We use then, as initial condition, an antikink (or kink) at rest.

Ratchet antikinks (or kinks) are attractors, if an initial condition

There are several types of crystalline defects of different dimension.

The nonlinear dynamics of Schottky defects and Frankel 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 modeled by an empty well of the substrate potential. The dynamics of this structure is described in terms of kinks.

- Intertials 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

where \( a, c, \alpha \), and \( \kappa \) are the damping and coupling constants, respectively. We assume that \( E(\theta) \) is a biharmonic force:

This driving force is asymmetric for almost all values of \( \theta \). 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:

- \( b \) is a measure of the potential width. For \( b = 0 \), 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 kink structures [7, 8]. For instance, in the case of a harmonic interaction potential, for the same set of parameters \((\omega, \kappa, E)\) an antikink and kink dynamics are exactly the same except for their opposite velocities.

- The anharmonicity implies, apart from a change in the profile, 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 antikink motion

An 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 \( \omega \) and \( b \) of the desired solution of the full dissipative lattice.

- In all simulations \( \omega = 0.5 \) and \( \kappa = 1 \) are fixed and periodic boundary conditions are chosen.

- The effect of increasing \( \kappa \) is 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, \( \theta \), \( E_0 \) and \( \omega \).

- An increase of the Peierls-Nabarro barrier can explain the law 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 \( b \).

Effect of the anharmonicity on kink motion

- For fixed \( \omega \), \( E_0 \), and \( \kappa \) 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 \( \theta \).

  2. For \( b > b_c \), kinks can move in the same direction of the antikink with the same value of \( \theta \), and with a much higher velocity than these.

- 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 \( b \) and \( \theta \) (center) and \( \kappa \) (center and right), \( \omega \) and \( \kappa \). Colors mean the following in the last figure (black) directed motion, (red) reversed motion, (white) pinning.

Summary

- We have shown some aspects of the dynamics of vacancy and interstitial defects driven by biharmonic or fields. Vacancy and interstitial defects can be represented by kinks or antikinks respectively.

- For a harmonic interaction potential, the dynamics of both defects is is equivalent but of opposite velocities when all the parameters are the same. For anharmonic interaction potentials, this symmetry is broken.

- For antikink (antikinks), the motion is facilitated when the interaction potential becomes narrower.

- For interstitials, the motion is hindered when the interaction potential narrows. However, for a critical value of the potential width, reversed high velocity kink 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 faster faster). Above this critical value, vacancies and interstitials always move in opposite direction.

Acknowledgements and Bibliography

We have shown some aspects of the dynamics of vacancy and interstitial defects driven by biharmonic or fields. Vacancy and interstitial defects can be represented by kinks or antikinks respectively.

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References


