameters α, β, or γ taking values in the interval $[-1, \infty)$. This model proves very suitable for obtaining moving breathers [9], [10], [12], and it has been used extensively in DNA dynamics [14]. We consider $D_0 = 1/2$ and $m_0 = 1$.

Hamiltonian (1) leads to the dynamical equations

$$F(\{u_n\}) \equiv m_n \ddot{u}_n + V_n'(u_n) + C_n(2u_n - u_{n+1} - u_{n-1}) = 0. \tag{2}$$

2.1.1. *Linear modes.* The dynamical equations can be linearized if the amplitudes of the oscillations are small. Therefore, the linear modes can be calculated supposing that the localized mode is $u_n(t) = u_0 e^{i\omega_{\mathrm{L}} t} r^n$ [13]. There exist one linear localized mode and $N-1$ linear extended modes.

In the case of the local inhomogeneity in the well depth, the extended modes are

$$\omega(q, \alpha) = \sqrt{\omega_0^2 + 4C \sin^2 \frac{q(\alpha)}{2}}, \tag{3}$$

where $q(\alpha)$ is the extended-mode wave vector (which depends in a nonstraightforward way on α), ω_0 is the linear frequency (in our case, $\omega_0 = \sqrt{2D}$), and the frequency of the linear localized mode is given by

$$\omega_{\mathrm{L}}^2 = \omega_0^2 + 2C + \operatorname{sgn}(\alpha)\sqrt{\alpha^2\omega_0^4 + 4C^2}. \tag{4}$$

The sign of r indicates the vibration pattern of the linear localized mode. Thus, if $r > 0$, the particles of the mode vibrate in phase and have a wave vector $q = 0$. In contrast, if $r < 0$, the mode has a zigzag vibration pattern and a wave vector $q = \pi$. The parameter r is given by

$$r = -\operatorname{sgn}(\alpha) \frac{\alpha\omega_0^2 + \sqrt{4C^2 + \alpha^2\omega_0^4}}{2C}. \tag{5}$$

Therefore, α and r have opposite signs. This also implies that for the extended modes, $q \in (0, \pi]$ if $\alpha < 0$ and $q \in [0, \pi)$ if $\alpha > 0$.

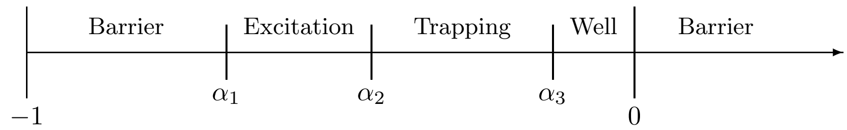

Fig. 1. Different regimes in the interaction of a moving breather with an impurity introduced as an inhomogeneity in the potential well depth in a soft substrate potential.

If we introduce the local inhomogeneity in the coupling parameter, the dependence of the linear localized mode frequency on the parameter β is

$$\omega_{\mathrm{L}}^2 = \begin{cases} \omega_0^2, & \beta < 0, \\ \frac{\beta+2}{4\beta} C(\sqrt{9\beta^2 + 20\beta + 4} - 2 + 3\beta), & \beta > 0, \end{cases} \tag{6}$$

and

$$r = \frac{3\beta + 2 - \sqrt{9\beta^2 + 20\beta + 4}}{3\beta}.$$

There are no linear localized modes for $\beta < 0$, whereas for $\beta > 0$, they exist with $q = \pi$.

In the case of the inhomogeneity in the mass, we find that

$$\omega_{\mathrm{L}}^2 = \frac{\omega_0^2 - \mathrm{sgn}(\gamma)\sqrt{(\gamma)^2\omega_0^2(\omega_0^2 + 4C) + 4C^2}}{m(1-(\gamma)^2)}, \tag{7}$$

$$r = \frac{|\gamma|(\omega_0^2 + 2C) - \mathrm{sgn}(\gamma)\sqrt{(\gamma)^2\omega_0^2(\omega_0^2 + 4C) + 4C^2}}{2C(|\gamma| - 1)}. \tag{8}$$

The parameters r and γ have the same sign. Then, if $\gamma < 0$, the localized mode has $q = \pi$ and the extended modes $q \in [0, \pi)$, and if $\alpha > 0$, the localized mode $q = 0$ and the extended modes $q \in (0, \pi]$.

2.1.2. *Numerical observations.* To study the interaction of a moving discrete breather with the local inhomogeneity of the system, we performed some numerical simulations. To obtain a stationary breather, we used common methods based on the anticontinuous limit [15]. If the initially chosen oscillator corresponds to the local inhomogeneity, a stationary breather centered at the impurity is obtained. It is called an *impurity breather*.

Once a stationary breather is obtained, it can be moved under certain conditions. There exists a systematic method for calculating moving solutions [8], [9]; it consists in adding a perturbation of magnitude λ collinear to the direction of the pinning mode to the velocities of the stationary breather and letting the system evolve in time. The pinning mode is an antisymmetric linear localized mode, which can appear in the set of linear perturbations of the system if the coupling is sufficiently strong [10]. A perturbation in the pinning-mode direction thus breaks the translational symmetry of the system and makes the breather move.

If the inhomogeneity is in the potential depth, four different regimes separated by critical values of the control parameter were found. This is shown in Fig. 1.

1. *Barrier.* The inhomogeneity acts as a potential barrier. As the moving breather reaches the impurity, it is generally reflected, leaving the impurity excited for a short time.
2. *Excitation.* The inhomogeneity is excited and the breather is reflected. The energy of the excited inhomogeneity is larger than the energy of the impurity breather. Therefore, the excited impurity vibrates with a frequency lower than ω_{b} because the on-site potential is soft.

3. *Trapping.* The breather is trapped by the inhomogeneity. When the moving breather is close to the inhomogeneity, it becomes trapped, and its center oscillates between the neighboring sites. Furthermore, the trapped breather emits a great amount of phonon radiation and seems chaotic.

4. *Well.* The inhomogeneity acts as a potential well. The breather accelerates as it approaches the inhomogeneity and decelerates after it has passed through the local inhomogeneity.

The transition between the different regimes is somehow diffuse, which means that the critical values of α cannot be determined exactly. Furthermore, they are slightly dependent on the breather velocity. These regimes were also found for different values of the breather frequency. For stronger coupling, the phonon radiation is significant and could mask some of the described effects.

To explain some of these results, we performed a continuation of a stationary breather centered at the local inhomogeneity, varying the parameter α. Then, a bifurcation appears for $\alpha = \alpha_{\mathrm{c}} > 0$ and another for $\alpha = \alpha_{\mathrm{res}} < 0$. The first is initiated by a localized Floquet eigenmode that abandons the unit circle and leads to a breather extinction, i.e., the impurity breather does not exist for $\alpha > \alpha_{\mathrm{c}}$. In the second case, the breather bifurcates with the zero solution through a pitchfork bifurcation in the space of time-reversible solutions of frequency ω_{b}.[1]

For $\alpha = \alpha_{\mathrm{res}}$, the frequency of the linear localized mode is the same as the frequency of the impurity breather with the moving breather frequency, i.e., $\omega_{\mathrm{L}} = \omega_{\mathrm{b}}$. The value α_{res} can be calculated from Eq. (4) as a function of ω_{b} and C:

$$\alpha_{\mathrm{res}} = -\frac{\sqrt{(\omega_{\mathrm{b}}^2 - \omega_0^2)(\omega_{\mathrm{b}}^2 - \omega_0^2 - 4C)}}{\omega_0^2}. \tag{9}$$

Hence, the trapped breather does not exist for $\alpha > 0$. This indicates that the condition $\alpha \in (\alpha_{\mathrm{res}}, 0)$ might hold for the trapped breather to exist.

The scenario for the trapped breathers for $\alpha < 0$ is as follows. In this case, the linear localized mode has $q = 0$, and also all the particles of the impurity breather vibrate in phase. This vibration pattern indicates that the impurity breather bifurcates from plane waves with $q = 0$ [16], i.e., the impurity bifurcates from the localized mode, and it will be the only localized mode that exists when the inhomogeneity is excited for $\alpha > \alpha_{\mathrm{res}}$. Therefore, when the moving breather reaches the inhomogeneity, the breather can excite the localized mode. In fact, we have performed a successful continuation from the impurity breather to the localized mode at constant action and α.

For $\alpha < \alpha_{\mathrm{res}}$, the trapped breather cannot be generated, and the moving breather is always reflected. In addition, the impurity breather does not exist.

If $\alpha > 0$, the scenario is different. In this case, the localized mode has $q = \pi$, but the impurity breather sites again vibrate in phase, i.e., the impurity breather does not bifurcate from the localized mode. Hence, there are two different localized excitations for $\alpha > 0$: the (linear) localized mode and the (nonlinear) impurity breather. But, actually, the equations that govern the system are nonlinear; therefore, the linear modes can only correspond to low-amplitude oscillations. In the case of the impurity breather, the linear regime corresponds to the tails. Consequently, if the moving breather reaches the inhomogeneous site, it will excite the impurity breather and the tails of the localized mode. But the latter vibrates in zigzag. As a consequence, there will be two different linear localized entities: the tails of the localized mode (vibrating in zigzag) and the tails of the impurity breather (vibrating in phase).

In the case of the inhomogeneity introduced in the coupling parameter, the breather can only be trapped for $\beta < 0$, as shown in Fig. 2. This result was verified numerically, and there is only a critical value of the parameter $\beta = \beta_1$.

[1] We note that dynamical equations (2) do not correspond to the standard dynamical system $\dot{x} = f(x,t)$, in which pitchfork bifurcations are usually described.

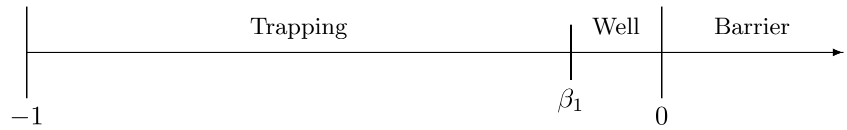

Fig. 2. Different regimes in the interaction of a moving breather with an impurity introduced as an inhomogeneity in the coupling parameter in a soft substrate potential.

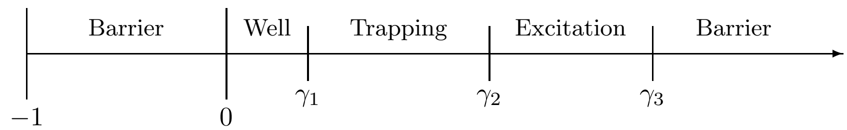

Fig. 3. Different regimes in the interaction of a moving breather with an impurity introduced as an inhomogeneity in the mass in a soft substrate potential.

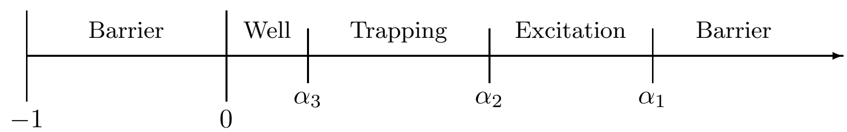

Fig. 4. Different regimes in the interaction of a moving breather with an impurity introduced as an inhomogeneity in the well depth with a hard substrate potential.

Finally, when we introduce the inhomogeneity in the mass, we observe a behavior qualitatively similar to the inhomogeneity in the potential depth. The trapping phenomenon occurs when an impurity breather exists with the same vibration pattern as the localized linear mode (see Fig. 3).

2.2. Hard substrate potential. We consider a hard substrate potential. We study a chain of nonlinear oscillators with a ϕ^4 hard on-site potential and linear coupling. The Hamiltonian is

$$H = \sum_n \left(\frac{1}{2}\dot{u}_n^2 + \frac{1}{2}\omega_{\mathrm{n}}^2 u_n^2 + \frac{1}{4}u_n^4 C\left(\frac{1}{2}(u_n - u_{n-1})^2 + \frac{1}{4}(u_n - u_{n-1})^4\right)\right),$$

and $\omega_{\mathrm{n}}^2 = \omega_0^2(1 + \alpha\delta_{n,0})$.

2.2.1. *Linear modes and numerical observations.* The linear modes are similar to those in the soft on-site potential case except that the vibration pattern of the impurity breather is inverted. In our numerical simulations, we found different behaviors summarized in Fig. 4. In all cases, the trapping phenomenon is observed in the region $\alpha > 0$, and the impurity breather has zero amplitude when $\alpha = \alpha_{\mathrm{res}}$.

3. Trapping hypothesis

As a consequence of our numerical observations, we conjecture that the existence of an impurity breather is related to the trapping phenomenon and the vibration pattern of the linear localized mode. We thus summarize our hypothesis:

The existence of an impurity breather for a given value of α is a necessary condition for the existence of trapped breathers. But if there exists a linear localized mode with a vibration pattern different from that of the impurity breather, then the trapped breather does not exist.

4. Conclusions

We have studied the interaction of moving discrete breathers with an local inhomogeneity in a Klein–Gordon chain with nonweak nonlinearity. The trapping occurs whenever the *trapping hypothesis* holds: an *impurity breather* of a frequency close to that of the moving breather must exist. In addition, there must not exist a (linear) localized mode with a vibration pattern different from that of the impurity breather.

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