Peierls-Nabarro potential for kinks in nonlinear chains

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Abstract. The aim of this work is to review various discrete models supporting topological solitons, in which the Peierls-Nabarro potential can be significantly lowered or even reduced to zero. These theoretical results are discussed in relation to the Peierls stresses for dislocations in a variety of crystals. Derivation of the discrete models free of the Peierls-Nabarro potential has been done by a number of authors with the use of analytical calculations. Peierls stresses for dislocations in crystals described in the literature have been estimated within the framework of molecular dynamics and \textit{ab initio} simulations. These theoretical results are discussed in connection with the variability of the Peierls stress in different crystals.

1. Introduction

Localized nonlinear excitations in the form of topological solitons play an important role in many areas of physics and are very often studied in discrete media [1-5]. For example, in solid state physics, they describe domain walls, dislocations, and crowdions in crystals. In all these applications, the mobility of topological solitons is an important problem, given that the discreteness of the medium destroys the translational invariance of the continuum. In continuum systems topological solitons can move radiating no energy, while in discrete media, typically, static solitons cannot be placed arbitrarily with respect to the lattice because the lattice creates for the solitons a potential energy profile (called Peierls-Nabarro potential) with minima for particular high-symmetry configurations. Motion of the solitons in discrete media is possible only if they get enough energy to leave the minimum of the Peierls-Nabarro potential or, in other words, to overcome this potential.

From a physical point of view, the mobility of topological solitons can be analysed from two different points of view. On the one hand, one can estimate the minimum external force required to set a standing soliton in motion, and, on the other, determine the deceleration rate of a moving soliton in the absence of external forces. In the first case, the mobility is higher when the minimum external force is lower, and in the second case, it is higher when the deceleration rate is smaller.

In the theory of dislocations the mobility of dislocations is estimated by the Peierls stress – the value of shear stress $\tau$ that is needed to overcome the Peierls-Nabarro potential [6]. In a recent study [7], the Peierls stresses have been estimated by a discretized Peierls-Nabarro model for a variety of crystals based on the results of \textit{ab initio} simulations and compared to the experimentally measured values reported in [8]. Remarkably, the Peierls stress can differ noticeably for crystals belonging to the same group. For instance, for copper the ratio $\tau/G$, where $\tau$ is the Peierls stress and $G$ is the shear modulus, is five times smaller than for gold (note that both Cu and Au are metals with fcc lattice). Strength of interatomic bonds in crystals correlates with such parameters as melting temperature and
heat of fusion. Both Cu and Au have very close melting temperatures of 1357 and 1337 K, respectively, and close values of heat of fusion, 13.3 and 12.6 kJ/mol, respectively. A natural question arises: why the height of the Peierls-Nabarro potential for two metals with the same crystal lattice and nearly same interatomic binding energy can be so different?

In order to address this question, we turn to the discussion of the Peierls-Nabarro potential in various nonlinear chains (simplified one-dimensional models of crystals). Note that the Frenkel-Kontorova chain was the first theoretical model used to study dislocations [1,2].

The aim of this article is to demonstrate that discreteness of media not always produces the Peierls-Nabarro potential, which is important for the discussion of dislocation mobility and mechanisms of plastic deformation of metals [24-31].

2. Exceptional discretizations of the $\phi^4$ model

Existence of the integrable lattices [9], where topological solitons propagate freely with any velocity below the speed of sound, suggests that discreteness of media does not exclude mobility of solitons. However, the number of known integrable lattices is very limited. On the other hand, several wide classes of non-integrable discretizations of the Klein-Gordon field have been derived and analyzed, where static kinks do not experience Peierls-Nabarro potential and the kink can be placed anywhere with respect to the lattice [10-23]. The first such model has been derived by Speight and Ward [10-12]. Their model conserves total energy but does not conserve momentum. Then Kevrekidis has derived a new class of models free of the static Peierls-Nabarro potential that conserve momentum but not energy [13]. Rather general approach to derivation of translationally invariant discrete kinks, based on the discretized first integral approach, has been offered in [18,21]. Such discretizations were named as exceptional in the work [18].

Let us give one example of derivation of an exceptional discretization of Klein-Gordon equation based on the discretized first integral approach [21].

The continuum Klein-Gordon model has the Hamiltonian

$$H = \frac{1}{2} \int \left[ \phi_+^2 + \phi_-^2 + 2V(\phi) \right] dx,$$

(1)

where $\phi(x,t)$ is the unknown field and $V(\phi)$ is the given on-site potential. The corresponding equation of motion has the form

$$\phi'' = \phi - V'(\phi) = D(\phi(x,t)).$$

(2)

Equation (2) will be discretized with respect to the variable $x_n=hn$, where $n=0, \pm1, \pm2, \ldots$, and $h>0$ is the lattice spacing. Let us write out the traditional discretization of equation (2),

$$\phi_n = \frac{(1/2)\phi_{n+1} - 2\phi_n + \phi_{n-1}}{h^2} - V'(\phi_n),$$

(3)

in which kinks do experience the Peierls-Nabarro potential. A method for constructing discrete models with kinks free of Peierls-Nabarro potential, based on the use of a discretized first integral, was proposed in [21]. Following this method, consider the first integral of the static Eq. (2), $\phi^2 - V(\phi) + C = 0$, where $C$ is the constant of integration. This first integral can be taken in a modified form

$$u(x) = \phi - \sqrt{2V(\phi) - C} = 0.$$

(4)

Next, we rewrite the Hamiltonian Eq. (1) in terms of $u(x)$,

$$H = \frac{1}{2} \int \left[ \phi_+^2 + \left[u(x)\right]^2 + 2\phi_+\sqrt{2V(\phi) - C} \right] dx.$$

(5)

The first integral Eq. (4) can be discretized as follows

$$u(\phi_n, \phi_{n+1}) = \frac{\phi_n - \phi_{n+1}}{h} - \sqrt{2V(\phi_{n+1}, \phi_n) - C} = 0,$$

(6)

where we assume that in the continuum limit ($h \to 0$) $V(\phi_{n+1}, \phi_n) \to V(\phi)$. Using Eq. (6), we obtain a discrete version of the Hamiltonian of Eq. (1)
\[ H = \frac{1}{2} \sum_n \left\{ \varphi_n^2 + \left[ u(h, \varphi_{n-1}, \varphi_n) \right]^2 \right\} + \frac{2}{h} \left( \varphi_n - \varphi_{n-1} - \sqrt{2V(\varphi_{n-1}, \varphi_n) - C} \right) \]  

If the potential is discretized as suggested in [10], namely,  
\[ \sqrt{2V(\varphi_{n-1}, \varphi_n) - C} = \frac{G(\varphi_n) - G(\varphi_{n-1})}{\varphi_n - \varphi_{n-1}}, \]  
then the second term in curly brackets in Eq. (7) will vanish as a result of telescopic summation. Under these conditions, the Hamiltonian takes the form  
\[ H = \frac{1}{2} \sum_n \left\{ \varphi_n^2 + \left[ u(h, \varphi_{n-1}, \varphi_n) \right]^2 \right\}. \]  
Further, using Eq. (8), we rewrite Eq. (6) in the form  
\[ u(h, \varphi_{n-1}, \varphi_n) = \frac{\varphi_n - \varphi_{n-1}}{h} - \frac{G(\varphi_n) - G(\varphi_{n-1})}{\varphi_n - \varphi_{n-1}}. \]  
Then the equation of motion is written in the form  
\[ \varphi_n = -u(h, \varphi_{n-1}, \varphi_n) \frac{\partial}{\partial \varphi_n} u(h, \varphi_{n-1}, \varphi_n) - u(h, \varphi_n, \varphi_{n+1}) \frac{\partial}{\partial \varphi_n} u(h, \varphi_n, \varphi_{n+1}). \]  
Equilibrium static solutions of this model can be found from the two-point map \( u(h, \varphi_n, \varphi_{n-1}) = 0 \), where the function \( u(h, \varphi_n, \varphi_{n-1}) \) is defined by Eq. (9). Such solutions can be constructed iteratively, starting from any admissible value \( \varphi_{n-1} \) or \( \varphi_n \), and therefore the Peierls-Nabarro potential is absent.

3. Results and discussion

Let us discuss some properties of the kinks in the exceptional discretization Eq. (10) in comparison with the standard discretization Eq. (3) taking as an example the \( \varphi^4 \) model with the on-site potential  
\[ V(\varphi) = \frac{1}{2} (1 - \varphi^2)^2. \]
This is a two-well potential with the minima at \( \phi = \pm 1 \) supporting the kink solution interpolating between these two minima.

Static kink solution for the standard discrete model can be found numerically with the use, for example, of the conjugate gradient method. There exist two static kink solutions, one centered on a lattice site and another one centered on the middle of a bond. One of such configurations has greater energy and it is unstable, while another one has minimal energy and it is stable. Actually difference between energies of these two high-symmetry states defines the height of the Peierls-Nabarro potential.

Exact static kink solution for the exceptional discretization, as mentioned above, can be found iteratively from the two-point map \( u(h, \phi_n, \phi_{n-1}) = 0 \), where the function \( u(h, \phi_n, \phi_{n-1}) \) is defined by Eq. (9), starting from any admissible value \(-1 < \phi_n < 1 \) or \(-1 < \phi_{n-1} < 1 \). The fact that the initial value of \( \phi_n \) can be chosen arbitrarily implies that the static kink can be placed arbitrarily with respect to the lattice, and all such configurations have precisely the same energy.

Most of the modes are the extended phonon modes with frequencies belonging to the spectrum of vacuum solution \( \phi = \pm 1 \). A few modes have frequencies below the phonon band, those are the modes localized on the kink.

In figure 1, panels at left, for the standard discretization Eq. (3) with the discreteness parameter \( h = 0.8 \), we present (a) the profiles of the static on-site and inter-site kinks, (b,c) the two eigenmodes localized on the kink and (d) the eigenfrequencies as the functions of the discreteness parameter \( h \). The eigenmodes form the phonon band with the borders shown by the black solid lines, with the additional frequencies of the modes localized on the kink. Results for the on-site (inter-site) kink are shown by dots (circles). In figure 2, panels at right, the same is given for the exceptional discretization Eq. (10).

Comparison of the left and right panels of figure 1 reveals the difference between the standard and exceptional discretizations of the \( \phi^4 \) field. The kink profiles [panels (a)] and the eigenmodes in the two models [panels (b) and (c)] are very similar. On the other hand, vibrational spectrums of the two models differ noticeably. In figure 1, left panels, the width of the phonon band decreases monotonically with increasing degree of discreteness \( h \). In figure 2, right panels, the upper and lower edges of the phonon band cross at \( h = 1 \). For this particular value of \( h \) the model becomes purely anharmonic. The most important difference is the variation with \( h \) of the lowest frequency mode \( \omega_1 \). In figure 1(d), left panels, one can see that for \( h < 0.5 \) frequency of the mode \( \omega_1 \) is nearly zero. For larger values of \( h \) the frequency of the stable inter-site kink configuration increases with \( h \) while frequency of the unstable on-site configuration becomes imaginary (\( \omega^2 < 0 \)).

In figure 2(d), right panels, frequency of the \( \omega_1 \) mode for both on-site and inter-site kinks is precisely zero for any \( h \). Actually, it is zero not only for the two symmetric but also for any asymmetric kink configuration. This reflects the absence of the Peierls-Nabarro potential in the exceptionally discretized model.

The difference in the behavior of the kinks in the standard and exceptional discretizations can be revealed by applying external force \( f \). The results of numerical simulation of the kink dynamics under external force \( f \) are presented in figure 2 (a,b) for the standard discretization Eq. (3) and in (c) for the exceptional discretization Eq. (10).

In the case of standard discretization, inter-site kink is initially at rest and at \( t = 0 \) the external force starts to grow with time linearly, as shown in (a). In (b), the kink kinetic energy is given as the function of time. It can be seen that before the force \( f \) reaches certain value, the kink is at rest since it is trapped by the Peierls-Nabarro potential. For \( h = 0.7 \) the depth of the Peierls-Nabarro potential is smaller than in the case of \( h = 0.8 \), that if why, in the latter case the kink starts to move at a greater value of the external force.

In the case of exceptional discretization at \( t = 0 \) constant in time force \( f \) is turned on. Three values of the force are considered, \( f = 10^{-5}, 10^{-4} \) and \( 10^{-3} \). Kink kinetic energy as the function of time is shown in figure 2(c). It can be seen that the kink starts to move immediately after the force is turned on even though the values of the external force are very small as compared to the force applied to the kink in the standard discrete model, see figure 2(a). Note that the dotted line in figure 2(c) shows the slope
equal to 2 (log-log scale is used here). Kink kinetic energy increases quadratically in time, which means that the kinks under constant external force demonstrate uniformly accelerated motion.

Figure 2. (a,b) Results for the standard discretization of the $\varphi^4$ field Eq. (3). (c) Results for the exceptional discretization Eq. (10). (a) External force as a function of time. (b) Kink kinetic energy as the function of time. Results for $h=0.7$ (blue solid line) and $h=0.8$ (red dashed line). (c) Kink kinetic energy as a function of time for constant in time external force $f$, as specified for each curve. The discreteness parameter is $h=0.7$ (blue solid line) and $h=0.8$ (red dashed line). The dotted line shows the slope equal to 2.

4. Conclusions

Theoretical models presented in Section 2 suggest that the discreteness of media does not necessarily produce a Peierls-Nabarro potential for topological solitons. Several wide classes of non-integrable discretizations of the Klein-Gordon field have been offered [10-23] in addition to a few integrable ones [9]. In such exceptional discretizations kinks are accelerated by any small external force. In terms of the dislocation theory, the Peierls stress is exactly zero for kinks in such models. The reason for vanishing of the Peierls-Nabarro potential in exceptionally discrete models is the many-body interactions. Indeed, in the classical discrete model Eq. (3), the particles interact via pairwise bonds, while in the discretization Eq. (10), one has three-body interactions.

Our main conclusion in the light of the theoretical results reviewed here is that in a discrete media with many-body interactions Peierls-Nabarro potential can be small, and indeed, the Peierls stress can differ noticeably for similar crystals [7,8]. This conclusion can be of interest in the theory of dislocations.

A final note is that discrete breathers and other localized phenomena can also experience the Peierls-Nabarro potential [32-40].

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