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Interaction of moving breathers with vacancies

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Abstract

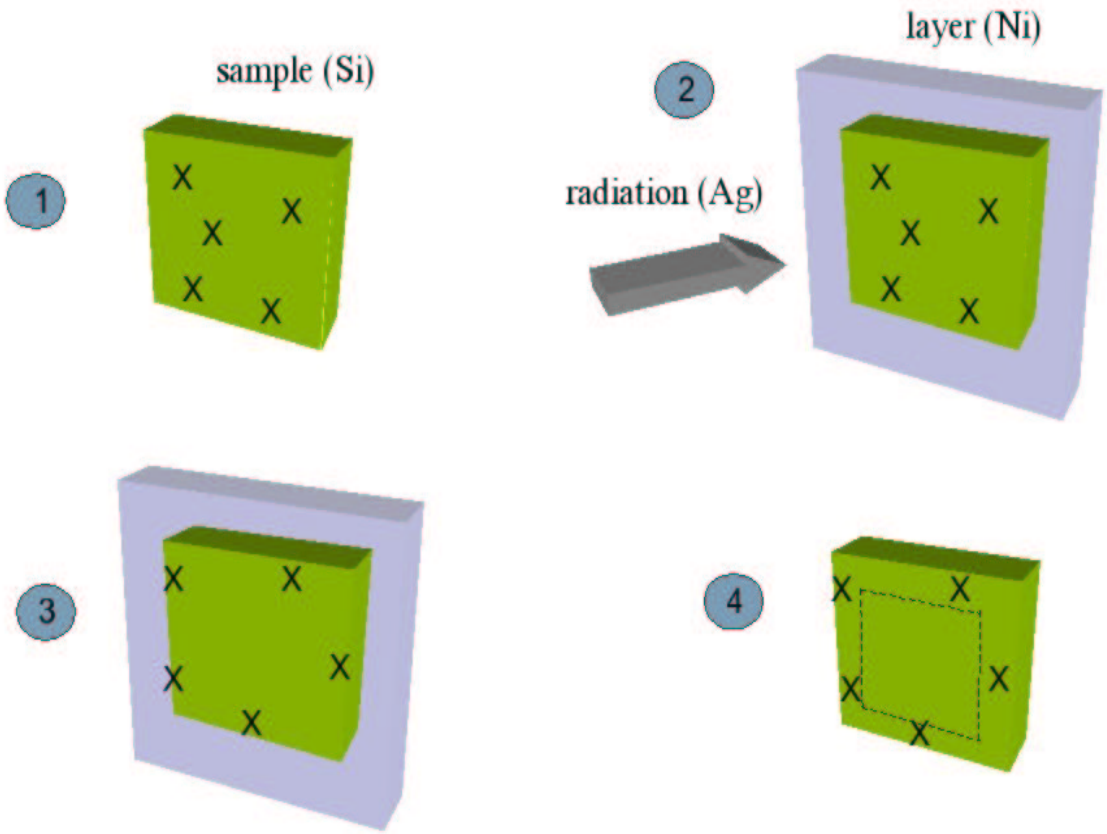
A vacancy defect is described by a Frenkel–Kontorova model with a discommensuration. We study the mechanism that can put into movement vacancies through the interaction of moving localized excitations (moving discrete breathers). We establish that the width of the interaction potential must be larger than a threshold value in order that the vacancy can move forward and that, for a certain range of parameters, there exists a threshold value of the translational energy of the moving breather. The occurrence of these phenomena are related to the properties of linear and nonlinear modes centred at the particles adjacent to the vacancy.

Experimental evidence: *defects migration*

The interaction of moving localized excitations can be connected with certain phenomena observed in crystals recently [1].

In fact (see the scheme below), it has been observed that, when a silicon crystal (1) is irradiated with an ion beam (2), after some time the defects are pushed towards the edges of the sample (3), so some sort of *cleaning* of the defects takes place (4).

The authors suggest that mobile localized excitations created in atomic collisions are a possible mechanism for the movement of defects.



Experimental scheme

The model

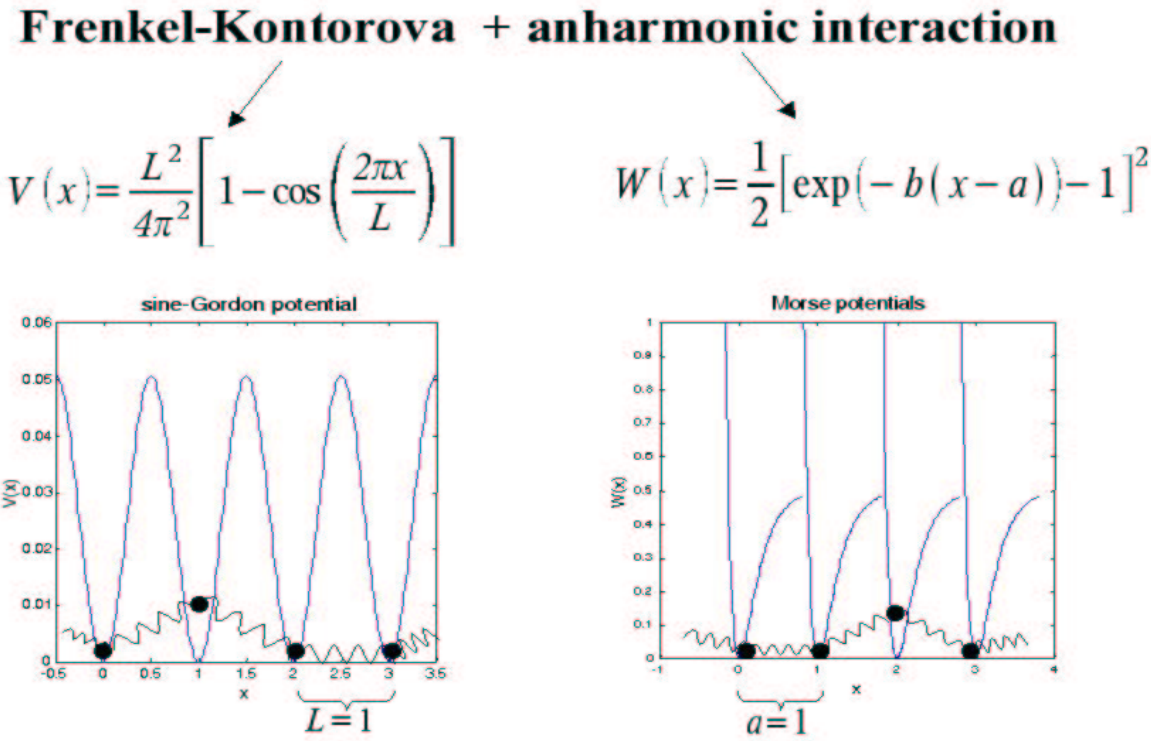
As stated above, a simple model which allows to describe a defect in a chain of atoms is the Frenkel–Kontorova chain [2]. The Hamiltonian is given by:

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

And the dynamical equations are:

$$F(\{x_n\}) \equiv \ddot{x}_n + V'(x_n) + C\,[W'(x_n - x_{n+1}) - W'(x_{n-1} - x_n)] = 0,$$

where $\{x_n\}$ are the absolute coordinates of the particles; C is the coupling constant; $V(x)$ is the periodic substrate potential, which is chosen of the sine-Gordon type; and $W(x)$ is the interaction potential, which is of the Morse type.



D is the depth of the interaction potential and L and a are the distances between neighbouring minima of the respective potentials. 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 moving breather

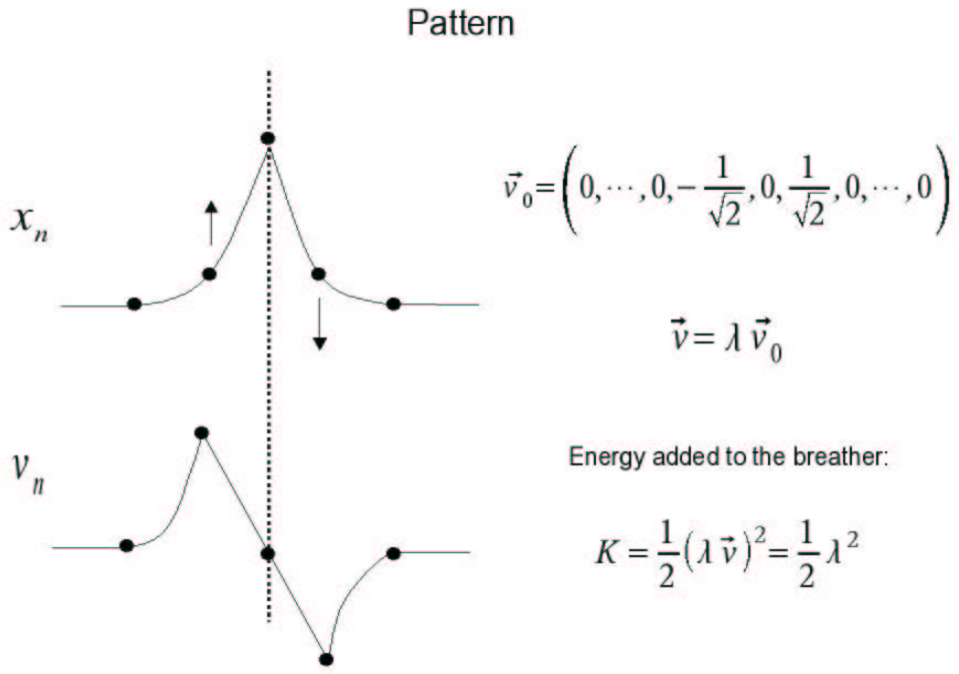
The basic phenomenon we are going to investigate in this work is how the width of the potential b^{-1} affects to the interaction of moving breathers with defects.

Thus, we consider some families of moving breathers with different values of b and velocities, which are launched towards the defects, always located to the right of the breather. This moving breather is generated using a simplified form of the marginal mode method [3,4],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.

The initial perturbation, $\{\vec{V}_n\}$, is chosen as:

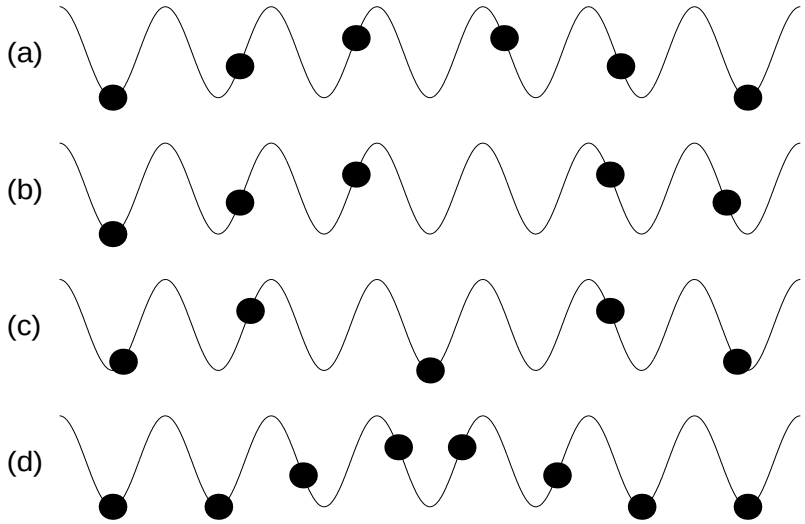
$$\vec{V} = \lambda(\ldots, 0, -1/\sqrt{2}, 0, 1/\sqrt{2}, 0, \ldots),$$

where the nonzero values correspond to the neighbouring sites of the initial centre of the breather (see the pattern). Thus the translational velocity of the breather is $K = \lambda^2/2$. 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.



Defects modelling

We consider two types of zero-dimensional defects: *vacancies* and *interstitials*. The dynamics of these structures is described by antikinks and kinks solutions, respectively [5,6]. In the following scheme is represented the Frenkel–Kontorova model with sine-Gordon potential for different defects:



where:

(a) is a single vacancy;

(b) are two adjacent vacancies;

(c) are two disjoint vacancies;

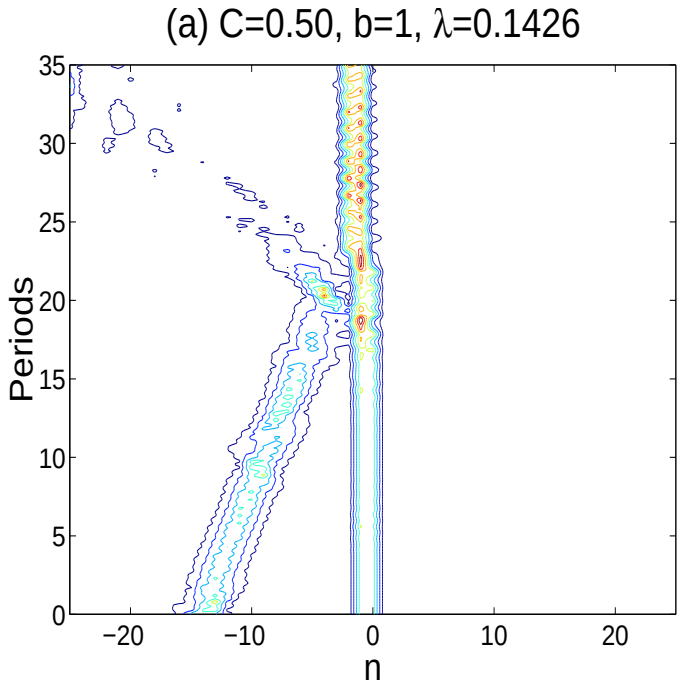
(d) is an interstitial.

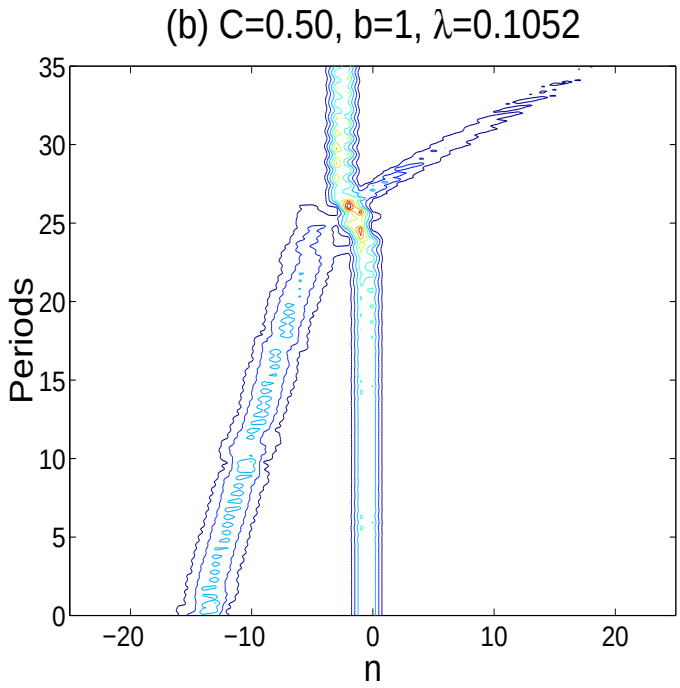
Single vacancy

- In this case, the breather excites the particle located at the left of the vacancy. As the well corresponding to the vacancy is empty, this particle can either:
  - *remain* at rest,
  - or *jump* to the vacancy site (i.e. the vacancy jumps backwards).
- However, if the interaction potential is wide enough, the particle at right of the vacancy, can feel the effect of the moving breather that makes the particle at the left of the vacancy vibrate with high amplitude and it can also *jump* to the vacancy site (i.e. the vacancy moves forwards).

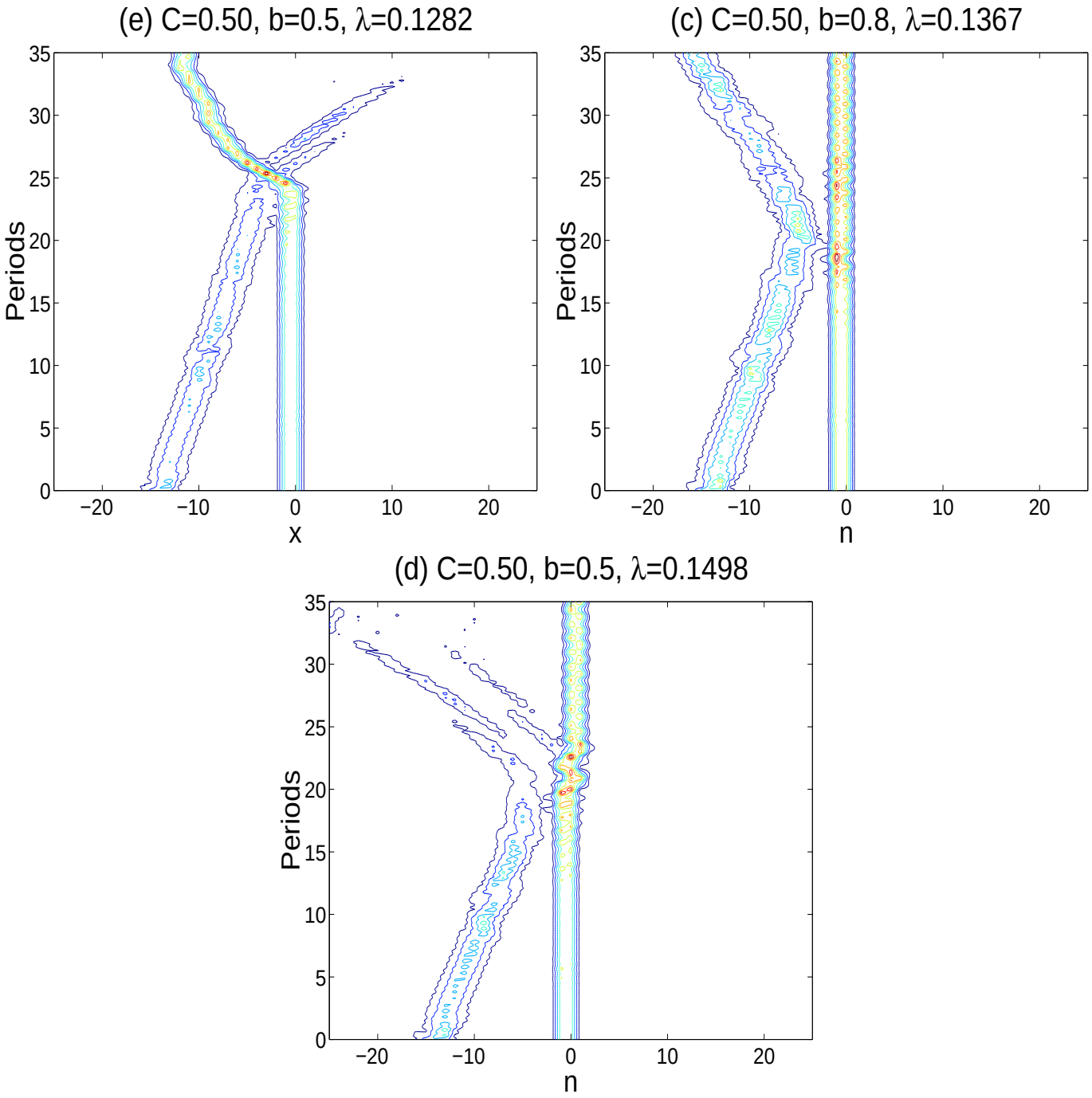
Single vacancy

- 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.
- In the following graphics, the energy density is represented for the particles in the interaction moving breather–vacancy.





Single vacancy



- The incoming breather only can pass through the vacancy if the vacancy moves backwards.

Single vacancy

Several simulations have been performed for each value of b. In particular, we have chosen 601 values of the parameter λ uniformly distributed in the interval $(0.10, 0.16)$. This dependence is qualitatively similar to the obtained if a Gaussian distribution of λ.

We can observe in Figures (2) and (3) the probability of the movement of the vacancy for some values of the parameter C.

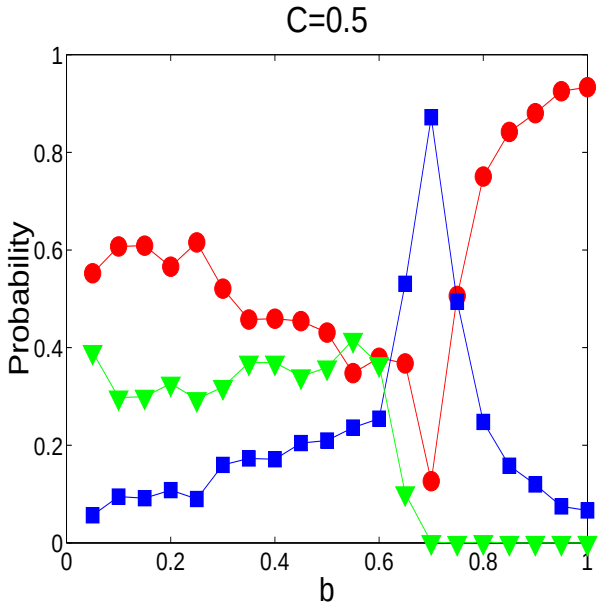


Fig 2: Probability that the vacancy remains at its site (blue), moves backwards (black), and moves forwards (green), for $C = 0.5$.

Furthermore, it can be observed that, for b higher than a critical value b_{forw}, the vacancy cannot move forwards, i.e., the forwards movement only occurs if the interaction potential is wide enough.

With the aid of the figures, it can be deduced that $b_{\text{forw}} \in (0.65, 0.70)$ for $C = 0.5$ and $b_{\text{forw}} \in (0.50, 0.55)$ for $C = 0.4$.

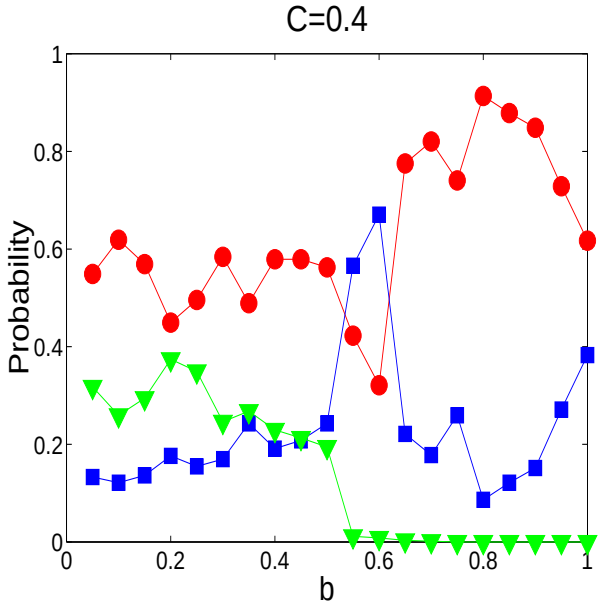


Fig 3: Probability that the vacancy remains at its site (blue), moves backwards (red), and moves forwards (green), for $C = 0.4$.

Threshold translational energy

Another important phenomenon is that for $b \in (b_{\rm barr}^{\rm min}, b_{\rm barr}^{\rm max})$, the translational energy of the breather must be higher than a critical value K_c in order that the vacancy can move. Furthermore, the relation $b_{\rm forw} \in (b_{\rm barr}^{\rm min}, b_{\rm barr}^{\rm max})$ is held.

The dependence of K_c with respect to b is shown in Figure 4.

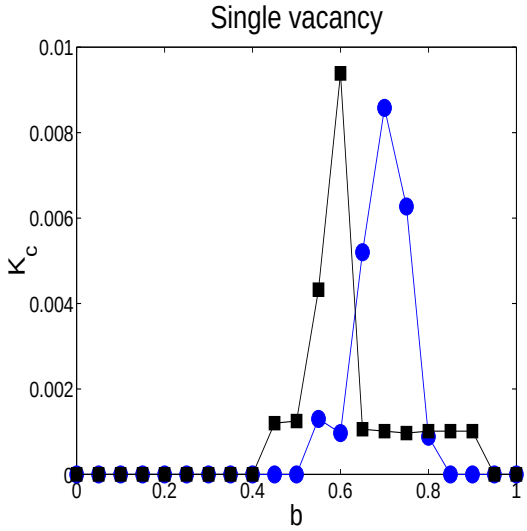


Fig. 4: Dependence of the threshold translational energy of the moving breather for a vacancy to be put into movement (K_c) with respect to b, for $C = 0.5$ (circles) and $C = 0.4$ (squares).

Defect breathers

Defect breathers are exact vibrating solutions obtained by exciting the particles closest to the defect, and three different kinds of them are considered: 1-site defect breathers (1DB), consisting on an only excited particle adjacent to the defect; 2-site defect breathers, which consist on the two particles adjacent to the defect excited at the same time, so that they can vibrate in-phase (2DBp) or anti-phase (2DBa).

If we define the variables $y_n = x_n - x_n^{(0)}$ which represent the deviation of the particles with respect to their equilibrium positions, it is possible to construct the bifurcation diagram (see Figure 5).

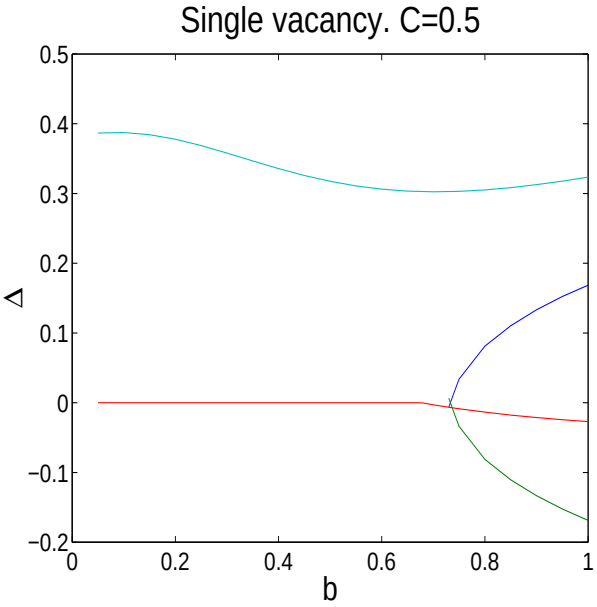


Fig. 5: Bifurcation diagram for the vacancy defect. The bifurcation variable is $\Delta = y_{n_{\rm v}^-} - y_{n_{\rm v}^+}$, for $C = 0.5$.

Conclusions

- The interaction moving breather-vacancy is highly dependent of the relative phase of the incoming breather and the particles adjacent to the vacancy.
- For some values of the width of the interaction potential, the translational energy of the breather must be higher than a critical value K_c in order that the vacancy can move. It is explained by the existence of unstable defect breathers.
- The existence of linear defect modes is needed for the forward movement of the vacancy.
- The incident breather always losses energy.
- The breather can be reflected, trapped (with emission of energy) or refracted by the vacancy, in analogy to the interaction moving breather-mass defect [8].
- The refraction of the breather (i.e. the breather can pass through the vacancy) can only take place if the vacancy moves forwards.

Acknowledgments

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