# Influence of moving breathers on vacancies migration

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**Abstract**

A vacancy defect is described by a Frenkel–Kontorova model with a discommensuration. This vacancy can migrate when interacts with a moving breather. We establish that the width of the interaction potential must be larger than a threshold value in order that the vacancy can move forward. This value is related to the existence of a breather centred at the particles adjacent to the vacancy.

*Key words:* Discrete breathers, Mobile breathers, Intrinsic localized modes, Defects
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## 1 Introduction

The interaction of moving localized excitations with defects is presently a subject of great interest and can be connected with certain phenomena observed in crystals and biomolecules. Recently, Sen *et al* [1] have observed that, when a silicon crystal is irradiated with an ion beam, the defects are pushed towards the edges of the sample. The authors suggest that mobile localized excitations called quodons, which are created in atomic collisions, are responsible for this phenomenon. The interpretation is that the quodons are moving discrete breathers that can appear in 2D and 3D lattices and move following a

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quasi-one-dimensional path [2]. The interaction of moving breathers with defects is currently of much interest [3,4] (for a review on the concept of discrete breather see, e.g. [5]).

In this paper, we consider a simple one-dimensional model in order to study how a moving breather can cause a lattice defect to move. This study is new in the sense that most studies that consider the interaction of moving discrete breathers with defects, assume that the position of the latter are fixed and cannot move through the lattice. In particular, the defect we consider is a lattice vacancy, which is represented by an empty well or discommensuration in a Frenkel–Kontorova model [6]. The aim of this paper is to determine in which conditions the vacancy moves towards the ends of the chain. This is a previous step to reproduce the phenomenon observed in [1] for higher dimensional lattices.

## 2 The model

In order to study the migration of vacancies, we consider a Hamiltonian Frenkel–Kontorova model with anharmonic interaction potential [7]:

$$H = \sum_n \frac{1}{2}\dot{x}_n^2 + V(x_n) + C'\,W(x_n - x_{n+1}). \tag{1}$$

The dynamical equations are:

$$F(\{x_n\}) \equiv \ddot{x}_n + V'(x_n) + C'\,[W'(x_n - x_{n+1}) - W'(n_{n-1} - x_n)], \tag{2}$$

where $\{x_n\}$ are the absolute coordinates of the particles; $V(x)$ is the on–site potential, which is chosen of the sine-Gordon type:

$$V(x) = \frac{L^2}{4\pi^2}\left(1 - \cos\frac{2\pi x}{L}\right), \tag{3}$$

with $L$ being the distance between neighboring minima of the on–site potential. The choice of a periodic potential allows to represent a vacancy easily. Thus, if we denote the vacancy site as $n_{\rm v}$ (see figure 1), the displacements of the particles with respect to their equilibrium position are:

$$\begin{cases} u_n = x_n - nL & n < n_{\rm v} \\ \\ u_n = x_n - (n+1)L & n > n_{\rm v}. \end{cases} \tag{4}$$

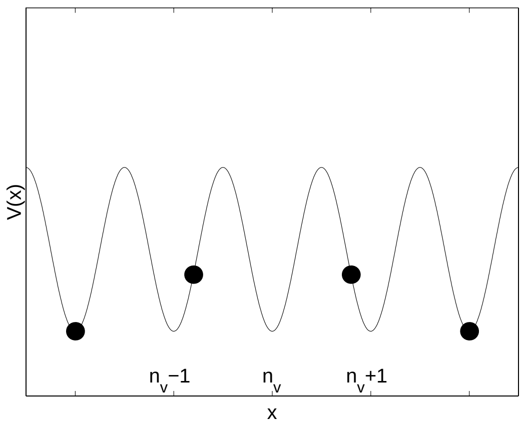


Fig. 1. Scheme of the Frenkel–Kontorova model with sine-Gordon on–site potential. The balls represent to the particles, which interact through a Morse potential. The vacancy is located at the site $n_\mathrm{v}$.

The interaction potential $W(x)$ is of the Morse type:

$$W(x) = \frac{1}{2}[\exp(-b(x-a)) - 1]^2, \tag{5}$$

where $a$ is the distance between neighboring minima of the interaction potential. In order to avoid discommensurations, we choose $L = a = 1$. $b$ is a parameter which is related to the width of the interaction potential, so that the interaction between particles is stronger when $b$ decreases.

The reason of the choice of this potential is twofold. On the one hand, it represents a way of modelling the interaction between atoms in a lattice so that, if the distance between particles is large, the interaction between them is weak. On the other hand, if a harmonic interaction potential were chosen, apart from being unphysical in this model, the movement of the breather would involve a great amount of phonon radiation, making it impossible to perform the study developed in this paper.

The linearized dynamical equations are:

$$\ddot{x}_n + x_n + C(2x_n - x_{n+1} - x_{n-1}) = 0, \tag{6}$$

with $C = C'\,b^2$.

Throughout this paper, the results correspond to a breather frequency $\omega_\mathrm{b} = 0.9$. Values of $\omega_\mathrm{b} \in [0.9, 1)$ lead to qualitatively similar results. Values of $\omega_\mathrm{b} \lesssim 0.9$ are not possible as moving breathers do not exist [8].

## 3 Numerical Results

### *3.1 Preliminaries*

In order to investigate the migration of vacancies in our model, we launch a moving breather towards the vacancy located at the site $n_\mathrm{v}$. This moving breather is generated using a simplified form of the marginal mode method [9,10], which consists basically in adding to the velocity of a stationary breather a perturbation which breaks its translational symmetry, and letting it evolve in time. In these simulations, a damping term for the particles at the edges is introduced in order that the effects of the phonon radiation are minimized.

The initial perturbation, $\{\vec{V}_n\}$ is chosen as $\vec{V} = \lambda(\ldots, 0, -1/\sqrt{2}, 0, 1/\sqrt{2}, 0, \ldots)$, where the nonzero values correspond to the neighboring sites of the initial center of the breather. This choice of the perturbation allows it to be independent on the parameters of the system $b$ or $C$. If the pinning mode were chosen as an initial perturbation, it would depend on the parameters of the system.

### *3.2 Breather–vacancy interaction*

When a moving breather reaches the site occupied by the particle adjacent to the vacancy, i.e., the location $n_\mathrm{v}-1$, it can jump to the vacancy site or remain at rest. If the former takes place, the vacancy moves backwards. However, if the interaction potential is wide enough, the particle at the $n_\mathrm{v}+1$ site, can feel the effect of the moving breather at the $n_\mathrm{v}-1$ site and it can also move towards the vacancy site. In this case, the vacancy moves forwards. Figures 2 and 3 illustrate both phenomena.

Numerical simulations show that the occurrence of the three different cases depends highly on the relative phase of the incoming breather and the particles adjacent to the vacancy. However, some conclusions can be extracted: 1) The incident breather always loses energy; 2) The breather can be reflected, trapped (with emission of energy) or refracted by the vacancy, in analogy to the interaction moving breather-mass defect [3]; 3) the refraction of the breather (i.e. the breather can pass through the vacancy) can only take place if the vacancy moves forwards.

It is interesting that the vacancy can migrate along several sites if the interaction between particles is strong enough (see Figure 4).

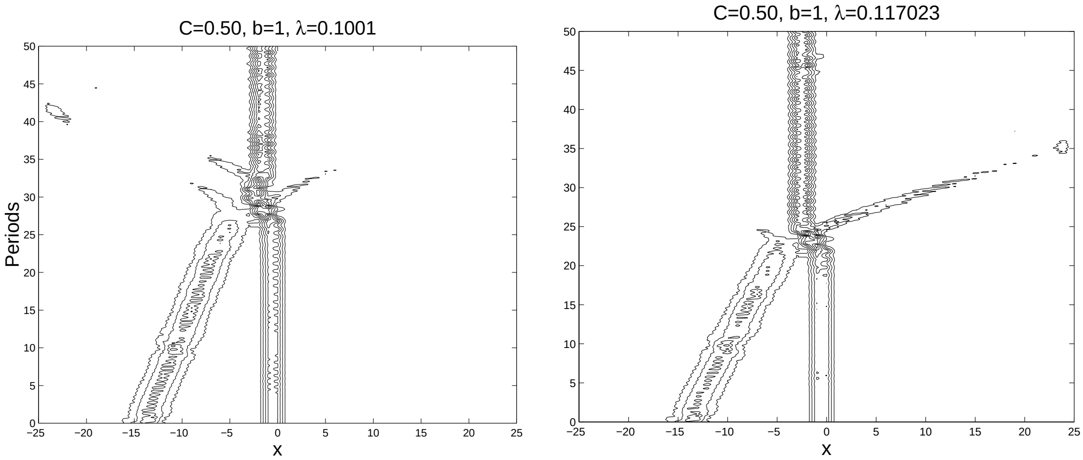


Fig. 2. Energy density plot of the interaction moving breather–vacancy. The vacancy is located at $n_{\rm v} = 0$. Note that the vacancy moves backwards (left) and, in the case of the figure to the right, the breather passes through the vacancy.

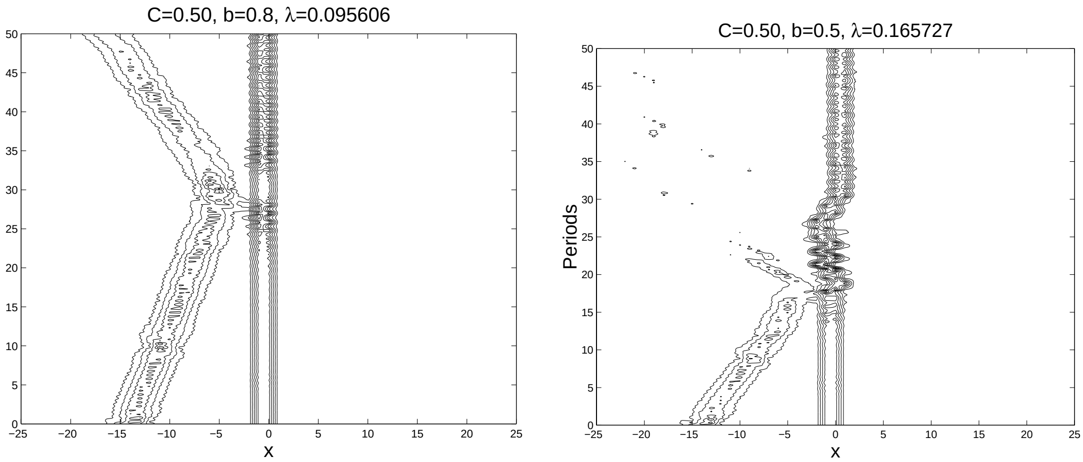


Fig. 3. Energy density plot of the interaction moving breather–vacancy. The vacancy is located at $n_{\rm v} = 0$. Note that, in the figure to the left, the breather is reflected and the vacancy remains at rest, while in the figure to the right, the vacancy moves forwards.

### *3.3 Numerical simulations*

As mentioned earlier, the moving breather–vacancy interaction is highly phase-dependent in a non obvious way. That is, the interaction depends on the velocity of the breather and the distance between the breather and the vacancy. Consequently, a systematic study of the state of the moving breather and the vacancy after the interaction cannot be performed.

Therefore, we have performed a simulation that consists in launching a large numbers of breathers towards the vacancy site. In particular, we have chosen

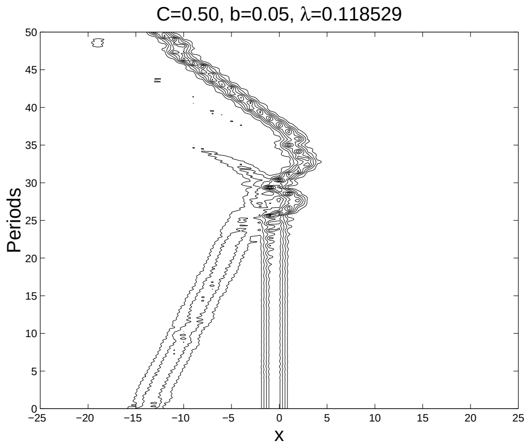


Fig. 4. Energy density plot of the interaction moving breather–vacancy. The vacancy is located at $n_{\rm v} = 0$. It can travel several sites along the lattice.

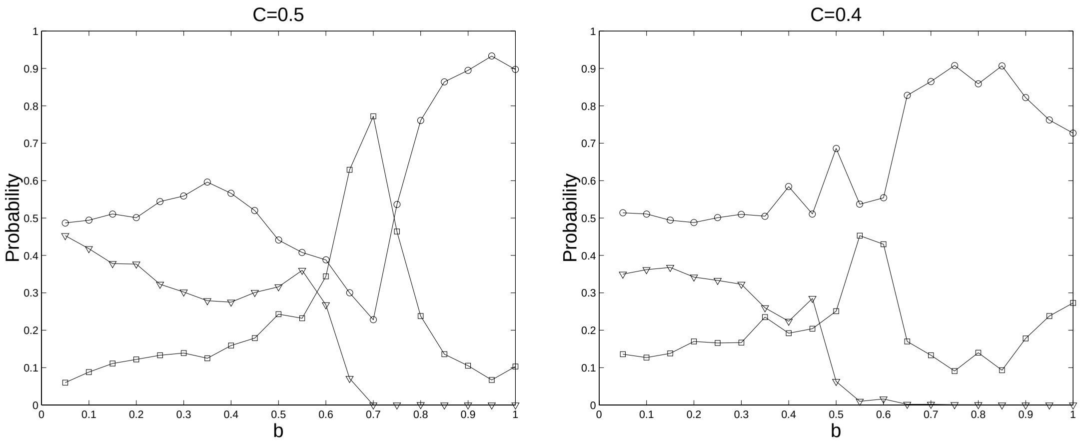


Fig. 5. Probability that the vacancy remains at its site (squares), moves backwards (circles) or moves forwards (triangles), for a Gaussian distribution of $\lambda$.

1000 breathers following a Gaussian distribution of the perturbation parameter $\lambda$ with mean value 0.13 and variance 0.03. Figure 5 shows the probabilities that the vacancy remains at its original site, or that it jumps backwards, or forwards for $C = 0.5$ and $C = 0.4$.

An important consequence can be extracted from this figure. There are two different regions for the parameter $b$, separated by a critical value $b(C)$. For $b > b(C)$, the probability that the vacancy moves forwards is almost zero, whereas for $b > b(C)$, this probability is finite. For example, $b(C = 0.5) \approx 0.70$ and $b(C = 0.4) \approx 0.55$.

Figure 6 represents this dependence for a uniform distribution of $\lambda \in (0.10, 0.16)$, and shows the occurrence of the same phenomenon. Thus, this result seems to be independent on how $\lambda$ is distributed.

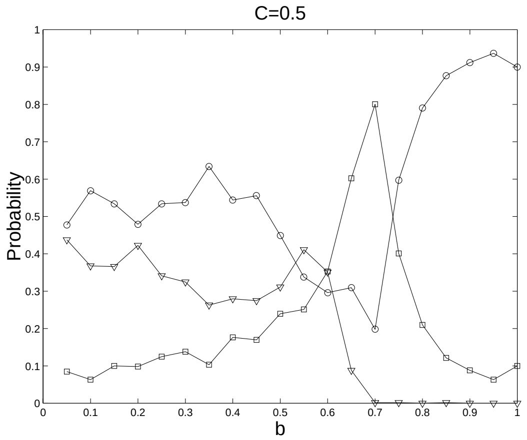


Fig. 6. Probability that the vacancy remains at its site (squares), moves backwards (circles) or moves forwards (triangles), for an uniform distribution of $\lambda$.

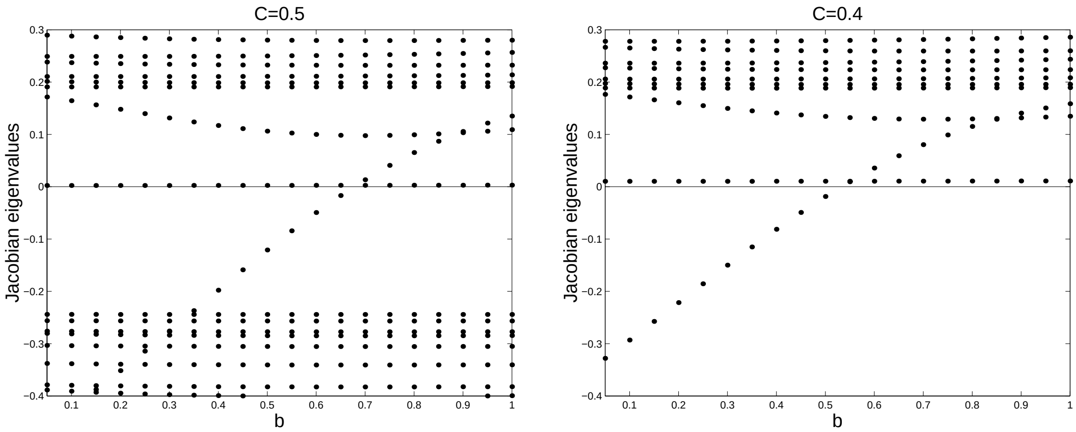


Fig. 7. Dependence of the Jacobian eigenvalues with respect to $b$. It can be observed that one eigenvalue changes its sign, and another is constant and close to zero. The first one is responsible for the bifurcation studied in the text, while the second one indicates the quasi-stability necessary for breather mobility [11].

### *3.4 Analysis of some results. Vacancy breather bifurcation.*

The non-existence of forwards vacancy migration can be explained through a bifurcation. If we analyze the spectrum of the Jacobian of the dynamical equations (2) defined by $\mathcal{J}\partial_x F(\{x_n\})$, bifurcations can be detected. A necessary condition for the occurrence of bifurcations is that an eigenvalue of $\mathcal{J}$ becomes zero. Figure 7 shows the dependence of the eigenvalues closest to zero with respect to $b$ for $C = 0.5$ and $C = 0.4$. It can be observed that, in both cases, there is an eigenvalue that crosses zero in $b \in (0.65, 0.70)$ for $C = 0.5$ and in $b \in (0.50, 0.55)$ for $C = 0.4$. These values agree with the points where the probability of the jump forward vanishes.

These bifurcations are related to the disappearance of the entities we call

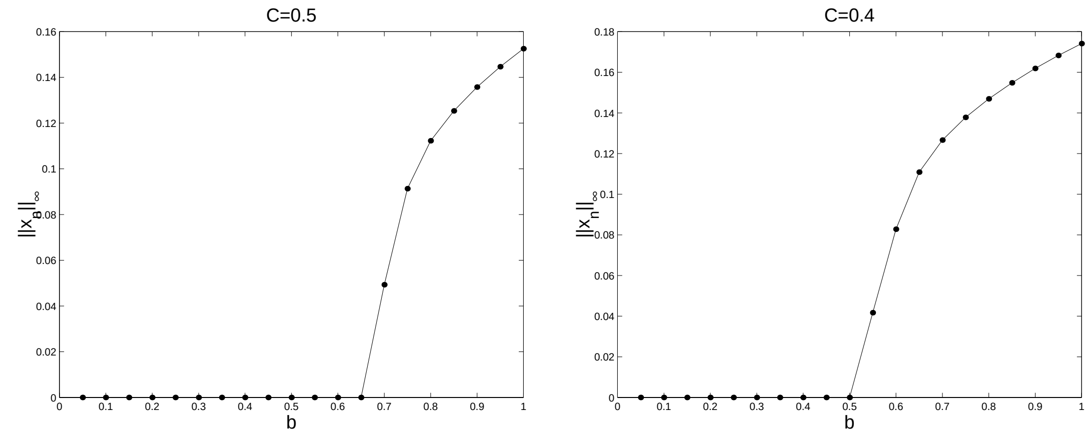


Fig. 8. Amplitude maxima of a vacancy breather versus $b$. It can be observed that the vacancy breather disappears at the bifurcation point (see figure 7). This is related to the vanishing of the forward movement probability.

*vacancy breathers*. These are defined as 1–site breathers centered at the site neighboring to the vacancy, e.g. the $n_\mathrm{v}-1$ or $n_\mathrm{v}+1$ sites. It can be observed (figure 8) that, for $b$ below the bifurcation value, vacancy breathers do not exist.

## 4 Conclusions

In this paper, we have observed that a moving breather con make a vacancy defect move forward, backward or let it at its site. We have also analyzed the influence of the width of the coupling potential and the coupling strength on the possibility of movement of a vacancy through the collision with a moving breather. In particular, we have observed that the width of the potential must be higher than a threshold for the vacancy being able to move forwards. This behaviour is relevant because experiments developed in crystals show that the defects are pushed towards the edges. We have also established that the non–existence of a breather centered at the sites adjacent to the vacancy is a necessary condition for the vacancy movement forwards.

The incident breathers can be trapped, in the sense that the energy becomes localized at the vacancy next neighbors, which radiate and eventually the energy spreads through the lattice. It can also be transmitted or reflected. The transmission can only occur if the vacancy moves backwards. The moving breather always losses energy but there is not a clear correlation between the vacancy and breather behaviours.

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