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Moving discrete breathers in a Klein–Gordon chain with an impurity

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Abstract

We analyse the influence of an impurity in the evolution of moving discrete breathers in a Klein–Gordon chain with non-weak nonlinearity. Three different types of behaviour can be observed when moving breathers interact with the impurity: they pass through the impurity continuing their direction of movement; they are reflected by the impurity; they are trapped by the impurity, giving rise to chaotic breathers, as their Fourier power spectra show. Resonance with a breather centred at the impurity site is conjectured to be a necessary condition for the appearance of the trapping phenomenon. This paper establishes a difference between the resonance condition of the non-weak nonlinearity approach and the resonance condition with the linear impurity mode in the case of weak nonlinearity.

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1. Introduction

Intrinsic localized modes or *discrete breathers* result from the combination of nonlinearity with spatial discreteness. They can be obtained in Klein–Gordon lattices as exact solutions of dynamical equations [1–3]. In addition, these localized oscillations, under certain conditions, can move and they are usually called *moving breathers* [4–8].

The interaction of nonlinear localized oscillations with impurities in a system can play an important role in its transport properties. This problem has been studied over the last decades within different frameworks. The scattering of kinks and envelope solitons with impurities has been studied in one-dimensional atomic lattices with nonlinear interactions [9]. Another approach is concerned with the interaction between high-frequency continuous breathers and impurities in the sine-Gordon model [10, 11]. This approach has been extended to the low-frequency case in [12], and to the case of kinks in the continuous sine-Gordon and

ϕ^4 models [13, 14]. The scattering of a kink by an impurity in the Frenkel–Kontorova model has been considered in [15, 16]. References [9, 15] describe solitons that can be reflected by the impurity or pass through it, depending on the velocity. However, in [10, 11, 13, 14], it is observed that solitons can also be trapped for intermediate velocities.

The interaction of a moving discrete breather with an impurity in a Klein–Gordon chain has been considered by Forinash *et al* [17]. In this case, it is assumed that the system has weak nonlinearity and three different types of behaviour can be observed: (a) the moving breather passes through the impurity, (b) it is reflected or (c) it is trapped by the impurity, originating a depository of energy. All these effects are related to resonances with the impurity modes.

In this paper, we are interested in the last approach, i.e. to study the features of the interaction of moving discrete breathers with an impurity at rest in a Klein–Gordon chain of oscillators with non-weak nonlinearity.

Although the behaviour in all of these approaches is qualitatively similar, there are some significant differences concerning the appearance of the trapping phenomenon. In the case of solitons, the different phenomena are velocity-dependent. In discrete lattices, the breather and the impurity mode are related entities [18, 19], i.e. they can be connected through a continuous path. Therefore, the interplay between a breather and an impurity mode can be much stronger than between a soliton and an impurity. In Forinash's approach, the necessary condition for the appearance of the trapping phenomenon is that the breather frequency resonates with the linear impurity mode one.

In our case, that is, a Klein–Gordon chain with non-weak nonlinearity, the necessary condition for the appearance of trapping is that there must exist a breather at the impurity with a frequency close to that of the moving breather. This fact guarantees the existence of a wide range of parameters for which trapping is possible. Nevertheless, this condition is not sufficient, as the trapping phenomenon does not occur when the tails of the breather centred at the impurity site and the linear impurity mode have different vibration patterns. We propose the hypothesis that both tails must have the same vibration pattern in order for the trapping to occur.

2. Model and solutions generation

2.1. Formulation of the model

In order to study the effects of impurities on the movement of breathers, we consider a simple model where moving breathers can be generated, that is, a Klein–Gordon chain with nearest-neighbour attractive interactions [4, 5]. Its Hamiltonian is given by

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

where u_n represents the displacement of the nth particle with respect to its equilibrium position, C is a coupling constant and $V_n(u_n)$ is the substrate potential at the nth site. We choose V as the Morse potential, i.e. $V_n(u) = D_n(\mathrm{e}^{-u} - 1)^2$, which proves to be very suitable for obtaining moving breathers [5, 6, 8]. D_n represents the well depth in the nth site. In this model, the inhomogeneity is introduced assuming a different well depth in only one site, i.e. $D_n = D_o(1 + \alpha\delta_{n,0})$, then we refer to the particle located at $n = 0$ as an impurity. α is a parameter which tunes the magnitude of the inhomogeneity. It takes its values in the interval $[-1, \infty)$. Hereafter, we will consider $D_o = 1/2$.

The results presented here correspond to free ends boundary conditions, although periodic boundary conditions lead to the same results.

This model has been used extensively in DNA dynamics; in this context it is usually referred to as the Peyrard–Bishop model [20]. In the framework of this model, the variables u_n represent the stretching of the hydrogen bonds connecting each pair of bases, D is the dissociation energy and C is the stacking coupling constant.

The inhomogeneity can also be introduced in a similar way varying the mass of a particle, or the coupling constant. The results in the first case are equivalent to those obtained for the inhomogeneity in the potential well. There are, however, several differences when the inhomogeneity is introduced through the coupling constant, and we will make some comments about them at the end of this paper.

The Hamiltonian (1) leads to the dynamical equations

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

which 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.

2.2. Linear modes

The dynamical equations can be linearized if the amplitudes of the oscillations are small. Thus, equation (2) is transformed in the system of coupled equations:

$$\ddot{u}_n + \omega_n^2 u_n + C(2u_n - u_{n+1} - u_{n-1}) = 0 \tag{3}$$

where ω_n is the natural frequency of the nth oscillator in the harmonic limit. It is given by $\omega_n = \sqrt{2D_n}$, which implies that $\omega_n^2 = \omega_o^2(1 + \alpha\delta_{n,0})$, with $\omega_o = 1$, as D_o has been chosen to be $1/2$.

These equations have $N - 1$ non-localized solutions (N being the number of particles) corresponding to *linear extended modes* and one localized solution, which corresponds to a *linear impurity mode*. Hereafter, unless stated otherwise, the term mode will be reserved to linear modes.

The frequencies of the extended modes can be calculated supposing that they are plane waves ($u_n(t) = u_o \exp(\mathrm{i}\omega(q)t - nq)$) and that the impurity mode decays in the space following a dependence of the form $u_n(t) = u_o \exp(\mathrm{i}\omega_L t) r^{|n|}$ [17], where r is a spatial decay parameter. Thus, the frequencies of the extended modes are given by

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

where $q(\alpha)$ is the extended modes wave vector, which depends in a non-straightforward way on α.

The frequency of the impurity mode is given by the relation [17]:

$$\omega_L^2 = \omega_o^2 + 2C + \mathrm{sign}(\alpha)\sqrt{\alpha^2\omega_o^4 + 4C^2}. \tag{5}$$

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

$$r = -\mathrm{sign}(\alpha)\frac{\alpha\omega_o^2 + \sqrt{4C^2 + \alpha^2\omega_o^4}}{2C}. \tag{6}$$

Therefore, α and r have opposite signs. This fact also implies that, for the extended modes, $q \in (0, \pi]$ if $\alpha < 0$ and $q \in [0, \pi)$ if $\alpha > 0$. Figure 1 shows the dependence of

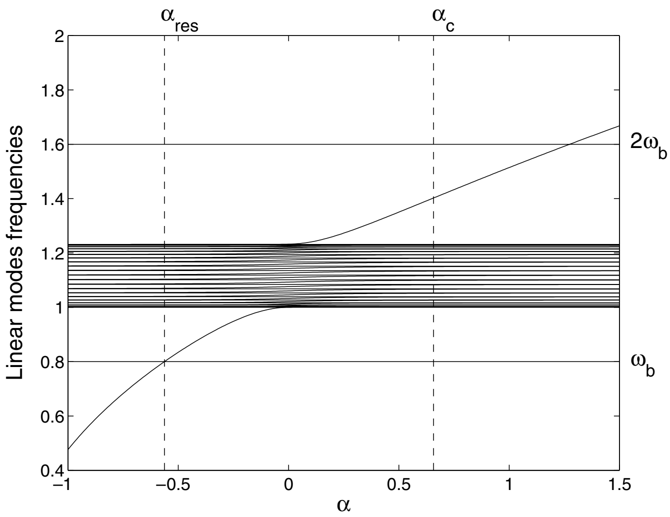

Figure 1. Frequencies of the linear modes versus the parameter α, for $C = 0.13$. The dependence is qualitatively similar for every value of C. At $\alpha = \alpha_{\rm res}$ and $\alpha = \alpha_c$, two different bifurcations occur, the first one being due to the resonance between the impurity mode and the breather.

the frequencies of the linear modes with α, where the isolated frequencies correspond to the impurity modes.

As is explained below, the values of the frequency and wave vector of the impurity mode will be the key to explain the occurrence of the trapping phenomenon.

2.3. Stationary and moving breathers

A stationary breather can be obtained by solving the full dynamical equations. It can be achieved using common methods based on the anti-continuous limit [21]. The implementation of these methods basically consists in calculating the orbit of an isolated oscillator at fixed frequency ω_b, and using this solution as a seed to solve the complete dynamical equations by means of a Newton–Raphson continuation method.

If the oscillator initially chosen is that corresponding to the impurity, a static breather centred at the impurity is obtained. It will be 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 [4, 5] which consists in adding to the velocities of the stationary breather a perturbation of magnitude λ collinear to the direction of the pinning mode and letting the system evolve in time. The pinning mode is an anti-symmetric linear localized mode, which may appear in the set of linear perturbations of the system provided the coupling is strong enough [6]. Thus, a perturbation in its direction breaks the translational symmetry of the system and makes the breather move.

The results presented here correspond to a frequency $\omega_b = 0.8$ and a coupling $C = 0.13$, although other values of the same order give qualitatively similar results. In this way, we obtain moving breathers with low phonon radiation for values of the perturbation $\lambda \lesssim 0.2$. It is worth remarking that the nonlinearity of our system is higher than that considered in [17], as, in that paper, the frequencies of the localized excitations oscillate between 0.922 and 0.980 (in our frequency units, i.e. normalized to the linear frequency at zero coupling $\omega_o = 1$), which are very close to the linear ones.

We have considered different values of the parameter α in the range $-1 \leqslant \alpha \leqslant 1$.

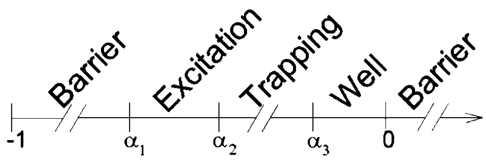

Figure 2. Different regimes in the interaction of a moving breather with an impurity introduced as an inhomogeneity in the potential well depth.

3. Interaction of moving breathers with an impurity

3.1. Numerical observations

We have studied the behaviour of moving breathers when they interact with an impurity. The study has been performed varying the value of the inhomogeneity parameter α. Four different regimes, separated by critical values of the parameter α, have been found (see figure 2):

(i) *Barrier*. The impurity acts as a potential barrier. This occurs either with $\alpha > 0$ or $\alpha \in (-1, \alpha_1)$ with $\alpha_1 < 0$. As the moving breather reaches the impurity, it is generally reflected, leaving the impurity excited for a short time, whose amplitude decreases with $|\alpha|$. The only exception to this behaviour occurs for $\alpha \gtrsim 0$. In this case, the breather can pass through the impurity provided the translational velocity is high enough.

(ii) *Excitation*. The impurity is excited and the breather is reflected. This occurs for $\alpha \in (\alpha_1, \alpha_2)$. The energy of the excited impurity is larger than the energy of the impurity breather. Thus, the excited impurity vibrates with a frequency lower than ω_b as the on-site potential is soft. This behaviour is shown in figure 3.

(iii) *Trapping*. The breather is trapped by the impurity. This occurs in the interval $\alpha \in (\alpha_2, \alpha_3)$. When the moving breather is close to the impurity, it becomes trapped while its centre oscillates between the neighbouring sites, as figure 4 shows. Furthermore, the trapped breather emits a large amount of phonon radiation and seems to be chaotic, as can be appreciated from its Fourier power spectrum (figure 5).

(iv) *Well*. The impurity acts as a potential well. This occurs for $\alpha \in (\alpha_3, 0)$ and consists of an acceleration of the breather as it approaches the impurity, and a deceleration after the impurity has been passed through.

The transition between the different regimes is somehow diffuse which means that the critical values of α cannot be exactly determined. Furthermore, they are slightly dependent on the breather velocity. An estimation of the critical values for $\omega_b = 0.8$, $C = 0.13$ and $\lambda = 0.1$ leads to: $\alpha_1 \approx -0.54$, $\alpha_2 \approx -0.49$ and $\alpha_3 \approx -0.02$. As commented above, these regimes have also been found for different values of the breather frequency. For stronger coupling, the phonon radiation is significant and could mask some of the described effects.

3.2. Discussion

Some of the results in the last subsection can be explained from the properties of the impurity breather. Particularly, if a continuation of a stationary breather is performed varying the parameter α, a bifurcation appears for $\alpha = \alpha_c > 0$ and another one for $\alpha = \alpha_{\text{res}} < 0$ (see figure 1). The first one is originated by a localized Floquet eigenmode which abandons the unit circle and leads to a breather extinction, i.e. the impurity breather does not exist for $\alpha > \alpha_c$. In the second case, the breather bifurcates with the zero solution through a pitchfork bifurcation

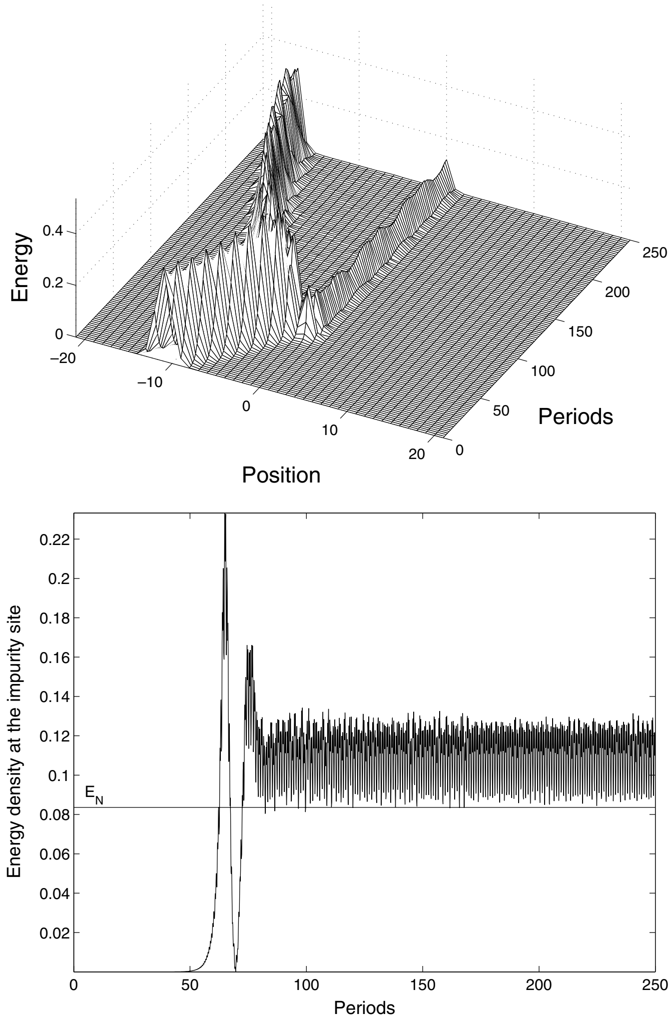

Figure 3. Interaction of a breather with an impurity for $\alpha = -0.52$ and $\lambda = 0.1$, which corresponds to the impurity excitation case. Top: evolution of the moving breather. Bottom: evolution of the energy density of the impurity. E_N is the energy of the impurity breather.

(see figure 6) in the space of time-reversible solutions of frequency ω_b.[3] In this bifurcation, the outer branches correspond to impurity breathers either with $u_n(0) > 0$ or $u_n(0) < 0$, while the central branch corresponds to the zero solution, i.e. all the oscillators are at rest.

For $\alpha = \alpha_{\rm res}$ the frequency of the impurity mode is the same as the frequency of the impurity breather with the moving breather frequency, i.e. $\omega_L = \omega_b$. $\alpha_{\rm res}$ can be calculated from equation (5) as a function of ω_b and C:

$$\alpha_{\rm res} = -\frac{\sqrt{\left(\omega_b^2 - \omega_o^2\right)\left(\omega_b^2 - \omega_o^2 - 4C\right)}}{\omega_o^2}. \tag{7}$$

[3] Note that the dynamical equations (2) do not correspond to a standard dynamical system $\ddot{x} = f(x, t)$, where usually pitchfork bifurcations are described.

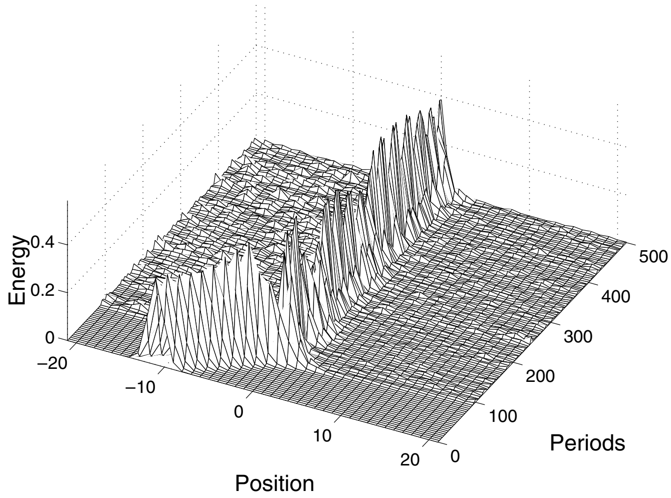

Figure 4. Evolution of the moving breather for $\alpha = -0.3$ and $\lambda = 0.1$, which corresponds to the trapping case. The moving breather becomes trapped by the impurity; afterwards, the breather emits phonon radiation and its energy centre oscillates between the sites adjacent to the impurity.

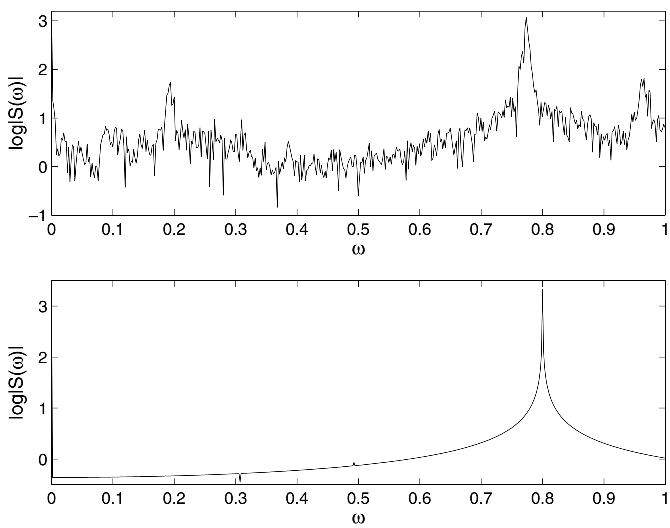

Figure 5. Fourier power spectra for the trapped breather of figure 4 (top) and a stationary breather with the same values of C and ω_b (bottom). The spectrum in the top panel is characteristic of chaos.

Thus, for $C = 0.13$ and $\omega_b = 0.8$, $\alpha_{\mathrm{res}} = -0.5628$, which is lower than α_1. However, the trapped breather does not exist for $\alpha > 0$. It indicates that the condition $\alpha \in (\alpha_{\mathrm{res}}, 0)$ might hold so that the trapped breather exists.

The scenario for the trapped breathers when $\alpha < 0$ is the following: in this case, the impurity 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 $q = 0$ [22], i.e. the impurity bifurcates from the impurity mode and it will be the only localized mode that exists when the impurity is excited for $\alpha > \alpha_{\mathrm{res}}$.

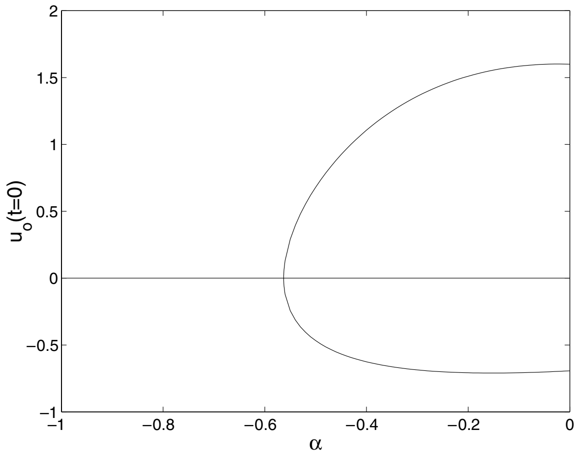

Figure 6. Pitchfork bifurcation for $\omega_b = 0.8$ and $C = 0.13$. $\alpha_{\rm res} = -0.5328$.

Thus, when the moving breather reaches the impurity, it can excite the impurity mode. In fact, we have performed a successful continuation from the impurity breather to the impurity mode at constant action and α [18, 19], and varying the parameter s which tunes the nonlinearity of the system. This parameter is introduced by changing the on-site potential to the expression $V_n^*(u_n) = D_n(1-s)u_n^2 + sV_n(u_n)$, where $V_n(u_n)$ is the original potential (1).

When $\alpha_{\rm res} < \alpha < \alpha_2$, the impurity breather is unable to create a trapped entity. The energy of the impurity mode decreases with $|\alpha|$, thus there must be a minimum value of the impurity breather energy for the existence of trapping. The narrow window of impurity excitations observed in the interval (α_1, α_2) can be due to a resonance of the moving breather with the impurity breather with a frequency slightly smaller than ω_b.

For $\alpha < \alpha_{\rm res}$, the trapped breather cannot be generated, and the moving breather is always reflected. In addition, the impurity breather does not exist. Therefore, there might be a connection between both facts, i.e. the existence of the impurity breather seems to be a necessary condition for obtaining a trapped breather.

If $\alpha > 0$, the scenario is different. In this case, the impurity mode has $q = \pi$ but the impurity breather sites vibrate again in phase, that is, the impurity breather does not bifurcate from the impurity mode. Thus, there are two different localized excitations for $\alpha > 0$: the (linear) impurity mode and the (nonlinear) impurity breather. But, actually, the equations that govern the system are nonlinear, so the linear modes can only correspond to low-amplitude oscillations. In the case of the impurity breather, the linear regime corresponds to the tails. Thus, if the moving breather reaches the impurity site, it will excite the impurity breather and the tails of the impurity mode. But the latter vibrates in a zigzag maroner. As a consequence, there will be two different linear localized entities: the tails of the impurity mode (vibrating in zigzag) and the tails of the impurity breather (vibrating in phase). Therefore, we conjecture that the existence of both linear localized entities at the same time may be the reason why the impurity is unable to trap the breather when $\alpha > 0$.

It may be considered whether the resonances with the harmonics of the breather frequency could have consequences in the interaction of the moving breather with the impurity. In our system, these resonances occur for $\alpha > \alpha_c$, and therefore, the impurity breather does not exist, so that no trapping effects take place, leading only to breather reflections.

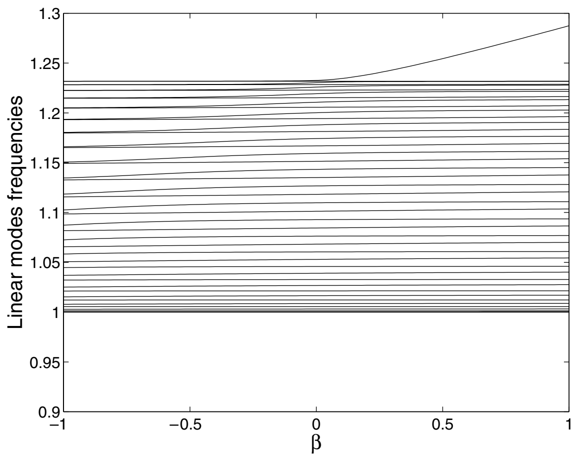

Figure 7. Frequencies of the linear modes versus the parameter β, for $C = 0.13$. The dependence is qualitatively similar for every value of C.

We summarize here our hypothesis for the existence of trapping:

Trapping hypothesis. *The existence of an impurity breather for a given value of α is a necessary condition for the existence of trapped breathers. However, if there exists an impurity mode with a different vibration pattern than that of the impurity breather, the trapped breather does not exist.*

4. Inhomogeneity in the coupling parameter

In order to check whether the hypothesis proposed in the last section holds for different situations, we consider a chain of oscillators for which the inhomogeneity is introduced through the coupling constants. In this case, the Hamiltonian can be written as

$$H = \sum_n \left(\frac{1}{2}\dot{u}_n^2 + V(u_n) + \frac{1}{4}C_n[(u_n - u_{n-1})^2 + (u_n - u_{n-1})] \right) \tag{8}$$

which leads to the following dynamical equations:

$$\ddot{u}_n + V'(u_n) + \tfrac{1}{2}[C_n(2u_n - u_{u+1} - u_{u-1}) + (C_{n+1} + C_{n-1})u_n - C_{n+1}u_{n+1} - C_{n-1}u_{n-1}] = 0. \tag{9}$$

The inhomogeneity is implemented so that $C_n = C(1 + \beta\delta_{o,n})$. The parameter β takes its values in $[-1, \infty)$.

The impurity modes can be calculated making the following ansatz:

$$\begin{cases} u_1(t) = \lambda u_o\, \mathrm{e}^{\mathrm{j}\omega_L t} \\ u_n(t) = u_1 r^{|n|}\, \mathrm{e}^{\mathrm{j}\omega_L t} \end{cases} \tag{10}$$

resulting in the dependence of the impurity mode frequency with the parameter β (represented in figure 7):

$$\omega_L^2 = \begin{cases} \omega_o^2 & \text{for} \quad \beta < 0 \\ \frac{\beta+2}{4\beta} C\left(\sqrt{9\beta^2 + 20\beta + 4} - 2 + 3\beta\right) & \text{for} \quad \beta > 0. \end{cases} \tag{11}$$

There are no impurity modes for $\beta < 0$, whereas for $\beta > 0$, they exist with $q = \pi$. Following the trapping hypothesis, the breather can only be trapped for $\beta < 0$. This result

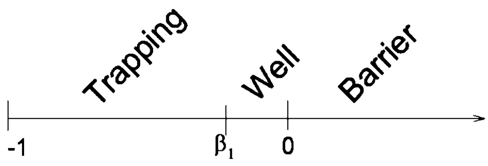

Figure 8. Different regimes in the interaction of a moving breather with an impurity introduced as an inhomogeneity in the coupling constant.

has been checked numerically. Figure 8 shows the different regimes of the moving breather–impurity interaction. There is only a critical value β_1, whose value is $\beta_1 \approx -0.12$ for $\lambda = 0.1$.

5. Conclusions

We have studied the interaction of moving discrete breathers with an impurity in a Klein–Gordon chain with non-weak nonlinearity. When the breathers reach the impurity, three different behaviours are observed. The scenario is as follows: (a) the impurity can act as a potential barrier or as a potential well; (b) the breathers can be reflected by the impurity, leaving it excited; (c) the impurity can trap the breathers.

The occurrence of the trapping has been found to be essentially independent on the breather velocity. At the borderline of the trapping region, the behaviour is slightly influenced by the velocity of the incident moving breather, as the critical value which separates the different regimes depends slightly on it. It implies that, in the case of an inhomogeneity in the on-site potential, there are two different situations: (a) at the borderline between the reflection and trapping areas, the breather is reflected for low velocities, whereas it is trapped for high velocities; (b) at the borderline between the trapping and crossing areas, the breather is trapped for low velocities, and passes through the impurity for high velocities. This result is different from that observed in the case of the interaction of a soliton with an impurity, where for the same value of the inhomogeneity parameter, it could pass through the impurity, be trapped or be reflected depending on its velocity.

In our study, we have found that the trapping occurs whenever the *trapping hypothesis* holds: an *impurity breather* of frequency close to the moving breather must exist. In addition, a (linear) impurity mode with a vibration pattern different from the impurity breather mode must not exist.

This result is different from that obtained in Forinash's approach, i.e. a Klein–Gordon chain with weak nonlinearity [17]. In this case, the trapping occurs provided the breather frequency resonates with a (linear) *impurity mode*, whereas in our case, the trapping may occur for a range of breather frequencies because the frequency of the impurity breather is not unique. Furthermore, this approach cannot explain the existence of trapping when the inhomogeneity is introduced through the coupling constant, as in this case the breather frequency does not resonate with the impurity mode frequency but the moving breather is trapped by the impurity.

Another significant difference with respect to Forinash's paper is that, in our case, the numerical results are justified in the light of the concept of the impurity breather. Furthermore, in [17], the range of parameters considered is $\alpha < 0$, whereas we have also studied the case of $\alpha > 0$ and the impurity implemented as an inhomogeneity in the coupling constant.

The model used here has been proposed by Peyrard and Bishop to explain DNA denaturation [20]. This suggests that our results can be applied to investigate some properties of DNA chains. For instance, if a moving breather is generated in a DNA chain, it can be trapped by an impurity, and acts as a precursor of the transcription bubble [23]. These trapped breathers may act as energy reservoirs and can transfer this energy to moving breathers generating high-energy localized excitations.

Impurities in DNA can have two different origins. The first consists in a modification of the dissociation energy due to the action of a transcription enzyme through a chemical effect, as explained in [23]. The second relies on the fact that the A–T base pairs have two hydrogen bonds whereas the C–G base pairs have three hydrogen bonds. Thus, it can be supposed that in the first case, the well depth of the Morse potential is about $2/3$ of the second case, within the framework of the Peyrard–Bishop model. According to the results in this paper, trapping does not occur when the well at the impurity is deeper than at the homogeneous part of the chain. It implies that trapping can only occur in a chain of C–G pairs with an impurity of A–T. Nevertheless, the main weakness of this analysis is the assumption of DNA homogeneity, as the role of the inhomogeneity due to the genetic code is known to be crucial in the dynamics [24]. However, the study of the effects of impurities is the first step in understanding the dynamics of moving breathers in DNA sequences.

Acknowledgments

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