RATCHET EFFECT IN SOLIDS: DEFECT TRANSPORT DRIVEN BY BIHARMONIC FORCES

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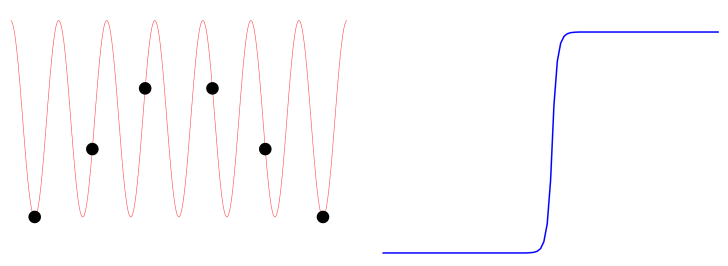
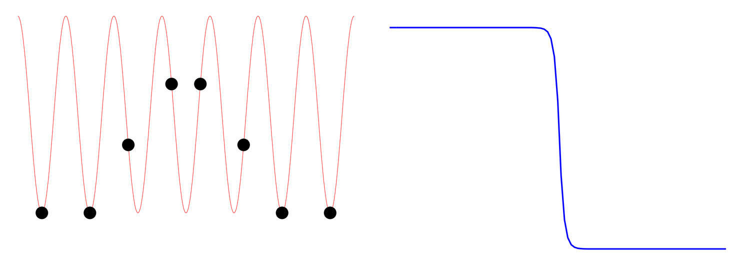
Defects in solids

- There are several types of crystalline defects of different dimensions. Among them, the zero-dimensional defects are also called point defects. This kind of defects includes impurities, vacancies (Schottky defects), interstitials (Frenkel defects), polarons, excitons, ...
- The nonlinear dynamics of Schottky and Frenkel defects can be described using the Frenkel-Kontorova (FK) model, which basically consists in a one-dimensional chain of interacting particles, subjected to a periodic substrate potential.
- The properties of this kind of defects are very important in the design of new materials [1]. Furthermore, the study of the transport properties is a subject of outstanding recent interest [2, 3].
- Vacancies can be modelled by an empty well of the substrate potential. The dynamics of this structure is described in terms of kinks:



- Interstitials correspond to a doubly occupied well. These structures are described by antikinks:



The mathematical model

- We have used a driven and damped Frenkel-Kontorova model with an anharmonic interaction potential:

$$\ddot{u}_n+\alpha\dot{u}_n+\frac{1}{2\pi}\sin(2\pi u_n)+\kappa[W'(u_n-u_{n+1})-W'(u_{n-1}-u_n)]=E(t)$$

- Here, α and κ are the damping and coupling constants, respectively. We assume that $E(t)$ is a biharmonic ac force:

$$E(t)=\frac{E_0}{2\pi}[\cos(\omega t)+\cos(2\omega t+\theta)]$$

- This driving force is asymmetric for almost all values of θ. Thus, it breaks the time symmetry of the system leading to soliton transport through a ratchet effect [4].

The anharmonic potential

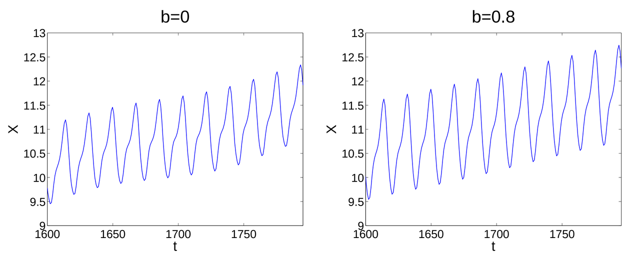
- The ratchet dynamics of solitons with a harmonic interaction potential was widely studied in [4]. The aim of our work is to study the effect of an anharmonic interaction potential. We have chosen a Morse potential:

$$W(x)=\frac{1}{2b^2}[\exp(-bx)-1]^2$$

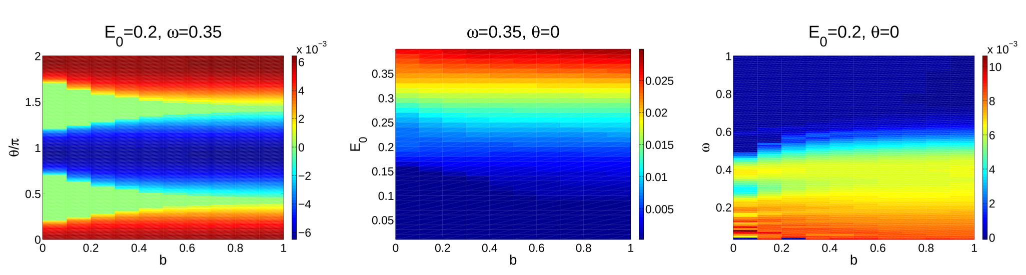
- b^{-1} is a measure of the potential width. For $b\to 0$, the harmonic potential is recovered. Results for Hamiltonian lattices [5, 6] show that kinks motion is strongly dependent on this parameter.
- The main effect of the anharmonicity is the symmetry breaking between antikink and kinks structures [7, 8]. For instance, in the case of a harmonic interaction potential, for the same set of parameters (α,κ,E,ω) antikink and kink dynamics are exactly the same except for their opposing velocities.
- The anharmonicity implies, apart from a change in the profiles, a diminution of the Peierls-Nabarro barrier in the case of antikinks, whereas, for kinks, this barrier increases. This effect, as we show in the poster, makes the kink dynamics richer than the antikink one.

Effect of the anharmonicity on antikinks motion

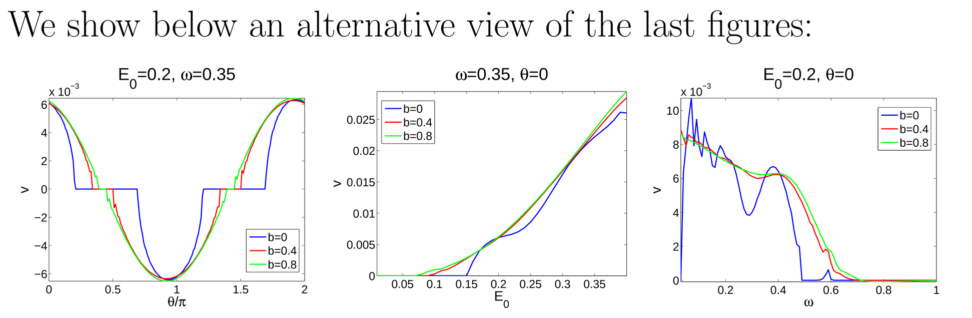
- As ratchet antikinks (or kinks) are attractors, if an initial condition close to the attractor is chosen, in a finite time, the attractor is found.
- We use then, as initial condition, an antikink (or kink) at rest, solution of the Hamiltonian lattice equations, with the same κ and b of the desired solution of the full dissipative lattice.
- In all simulations $\alpha=0.5$ and $\kappa=1$ are fixed and periodic boundary conditions are chosen.
- The effect of increasing b is, in general, to increase antikinks velocity. Figures below show the time evolution of the energy center for two antikinks with $E_0=0.2$, $\omega=0.35$ and $\theta=0$:



- The velocity dependence is better visualized in the following density plots. The graphs represent the velocity (in the colored bar) as a function of b and, from left to right, θ, E_0 and ω.



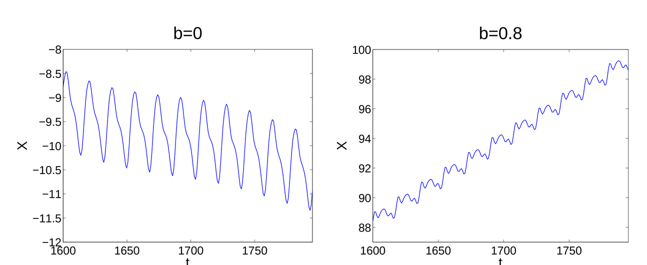
- We show below an alternative view of the last figures:



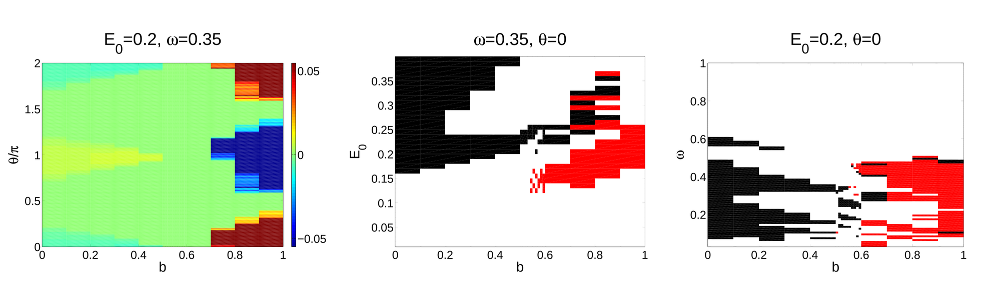
- We can observe the following facts from the figures:
  1. For θ variable and b fixed, there is a region where the antikink remains pinned. This region is smaller as b increases.
  2. For E_0 variable and b fixed, there is a threshold value of the driving amplitude for antikink motion. This threshold value decreases with b.
  3. For ω variable and b fixed, there is a maximum value of the driving frequency for antikink motion. This maximum increases with b.
- The increase of the mobility with the anharmonicity (i.e. with parameter b) can be related with a decrease of the Peierls-Nabarro barrier.

Effect of the anharmonicity on kinks motion

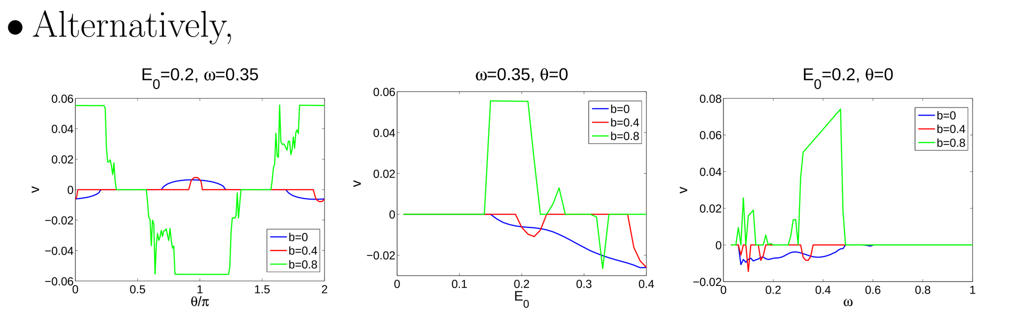
- For fixed α, κ, θ, E_0 and ω, two different regimes are observed in kink motion separated by a critical value b_c:
  1. For $b<b_c$: the velocity decreases with b and has the opposite sign of the antikinks with the same value of θ.
  2. For $b>b_c$: kinks can move in the same direction of the antikinks with the same value of θ, and with a much higher velocity than those.
- Figures below show the time evolution of the energy center for two antikinks with $E_0=0.2$, $\omega=0.35$ and $\theta=0$:



- Next figures show, from left to right, the following magnitudes: (left) the dependence of the velocity is displayed versus θ and b; (center & right) the direction of motion is represented versus b and E_0 (center) or ω (right). Colors mean the following in the last figures: (black) directed motion; (red) reversed motion; (white) pinning.



- Alternatively,



- Some facts can be observed from these figures:
  1. For θ variable and b fixed, there is a region where the kink remains pinned. This region is bigger as b increases, so that the kink cannot move for $0.5\lesssim b\lesssim 0.6$. For values of b above this range, kink motion is recovered, but in the inverse direction.
  2. For E_0 or ω variable and b fixed, there is a critical value of b separating regions with only directed motion and regions with possible inverse motion. This value is $b_c=0.54$ for E_0 variable and $b_c=0.60$ for ω variable.
  3. Differently from the antikink case, where the pinning was not observed for E_0 or ω variable (with $\theta=0$), in the kink case, the most observed regime is the pinning.

- An increase of the Peierls-Nabarro barrier can explain the lose of mobility when b increases. However, the appearance of inverse kink motion cannot be understood with this explanation. This anomalous motion might be related to a topological change of the Peierls-Nabarro barrier for high values of b.

Summary

- We have shown some aspects of the dynamics of vacancy and interstitial defects driven by biharmonic ac fields. Vacancy and interstitial defects can be represented by kinks or antikinks respectively.
- For a harmonic interaction potential, the dynamics of both defects is equivalent but of opposite velocities when all the parameters are the same. For anharmonic interaction potentials, this symmetry is broken.
- For interstitials (antikinks), the motion is facilitated when the interaction potential becomes narrower.
- For vacancies (kinks), the motion is hindered when the interaction potential narrows. However, for a critical value of the potential width, reversed high-velocity vacancy motion is observed.
- There is a value of the interaction potential width below which there can be found vacancies and interstitials moving in the same direction (moving the former faster). Above this critical value, vacancies and interstials always move in opposite direction.

Acknowledgements and Bibliography

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