

Front propagation in bi-stable non-degenerate systems: model dependence and universality

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Summary. Propagation of transition waves in lattices with bi-stable on-site potential is addressed. Inclusion of nearest neighbour cubic coupling drastically affects the dynamics and cannot be considered as small perturbation. Although the full nonlinear model is unsolvable analytically, it possesses features that enable approximate assessment. Strong energy concentration in the front zone and dominance of the nonlinear term allow derivation of an equivalent SDOF model. This leads to correct scaling predictions for the front velocity. The potential's exact shape weakly effects the propagation and the SDOF model can be generalized to arbitrary potentials.

Introduction

In condensed matter, various processes can be described by movement of a defect of some kind. At the microlevel, in the situation when no dissipation is assumed, the lattice waves that are responsible for the removal of the released energy and are known as “radiative damping” [1]. The discrete approach is essential, since it enables to determine the relationship between the velocity of the transition front and the driving force, in contrast to continuum models. The implementation of discrete models with multi-equilibria potential goes back to the early work of Frenkel and Kontorova [2]. Various derivatives of this model are used to describe processes as dislocation in metals, twin boundaries, domain walls in ferro-electrics, fracture and phase transitions. Other applications can be found in the review of Braun and Kivshar [3]. A common configuration that has been adopted in several works is that of a bi-stable on-site potential [4, 1]. Clearly, the case of interest is the one with energetic difference between the minima that dictates the direction of propagation. The linearly coupled chain with a bi-stable on-site potential was studied in several works. The simplest model where both wells have same curvature was proposed in the work of Atkinson and Cabrera [5]. In this case, an analytical solution is obtained through Fourier transform. The technique was further used in several works [6, 1].

Nonlinearly coupled chains remain less explored. A recent study [7] addressed the nonlinear case with on-site dissipation and suggested a law that connected the transported energy with the velocity and dissipation. Current work explores the strongly nonlinear case without assuming on-site dissipation and allows estimation of the phase velocity.

The model and analytical treatment

The idea of the model is adopted from [4, 1] where the problem of a chain with a linear inter-particle interaction and an on-site bi-parabolic potential is addressed. Here we expand this model in two ways. First, we include a cubic nonlinear inter-particle coupling. Second, we don't specify the exact shape of the on-site potential, but only its key characteristics. Hamiltonian of the system is given by Eq. (1).

$$H = \sum_{n=1}^{\infty} \left[1/2 \dot{\varphi}_n^2 + 1/2 (\varphi_{n+1} - \varphi_n)^2 + 1/4 \beta (\varphi_{n+1} - \varphi_n)^4 + U(\varphi_n) \right] \quad (1)$$

φ_n is the displacement of the n^{th} particle from the initial equilibrium state. β is the stiffness of nonlinear nearest-neighbour springs. The shape of the nondegenerate bi-stable on-site potential $U(\varphi)$ is defined by the energetic effect Q , the height of barrier B and the coordinate of the stable state φ^* . See two examples in Figure 1.

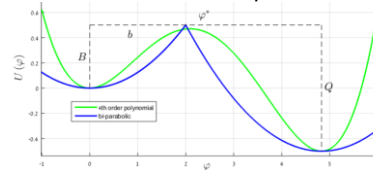


Figure 1 - On-site nondegenerate potential U

A typical dynamical response is shown in Figure 2 in $n - \varphi$ and $t - \varphi$ planes. Unlike in the case with linear coupling where analytical solution is available [1], in the current model the concept of analysis is different as the nonlinearity dramatically changes the physics. First, we examine the distribution of the linear and the nonlinear portions of strain energy along the chain (Figure 3). It is seen that the nonlinear term is dominant in the transition area when compared to the linear coupling and the on-site potential contributions. This leads to the following approximate reformulation:

$$\ddot{\varphi}_i + \beta \left[(\varphi_i - \varphi_{i+1})^3 + (\varphi_i - \varphi_{i-1})^3 \right] \approx 0 \quad i \in \text{transition area} \quad (2)$$

Second, the transitional area is steep and only very few particles participate in the transition simultaneously (see zoom in Figure 2), but sufficient description may be obtained by considering the rapid jump of a single particle from the meta-stable to the stable state. Third, the gradient in the transitional region is steep when compared to adjacent layout within the two wells (see zoom-ins in Figure 2), so this particle can be isolated from the chain. When a particle emerges from the metastable state it is approximately connected to $\varphi \approx 0$ and when it reaches the stable state, it is connected to $\varphi \approx \Delta$ due to low wavenumbers in the tail region (see Figure 2a for notation).

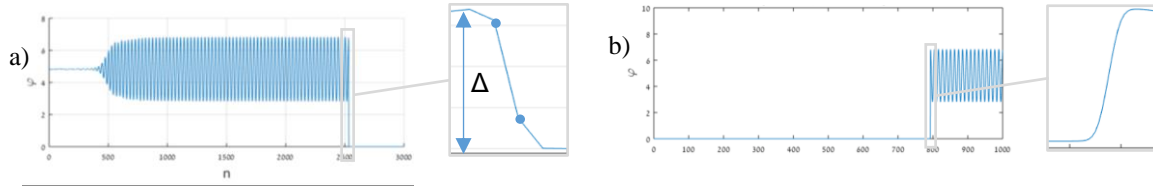


Figure 2 -a) Dynamic response a) $\varphi = \varphi(n)$ at $t = 1000$. b) $\varphi_{2000} = \varphi_{2000}(t)$ for $Q/B = 1, \omega_0 = 0.5, \beta = 0.4$

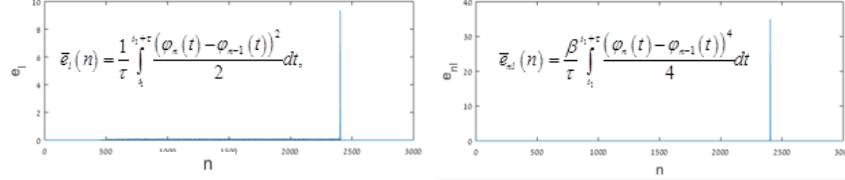


Figure 3 –Interaction energy: a) linear coupling b) nonlinear coupling, for: $Q/B = 1, \omega_0 = 0.5, \beta = 0.4, t = 950$
The resulting single DOF equation is presented in (3):

$$\ddot{\varphi} + \beta \left[\varphi^3 + (\varphi - \Delta)^3 \right] \approx 0 \quad (3)$$

The SDOF equation of motion is integrable and can be solved to obtain the phase velocity:

$$V = \left[t(\varphi = \Delta) - t(\varphi = 0) \right]^{-1} = \left[\sqrt{2} K(\sqrt{2}/4) \right]^{-1} \Delta \sqrt{\beta} \Rightarrow V \sim \Delta \sqrt{\beta} \quad (4)$$

Where $K(\sqrt{2}/4)$ is a complete elliptic integral of the first kind. Numerical and the analytical dependence of phase velocity on β and Δ is presented in Figure 4. A good match to the numerical results is achieved, which asymptotically improves at higher velocities. An error of about 0.285 was found in both comparisons in the constant coefficient.

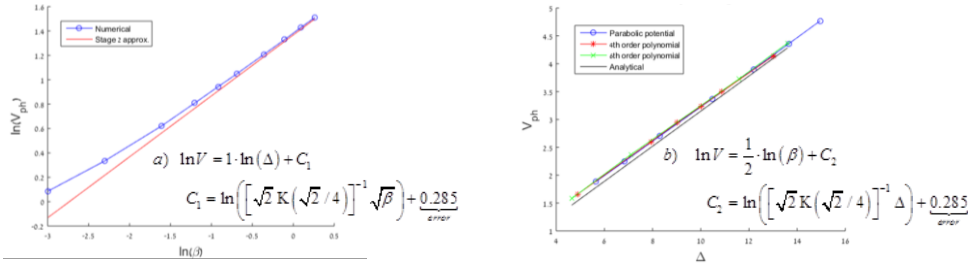


Figure 4 a) $\ln(V_{ph}) = f(\ln(\Delta))$ for $\beta = 0.3, \omega_0 = 0.5$, b) $\ln(V_{ph}) = f(\ln(\beta))$ for $Q/B = 1, \omega_0 = 0.5$

It was assumed that the only characteristics of the on-site potential that affects the velocity is the fixed value Δ which is dictated by the oscillation regime in the tail region. To examine this claim, we compare 3 different potentials: bi-parabolic 4th and 6th order polynomials with same general characteristics (B, Q, φ^*). The comparison in Figure 4b leads to an important conclusion, that the model (4) can be generalized to different potentials.

It was shown that the velocity linearly depends on Δ . It, however, is not always known, for it depends on the specific oscillation regime within the stable well. For a special case of bi-parabolic potential Δ can be analytically evaluated:

$$\Delta \approx \varphi^* + \sqrt{2Q}/\omega_0 \quad (5)$$

Conclusions

Current work examined front propagation in a lattice with an on-site bi-stable potential. It was found that an addition of even a small nonlinearity to the nearest-neighbour interaction led to far supersonic velocities and strong localization of the front. The extremely steep behaviour in the transitional zone allowed reduction of the system to an effective single DOF model. Then, the dominance of the nonlinear term allowed to reduce even more the complexity into an integrable form. This led to a conclusion that the phase velocity is governed by two parameters: nonlinear coupling coefficient and the coordinate of entrance into the stable state. This scaling relationship turned out to be universal for on-site potentials with similar main shape characteristics.

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