Interaction of moving discrete breathers with vacancies

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Abstract

In this paper a Frenkel–Kontorova model with a nonlinear interaction potential is used to describe a vacancy defect in a crystal. According to recent numerical results [Cuevas *et al.* Phys. Lett. A 315, 364 (2003)] the vacancy can migrate when it interacts with a moving breather. We study more thoroughly the phenomenology caused by the interaction of moving breathers with a single vacancy and also with double vacancies. We show that vacancy mobility is strongly correlated with the existence and stability properties of stationary breathers centered at the particles adjacent to the vacancy, which we will now call vacancy breathers.

Key words: Discrete breathers, Mobile breathers, Intrinsic localized modes, Vacancies, Breather-kink interaction.
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1 Introduction

Discrete breathers (DBs) are classical, spatially localized, time-periodic, numerically exact solutions which can be sustained by many non-linear lattices [1]. Their existence, which is proven by rigorous theorems [2] and a large amount of numerical results, is not restricted to special or integrable models. On the contrary, they can be found, in principle, in any discrete, nonlinear system and in any dimension [3,4]. They have been observed in experiments involving different systems, as Josephson-junctions arrays [5,6], waveguide arrays [7,8], molecular crystals [9] and antiferromagnetic systems [10]. They are also thought to play an important role in DNA denaturation [11].

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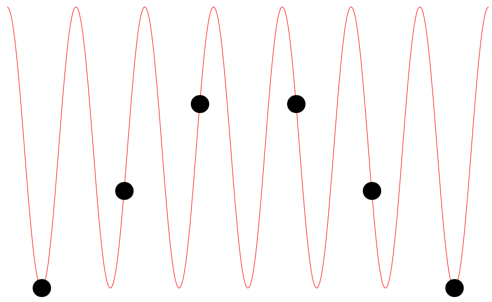

Fig. 1. Scheme of the equilibrium state of the Frenkel–Kontorova model with sine–Gordon substrate potential and Morse nearest neighbor interaction. The empty well represents a vacancy.

Usually they are pinned to the lattice but under certain circumstances may become highly mobile [12]. In this case, an interesting problem arises: the interaction between moving discrete breathers (MBs) and local inhomogeneities. This problem has been addressed within different frameworks: scattering of breathers or solitons by impurities [13–15], by lattice junctions [16] and by bending points [17] of a given chain.

Vacancies in a crystal are another type of local inhomogeneities. By using numerical methods, some of the authors found that a localized energy packet in the form of a moving discrete breather can put a vacancy into movement [18]. This vacancy migration induced by localized excitations had already been suggested as an explanation for some experimental results [19].

The aim of this paper is to find an explanation to the somehow qualitative results established in [18]. The main result is that vacancies mobility is highly dependent on the existence and stability of the breathers adjacent to the vacancy, hereafter called vacancy breathers (VBs).

2 The model

The simplest way to model a vacancy in a crystal consists in considering a one-dimensional chain of interacting particles submitted to a periodic substrate potential. It is known in other context as the Frenkel-Kontorova (FK) model [20]. A vacancy can be represented by an empty well of the substrate potential as Fig. 1 shows.

The Hamiltonian of this system is [15]

$$H = \sum_{n=1}^{N} \frac{1}{2} m \dot{x}_n^2 + V(x_n) + W(x_n - x_{n-1}) \quad , \tag{1}$$

being x_n the absolute coordinate of the n-th particle. We have chosen the sine-Gordon potential

$$V(x_n) = \frac{a^2}{4\pi^2} [1 - \cos(2\pi x_n / a)] \tag{2}$$

as the simplest periodic, substrate potential, with linear frequency normalized to the unity $\omega_0 = \sqrt{V''(0)} = 1$. We have chosen the Morse potential for the interaction between particles because its force weakens as the distance between particles grows and its hard part prevents the particles from crossing. It is given by

$$W(x_n - x_{n-1}) = \frac{C}{2b^2} [e^{-b(x_n - x_{n-1} - a)} - 1]^2. \tag{3}$$

The parameter $C = W''(a)$ is the curvature of the Morse potential. We have taken $C = 0.5$ in order that MBs exist in this system for a breather frequency $\omega_b = 0.9$. The strength of the interaction potential can be modulated, without changing its curvature, by varying b, being b^{-1} a measure of the well width and $C/2b^2$ the well depth. We have also normalized the lattice period a and the masses to the unity. The dynamical equations are given by

$$\ddot{x}_n + V'(x_n) + [W'(x_n - x_{n-1}) - W'(x_{n+1} - x_n)] = 0. \tag{4}$$

In this system, it is possible to generate DBs numerically using the standard methods from the anticontinuous limit [21]. We can also induce translational motion of DBs by using a simplified form of the marginal mode method [12]. It consists of adding a perturbation $\vec{v} = \lambda(..., 0, -1/\sqrt{2}, 0, 1/\sqrt{2}, 0, ...)$ to the velocities of the stationary breather, with the nonzero values at the neighboring sites of the initial breather center. The resulting DB kinetics is very smooth and resembles that of a classical free particle with constant velocity. Therefore, we can consider the total energy of a MB as the sum of a the internal energy, equal to the one of the stationary breather, plus the translational energy, equal to the energy of the perturbation added $K = \lambda^2/2$.

In order to facilitate systematic studies, we have introduced dissipation at the boundaries.

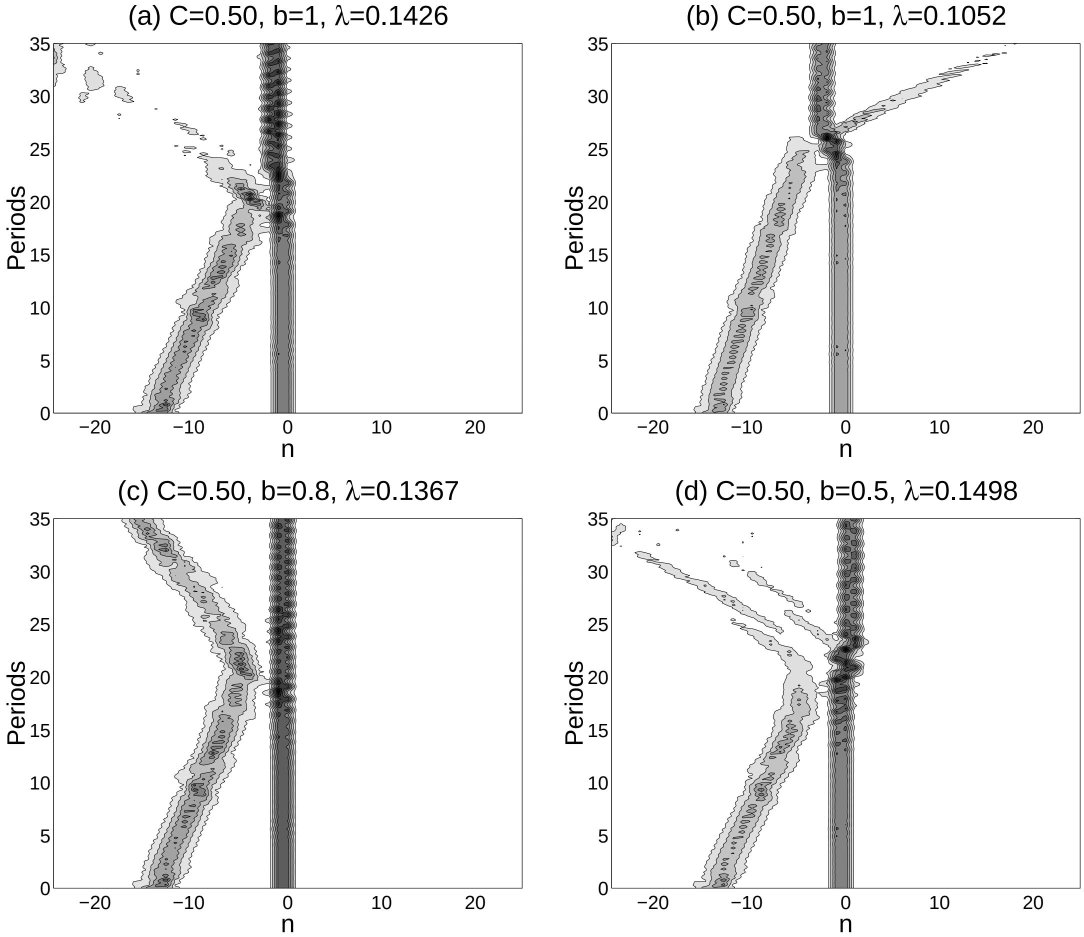

Fig. 2. Energy density plot for the interaction moving breather–vacancy. The particle to the right of the vacancy is located at $n = 0$. In (a), (c) and (d) the moving breather is reflected and the vacancy moves backwards, remains at rest and moves forwards respectively. In (b) the breather is transmitted and the vacancy moves backwards.

3 Interaction of moving breathers with a single vacancy

In order to investigate vacancy mobility, we have generated DBs far from a vacancy and then launched this breather against it. Our numerical calculations show that the outcome of the scattering is extremely sensitive to the initial conditions [18]. The incident breather can be reflected, trapped or transmitted (see Fig. 2), always losing energy as it occurs in the interaction between a MB and an impurity [13], whereas the vacancy can either move forward or backward or remain at rest. This scenario is very different to the one arising in the continuum limit where the vacancy (anti-kink) always moves backwards and the breather is always transmitted after the collision.

We have studied the dependence of the vacancy mobility on the parameter b, which controls the strength of the interaction between neighboring particles

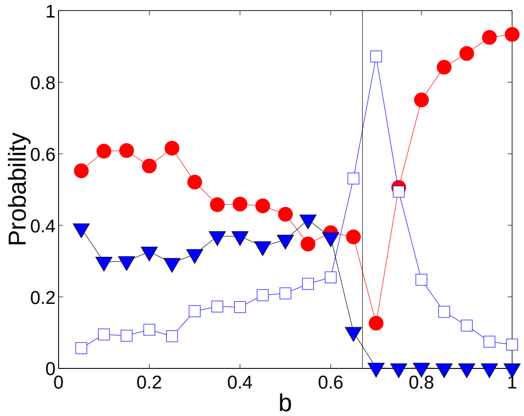

Fig. 3. Probability for the vacancy to remain at its site (squares), move backward (circles) or forward (triangles). The interaction weakens when b increases. Note that no forward movement of the vacancy occurs to the right of the vertical line.

of the chain. For each value of b we have analyzed a set of 601 numerical experiments of scattering corresponding to different initial conditions. As initial conditions we have considered a set of MBs with increasing kinetic energy, which were obtained choosing the values of the parameter λ uniformly distributed in the interval $[0.10, 0.16]$. The lower bound of this distribution is chosen so that the threshold value for vacancies movement (see below) is surpassed. The upper bound can be increased without any dramatic change in the results. However, an extremely high value of λ can destroy the moving breather.

Fig. 3 shows the probability that the vacancy moves forward, backward or remains at rest (averaged over the set of initial conditions) with respect to the parameter b. Note that, as it should be expected, the backward movement is the most probable behavior because in this case the incident breather pushes forward the particle to the left of the vacancy. In fact, the forward movement of the vacancy requires a strong enough interaction, i.e. b has to be smaller that a critical value $b_f \approx 0.7$.

Another interesting finding is shown in Fig. 4: the translational energy of the MB has to be higher than a minimal value K_{min} in a certain interval $b \in (0.5, 0.8)$ in order to move the vacancy. It is worth remarking that $K_{min} = 0$ means the minimum kinetic energy needed to move a breather, which is actually different to zero. However, we have included this notation in order to have a clear picture of the vacancy movement.

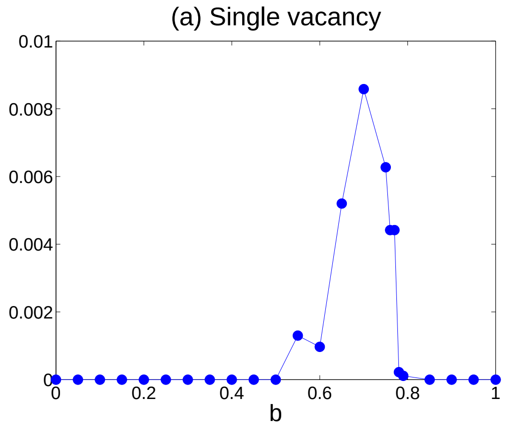

Fig. 4. Minimal translational energy (K_{min}) to move a vacancy.

4 Vacancy modes and vacancy breathers

We can try to understand these results by studying: a) the linear modes, which can be obtained by linearizing Eqs. 4 around the equilibrium state shown in Fig. 1; and b) the vacancy breathers, i.e., the nonlinear localized modes centered at the particles adjacent to the vacancy, with the same frequency as the incident MB.

Fig. 5a shows the dependence of the linear frequencies with respect to b. Note that the minimum linear frequency corresponds to a linear localized mode which we call linear vacancy mode (LVM). On the other hand, there are three types of VB: 1–site vacancy breathers (1VB), which consists of a single excited particle adjacent to the vacancy; and 2–site vacancy breathers, obtained by exciting the two particles adjacent to the vacancy, which can vibrate in-phase (2VBp) or anti-phase (2VBa). Fig. 5b shows the bifurcation pattern for these VBs. A letter at the beginning of the abbreviation specifies the breather stability: S stable, hU harmonically unstable, sU subharmonically unstable or oU oscillatory unstable. For example sU2VBa means a subharmonically–unstable, two–site, vacancy breather in anti–phase.

For weak interaction (b large) there exist stable one-site VBs at both sides of the vacancy as stated by the theory [1]. As b decreases the S1VB disappears through an inverse pitchfork bifurcation to two unstable two-site VB in phase (hU2VBp) which becomes stable (S2VBp). Further decrease of b brings about the annihilation of the S2VBp when the breather frequency coincides with the frequency of the LVM with the same profile.

The two–site VB in antiphase is stable (S2VBa) for the largest values of b represented in Fig. 5b. When the interaction increases (b decreases) this 2VB becomes oscillatory unstable (oU2VBa), and finally subharmonically unstable (sU2VBa).

From this bifurcation diagram we can deduce that the stability of the VBs is correlated to the existence of a kinetic energy threshold to move the vacancy, in the interval $b \in (0.5, 0.8)$. Comparison of Fig. 4 and 5b suggests that *the existence of a subharmonically or harmonically unstable, 2-site, vacancy breather is a necessary condition in order to get an optimum vacancy mobility (no kinetic energy threshold).*

Generally speaking, any approaching breather with any kinetic energy is able to move the vacancy if at least one the two 2VBs exists and is either subharmonically or harmonically unstable. We cannot expect, however, an exact agreement between the numerically exact bifurcation values for a given frequency with the observed changes in behavior for the simulations. The reason for that is that a moving breather is obtained by perturbation with an asymmetric mode. Therefore, it is no longer an exact solution of the dynamical equations, its frequency is shifted and it is not unique. The bifurcation values for other frequencies will change and interaction of phonons emitted by the MB are expected to have an (unknown) influence, hence the probability analysis of the simulations outcome. However, the only important exception to the first assessment in this paragraph in the region $b \in (0.73, 0.8)$ is noteworthy. The role of the unstable vacancy breather is probably to act as an intermediate structure with high oscillations for the particles nearest to the vacancy, which, being unstable, leads to one of them changing place. Clearly the stable S2VB does not play that role and its existence in the vicinity of that region seems to be the reason for that discrepancy –proximity in b for a $\omega_{\rm b} = 0.9$ also means proximity in $\omega_{\rm b}$ for the a given value of b, which can be excited by the bundle of the MB frequencies–.

Therefore our conclusion is that vacancy mobility is governed, for a particular choice of the substrate potential, by the strength of the interaction between the particles adjacent to the vacancy, which is correlated to the existence and stability properties of vacancy breathers. This correlation manifests in two different ways. Firstly, the interaction has to be strong enough to move the vacancy forward, or equivalently, there must exist no linear vacancy modes. Secondly, a threshold value of the translational energy of the incident MB in order to move the vacancy does not exist if an harmonically or subharmonically unstable VB exists.

Another choice of the interaction potential would alter the values of b which separate the different regimes. However, the correlation between the vacancy mobility and the strength of the potential would be similar.

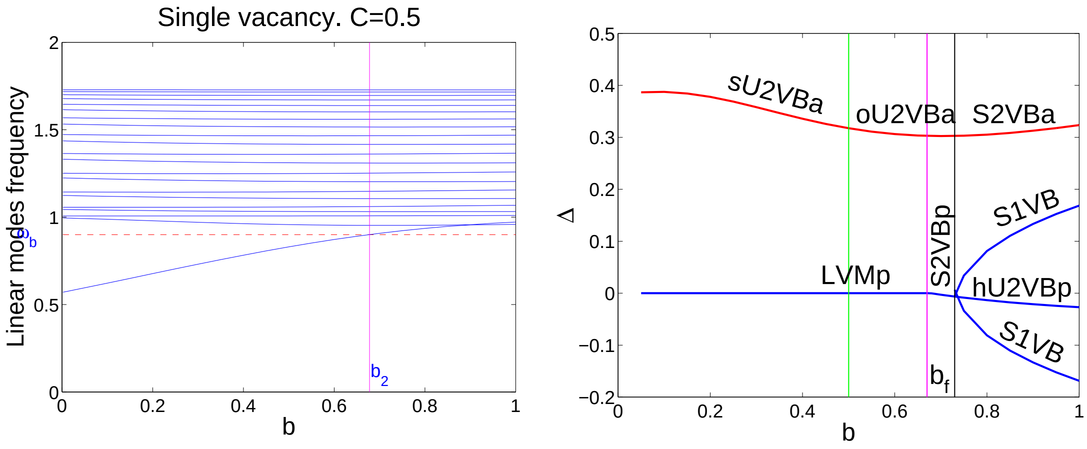

Fig. 5. a) Linear spectrum. Also represented is the breather frequency $\omega_{\mathrm{b}} = 0.9$. Note the existence of a localized linear mode. (b) Bifurcation diagram for the nonlinear localized modes obtained by exciting the particles adjacent to the vacancy. The bifurcation variable Δ is the difference between the relative displacements of the particles to the left and to the right of the vacancy. The vertical lines indicate bifurcation points. See the text for the breather codes.

5 Double vacancy

We have studied the mobility of a double vacancy (two empty neighboring wells of the substrate potential) to test our conjecture. The outcome is similar to the single vacancy case except for the fact that the left vacancy never moves forwards. Thus, if the right vacancy moves forwards, the double vacancy splits in two (see Fig. 6). Fig. 7 shows the linear spectrum and the bifurcation diagram for the VB in this case. In these figures the lowest value of b is approximately 0.5 since there are no equilibrium states for $b \lesssim 0.5$. This result also implies the non existence of double vacancies equilibrium states for a harmonic interaction potential. As b increases, we observe two–site VBs emerging from linear localized modes, and afterwards an inverse pitchfork bifurcation similar to the one described for a single vacancy. There is not any harmonically or subharmonically unstable VB for $b < 0.75$. Therefore, we should expect that there is a minimum value for the kinetic energy of the incident MBs able to move the double vacancy. This is confirmed by numerical computations as Fig.8 shows.

6 Summary

We have observed numerically the interaction of moving breathers with vacancies in the simplest, physically consistent model. We have found that the breathers can be reflected, transmitted and trapped, both by the single and

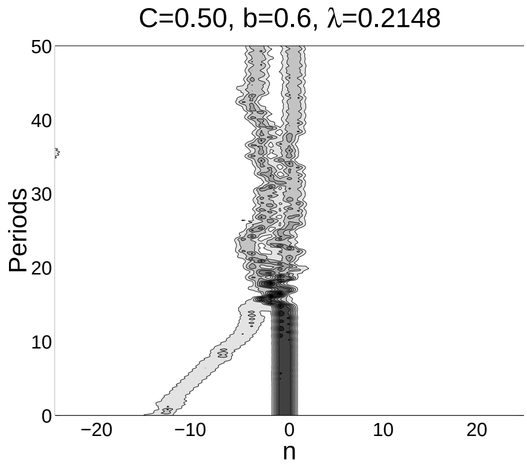

Fig. 6. Energy density plot for the interaction moving breather–double vacancy, in the vacancy splitting regime. The particle to the right of the vacancies is located at $n = 0$.

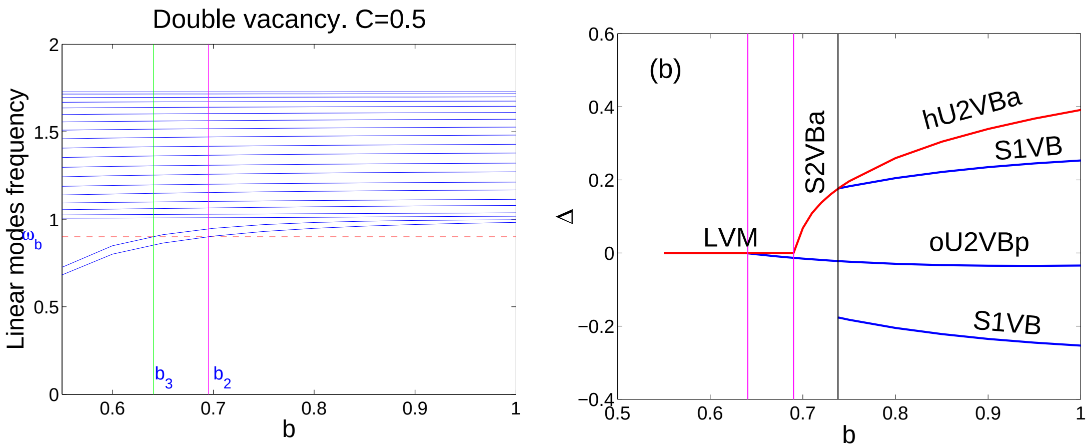

Fig. 7. Double vacancy case: a) Linear spectrum. The breather frequency $\omega_{\rm b} = 0.9$ is also represented. Note the existence of two localized linear modes. (b) Bifurcation diagram for the nonlinear localized modes obtained exciting the particles adjacent to the double vacancy. The bifurcation variable Δ is the difference between the relative displacements of the particles to the left and to the right of the double vacancy. The vertical lines indicate bifurcation points. See text for the breather codes.

the double vacancy. The single vacancy can move forward, backwards and remain and rest, but the double vacancy cannot move forward, instead it can split into two single vacancies, one at rest and the other moving forwards. This phenomenology is very different from the continuous analogue, where the breather is always transmitted and the vacancy (anti-kink) always moves backwards.

The vacancy migration is strongly correlated with the existence and stability of vacancy breathers, which we have studied in detail. In order to move the vacancy the interaction has to be strong enough and the energy of the incident

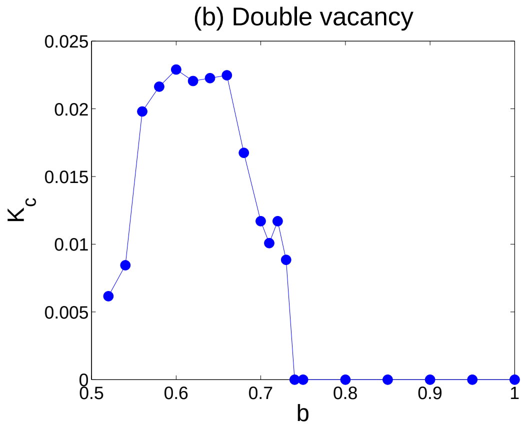

Fig. 8. Minimal translational energy (K_{min}) to move a double vacancy.

MB has to be above a threshold. This threshold disappears approximately around bifurcation points where vacancy breathers become unstable.

We think that the study of the properties of breathers next to a defect may help to understand the mobility of other class of point defects such as interstitials, which might be related with recent defect migration observed experimentally in ion-irradiated silicon.

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