Non-symmetric kinks in Klein-Gordon chains free of the Peierls-Nabarro potential

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Abstract. There exist several approaches to discretize Klein-Gordon field equations in a way that static kink solutions can be obtained from a two-point map, iteratively, starting from any admissible initial value. Such kinks can be placed anywhere with respect to the lattice, in other words, they do not experience the Peierls-Nabarro potential (PNP). So far, to the best of our knowledge, only symmetric PNP-free kinks have been analyzed for the \( \phi^4 \) and sine-Gordon equations. It is interesting to construct PNP-free discretisations for the \( \phi^6 \) equation supporting asymmetric kinks. In the present study, two versions of such discretisations are derived.

1. Introduction

Discrete Klein-Gordon equations supporting kinks free of the Peierls-Nabarro potential (PNP) have been considered in a number of studies [1-9]. Such discretizations are interesting for a number of reasons. One of them is the mobility of such kinks, possessing the zero-frequency Goldstone mode, even in the regime of strong discreteness. So far, only symmetric \( \phi^4 \) and sine-Gordon kinks have been analyzed. Recently, kinks in the continuum \( \phi^6 \), \( \phi^8 \), \( \phi^{10} \) and \( \phi^{12} \) models have been studied [10-13]. It is tempting to derive PNP-free discrete analogues of such fields, and in the present study we do this for the \( \phi^6 \) case.

With the use of the discretized first integral approach [9], we derive the Hamiltonian PNP-free discrete version of the \( \phi^6 \) equation, which is essentially the Klein-Gordon model proposed by Speight and Ward [1]. Then we obtain the momentum-conserving PNP-free discrete \( \phi^6 \) model suggested in [2].

Kink solutions of the discrete Klein-Gordon models find their applications, e.g., in the solid state physics, describing the dynamics and interaction of dislocations, dislocation kinks and jogs, domain walls, crowdions, crowdion clusters [14-17], etc. Kink mobility is a crucial issue in all such applications.

2. \( \phi^6 \) field

We consider the Hamiltonian of the \( \phi^6 \) field,

\[
H = E_K + E_P,
\]

with kinetic and potential energies given by
\[ E_K = \frac{1}{2} \int_{-\infty}^{\infty} \phi^2 \, dx, \]

and
\[ E_p = \frac{1}{2} \int_{-\infty}^{\infty} \left[ \phi_x^2 + \frac{k}{4} \phi^2 (1 - \phi^2)^2 \right] \, dx, \]

respectively. Here \( \phi(x,t) \) is the unknown function of spatial, \( x \), and temporal, \( t \), variables. The last term in (3) gives the energy of the six-order on-site potential, which we denote as
\[ V(\phi) = k \phi^2 (1 - \phi^2)^2 / 8. \] (4)

From the Hamiltonian (1)-(3) the following equation of motion can be derived
\[ \phi_{tt} = \phi_{xx} - V'(\phi) = \phi_{xx} - k \phi (1 - 4 \phi^2 + 3 \phi^4) / 4 \equiv D(\phi(x,t)). \] (5)

In the following we will discretize the equation of motion (5) on the lattice \( x = nh \), where \( n = 0, \pm 1, \pm 2, \ldots \), and \( h \) is the lattice spacing. The general form of the constructed discrete models will be as follows
\[ \ddot{\phi}_n = \Delta_2 \phi_n + F(\phi_{n-1}, \phi_n, \phi_{n+1}) \equiv D(h, \phi_{n-1}, \phi_n, \phi_{n+1}), \] (6)

where
\[ \Delta_2 \phi_n = \left( \frac{1}{h^2} \right) (\phi_{n-1} - 2 \phi_n + \phi_{n+1}), \] (7)

and, in the continuum limit \( (h \to 0) \),
\[ F(\phi_{n-1}, \phi_n, \phi_{n+1}) \to k \phi (1 - 4 \phi^2 + 3 \phi^4) / 4. \] (8)

Note that the standard discretization reads
\[ \phi_n = \Delta_2 \phi_n + k \phi_n (1 - 4 \phi_n^2 + 3 \phi_n^4) / 4, \] (9)

but in this model kinks typically have only two possible equilibrium center positions with respect to the lattice, one of them being stable and another one unstable.

PNP-free discretisations can be derived with the help of the first integral of the static version of (6), taken with zero integration constant \( (C = 0) \), which can be written either as
\[ u(x) = \phi_n^2 - k \phi (1 - \phi^2) / 2 = 0, \] (10)

or as
\[ u(x) = \pm \phi_n - \sqrt{k \phi (1 - \phi^2) / 2} = 0. \] (11)

2.1. Discretization conserving energy

We consider a discrete version of the first integral (11) in the form
\[ u(h, \phi_{n-1}, \phi_n) = \frac{\phi_n - \phi_{n-1}}{h} - \frac{\sqrt{E}}{2} \phi_{n-1} \phi_n \left( 1 - \phi_{n-1}^2 \phi_n + \phi_n^2 \right) = 0. \] (12)

The Hamiltonian (1)-(3) can be discretized as follows
\[ \mathcal{H} = \frac{h}{2} \Sigma_n (\dot{\phi}_n^2 + u^2), \] (13)

from which the following discrete equations of motion can be derived,
\[ \dot{\phi}_n = -u(\phi_{n-1}, \phi_n) \frac{\partial}{\partial \phi_n} u(\phi_{n-1}, \phi_n) - u(\phi_n, \phi_{n+1}) \frac{\partial}{\partial \phi_n} u(\phi_n, \phi_{n+1}). \] (14)

Substituting (12) into (14) one obtains the equations of motion of the discrete \( \phi^6 \) model conserving energy (13),
\[ \ddot{\phi}_n = \Delta_2 \phi_n + \sqrt{E} \left[ \phi_{n-1}^3 - \phi_n^3 + 3 \phi_n^2 (\phi_{n-1} - \phi_n) \right] + \frac{k}{12} \left[ -2 (\phi_{n-1}^5 + \phi_{n+1}^5) - 8 \phi_n (\phi_{n-1}^4 + \phi_{n+1}^4) + (9 - 15 \phi_n^2) (\phi_{n-1}^3 + \phi_{n+1}^3) + (24 \phi_n - 16 \phi_n^3 (\phi_{n-1}^2 + \phi_{n+1}^2) + (27 \phi_n^4 - 10 \phi_n^4 + 9) (\phi_{n-1} + \phi_n) - 6 \phi_n^5 + 24 \phi_n^3 - 18 \phi_n. \] (15)

From the construction, it is clear that static solutions of (15) can be found from (12), which is the cubic two-point map. Since in the discretized first integral (11) the integration constant was set to be zero, only kink solution can be found from (12). For this, one can take any initial value of the two-point map in the range \( 0 < \phi_n < 1 \) and find iteratively the equilibrium kink solution. The arbitrariness of the choice of the initial value means that the static equilibrium kink can be placed anywhere with respect to the lattice, meaning that the PNP is zero for the kink.
2.2. Discretization conserving momentum

Now we consider the first integral in the form of (10) and discretise it as follows,

\[ U(h, \phi_{n-1}, \phi_n) = \frac{(\phi_n - \phi_{n-1})^2}{h^2} - \frac{k}{4} \phi_{n-1} \phi_n (1 - \phi_{n-1} \phi_n)^2 = 0. \]  

(16)

The equation of motion (5) then can be discretized as follows, in the spirit of [2],

\[ \dot{\phi}_n = \frac{U(h, \phi_n, \phi_{n+1}) - U(h, \phi_{n-1}, \phi_n)}{\phi_{n+1} - \phi_{n-1}}. \]  

(17)

Substituting (16) into (17) one finds the discrete \( \phi^d \) model of the form

\[ \dot{\phi}_n^d = \Delta \phi_n - \frac{k}{4} [\phi_n - 2\phi_n^2 + \phi_n^3 + \phi_{n+1}^2 + \phi_{n-1}^2]. \]  

(18)

This model can be written as a conservation law:

\[ \frac{d}{dt} \left[ \phi_n (\phi_{n+1} - \phi_{n-1}) \right] = J(h, \phi_n, \phi_{n+1}, \phi_{n-1}, \phi_{n+1}' - \phi_{n-1}', \phi_n'), \]  

(19)

where

\[ J(h, \phi_n, \phi_{n+1}, \phi_n', \phi_{n+1}') = U(h, \phi_n, \phi_{n+1}) + \phi_n \phi_{n+1}' - \phi_{n+1} \phi_n', \]  

(20)

and consequently, as a result of direct summation, conserves the linear momentum [2],

\[ P = \sum_n \phi_n^d (\phi_{n+1} - \phi_{n-1}). \]  

(21)

Again, it is clear from the construction that static solutions of (18) can be found from the cubic two-point map (16). The integration constant in the discretized first integral (10) was set to be zero, so that only kink solution can be found from (16). Equilibrium kink solutions are found from the two-point map, iteratively, starting from any initial value in the range 0<\( \phi_k <1 \). Such kinks do not experience PNP, since they can be placed anywhere with respect to the lattice.

3. Numerical results

In figure 1, profiles of static kinks are plotted for the energy-conserving model (15) (open dots) and the momentum-conserving model (18) (filled dots). The case of \( k=2 \) is considered. Kink solutions were obtained for these models from the cubic two-point maps (12) and (17), respectively, using \( \phi_0=0.5 \) as the initial value. The results for the discreteness parameter \( h=0.5, 1.0, 2.0, \) and \( 3.0 \) are shown in (a)-(d), respectively. The asymmetry of the kinks with respect to the central point can be clearly seen. For large \( h \), the kink profiles in the two models are noticeably different, and they become closer to each other for smaller \( h \), because both models have the same continuum limit. Note the asymmetry with respect to the central point in the discrete \( \phi \) kink profile.
4. Conclusions

Two discrete $\phi^6$ models, supporting asymmetric kinks free of PNP were derived, one of them, (15), conserves energy (13) and the other one, (18), conserves momentum (21).

The obtained results demonstrate that, in principle, discrete kinks can be highly mobile in that sense that they can be accelerated by any weak external force. Discrete kinks (or domain walls [18]) play an important role in nanomaterials transporting mass, energy, momentum, or/and electric charge, depending on the application.

As a continuation of this work, one can study collisions between slowly moving kinks boosted with the use of the zero-frequency Goldstone mode. It is also important to study the effect of the discreteness parameter $\hbar$ on the linear phonon spectra of the two vacuums, $\phi_n=0$ and $\phi_n=\pm 1$, and on the existence and frequencies of the kink’s internal modes. It would be also interesting to analyze the interaction of moving kinks with PT-symmetric perturbations similar to what was done for the continuum case [19,20].

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