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Discrete Klein–Gordon models with static kinks free of the Peierls–Nabarro potential

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Abstract

For the nonlinear Klein–Gordon type models, we describe a general method of discretization in which the static kink can be placed anywhere with respect to the lattice. These discrete models are, therefore, free of the Peierls–Nabarro potential. Previously reported models of this type are shown to belong to a wider class of models derived by means of the proposed method. A relevant physical consequence of our findings is the existence of a wide class of discrete Klein–Gordon models where slow kinks *practically* do not experience the action of the Peierls–Nabarro potential. Such kinks are not trapped by the lattice and they can be accelerated by even weak external fields.

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1. Introduction

Discrete solitons and more specifically kink-like topological excitations are ubiquitous structures that arise in numerous physical applications ranging from dislocations or ferroelectric domain walls in solids, to bubbles in DNA, or magnetic chains and Josephson junctions, among others (see, e.g., [1] for a recent exposition of relevant applications). The mobility of such lattice kinks is one of the key issues in many of these applications, especially since the pioneering works of [2, 3] which illustrated that the kinematics on the lattice is dramatically different from the continuum analogue of such equations where constant speed propagation is typical. Instead, on the discrete substrate, kinks need to overcome the so-called Peierls–Nabarro potential (PNp), constantly radiating their energy and being eventually trapped by the lattice. The PNp refers to the energy difference between a stable inter-site centred discrete kink and an unstable, onsite centred discrete kink. Clearly, as a kink is travelling from one site to the next, it 'wobbles' over this potential energy landscape [4]. However, even though clearly travelling is intimately connected with overcoming the static PNp without 'radiating' energy [5], this connection is relatively subtle and the inter-dependence of these two features (static PNp and travelling) still remains elusive [6]. Typically, discrete kinks travelling with finite velocity have only been obtained for a discrete set of velocities [7] which makes the motion unstable with respect to perturbations. There exists a class of more exotic exact solutions (the so-called 'nanoptera') where the kink propagates together with a plane wave having the same velocity [7].

While the travelling problem is extremely interesting in its own right, in the present work, we will start by examining the construction of discrete models with PNp-free kinks, using a simplified (quasi)static approach. Two classes of discrete models where a static kink can be placed anywhere with respect to the lattice have been previously derived: one conserving energy [8] and another one conserving momentum [9]. In both cases, the static kink solution can be obtained from a two-site nonlinear map. In the present paper we demonstrate that, in general, a discrete version of the first integral of the static continuum Klein–Gordon field plays the role of this nonlinear map. Thus, we derive a wide class of such models including the two above-mentioned classes as special cases. The advantage of this approach is that the kinks are no longer (typically) trapped by the lattice. Instead, they can be accelerated by even weak external fields. This means that in the absence of a potential barrier, the energetic 'tilt' lent to the coherent structure by a very weak external field may result in the moving solutions observed (only for a super-critical field) in [10]. However, a note of caution should be added here. While one might naively expect that such solutions would be intimately connected with slow travelling, it has been demonstrated numerically that travelling solutions (when they can be found as e.g. in [7, 11] for Klein–Gordon lattices, using the methods of [12]) have a sharp lower bound in their wave speed [13]. The existence of such a threshold illustrates the fact that one should be particularly careful in trying to infer features of the travelling problem from such 'static' considerations. On the other hand, as the recent work of Barashenkov, Oxtoby and Pelinovsky demonstrates [14], discretizations without PNp are much more natural candidates for possessing travelling solutions for isolated wave speeds (not close to zero).

The presentation of our results will be structured as follows. Section 2 will contain the setup and notations used for the Klein–Gordon models. Section 3 will present the general methodology for obtaining static PNp-free discretizations. Section 4 will illustrate the connection to previously reported models. Section 5 will focus on the special case example of the ϕ^4 model, for which our numerical observations will be presented in section 6. Finally in section 7, we will summarize our findings and present our conclusions.

2. Setup

We consider the Lagrangian of the Klein–Gordon field,

$$L = \int_{-\infty}^{\infty} \left[\frac{1}{2}\phi_t^2 - \frac{1}{2}\phi_x^2 - V(\phi) \right] \mathrm{d}x, \tag{1}$$

and the corresponding equation of motion,

$$\phi_{tt} = \phi_{xx} - V'(\phi) \equiv D(x). \tag{2}$$

Topological solitons (kinks) are possible only if $V(\phi)$ has at least two minima ϕ_{01} and ϕ_{02}, where $V'(\phi_{0i}) = 0$ and $V''(\phi_{0i}) > 0$. Obviously, $\phi = \phi_{01}$ and $\phi = \phi_{02}$ are the stationary solutions to equation (2). We will study the properties of kinks that interpolate between these two stationary solutions.

Equation (2) will be discretized on the lattice $x = nh$, where $n = 0, \pm 1, \pm 2 \ldots$, and h is the lattice spacing.

For brevity, when possible, we will use the notations

$$\phi_{n-1} \equiv l, \qquad \phi_n \equiv m, \qquad \phi_{n+1} \equiv r. \tag{3}$$

We would like to construct a nearest-neighbour discrete analogue to equation (2) of the form

$$\ddot{m} = D(C, l, m, r), \tag{4}$$

where $C > 0$ is a parameter related to the lattice spacing h as $C = 1/h^2$, such that in the continuum limit ($C \to \infty$), $D(C, l, m, r) \to D(x) = \phi_{xx} - V'(\phi)$.

Note that in this context, the 'standard' discretization emerges in the form: $D(C, l, m, r) = C(l - 2m + r) - V'(m)$. Generalizations of this model will be discussed in the form

$$\ddot{m} = C(l - 2m + r) - B(l, m, r), \tag{5}$$

where $B(l, m, r)$ has $V'(\phi)$ as the continuum limit.

We will characterize a model as PNp-free if a *static* kink can be placed anywhere with respect to the lattice (continuum, rather than discrete, set of equilibrium solutions). This is equivalent to demanding that the kink must have an neutral direction, or (from Noether's theory [15]) a Goldstone translational mode. It is natural to categorize this definition of PNp-free model as 'static' or 'quasi-static', in the sense that it does not involve the kinematic or dynamical properties of the model.

In this paper, we aim to construct the models PNp-free in the static sense as a first (yet non-trivial) step towards understanding the nature of the discrete travelling problem (see also the comments above).

We will also focus on the existence of physically motivated conserved quantities for the derived models. Hamiltonian models are energy-conserving models and the models with $\mathrm{d}M/\mathrm{d}t = 0$, where

$$M = \sum_{n=-\infty}^{\infty} \dot{\phi}_n(\phi_{n+1} - \phi_{n-1}), \tag{6}$$

will be called momentum-conserving models. As was shown in [9], the discrete model of equation (4) conserves the momentum of equation (6), if it can be presented in the form

$$\ddot{m} = \frac{\mathcal{H}(m, r) - \mathcal{H}(l, m)}{r - l}. \tag{7}$$

This can be verified by calculating

$$\frac{\mathrm{d}M}{\mathrm{d}t} = \sum_n \ddot{\phi}_n(\phi_{n+1} - \phi_{n-1}) = \sum_n [\mathcal{H}(\phi_n, \phi_{n+1}) - \mathcal{H}(\phi_{n-1}, \phi_n)] = 0, \tag{8}$$

where we have used the fact that the terms $\dot{\phi}_n(\dot{\phi}_{n+1} - \dot{\phi}_{n-1})$ cancel out due to telescopic summation.

3. Static PNp-free discretization

Our aim here will be to discretize equation (2) in a symmetric way, so that the static kink solution can be found from a reduced first-order difference equation. According to [8], if we achieve that, then we are going to have a one-parameter family of solutions with the possibility of placing equilibrium kinks anywhere with respect to the lattice (and hence, PNp-free in the static sense).

The first integral of the steady-state problem in equation (2), $\phi_x - \sqrt{2V(\phi)} = 0$ (with zero integration constant), can be written in the form

$$w(x) \equiv p[g(\phi_x) - g(\sqrt{2V(\phi)})] = 0, \tag{9}$$

where p and g are continuous functions and $p(0) = 0$.

Our plan will then be the following:

- Discretize the first-order differential equation of equation (9) using a first-order difference scheme $w(l, m) = 0$.
- Then express the right-hand side of equation (2) as a sum of terms containing derivatives, e.g., $\mathrm{d}w/\mathrm{d}x$, $\mathrm{d}w/\mathrm{d}\phi$, etc.
- As a result, discretizations of such terms, e.g., $\mathrm{d}w/\mathrm{d}x \sim \sqrt{C}[w(m, r) - w(l, m)]$, vanish for $w(l, m) = 0$ (or otherwise stated: the construction of the equilibrium solution is converted to a first-order difference problem). Then, the static kink solutions (PNp-free, by construction) for the obtained discrete model can be found from this two-site problem.

In the following, we will consider a particular case of equation (9) with $p(\zeta) = \zeta$ and $g(\xi) = \xi^2$, for which we introduce the notation

$$u(x) \equiv \phi_x^2 - 2V(\phi) = 0, \tag{10}$$

and the following two-site discrete analogue

$$u(l, m) \equiv C(m - l)^2 - 2V(l, m) = 0. \tag{11}$$

We will also use the short-hand notations,

$$u_l = u(l, m), \qquad u_m = u(m, r). \tag{12}$$

We have assumed that the Klein–Gordon field supports kink solutions. Then, at least for the case of weak discreteness, equation (11) also supports static kinks because it is nothing but a discretization of the first integral of static version of equation (2) (see also [8]).

The next step is then to find a discretization of the right-hand side of equation (2), $D(x)$, which vanishes when equation (11) is fulfilled.

One simple possibility comes from the following finite difference:

$$D_1(l, m, r) \equiv \frac{u_m - u_l}{r - l} \rightarrow \frac{1}{2}\frac{\mathrm{d}u}{\mathrm{d}\phi} = D(x). \tag{13}$$

One can also consider, more generally, continuous functions $q(u, h)$ such that $q(0, h) = 0$ and, in the continuum limit, $q(u, 0) = u$ and $\frac{\mathrm{d}q}{\mathrm{d}u}(u, 0) = 1$. For example, one can take $q = (\mathrm{e}^{hu} - 1)/h$ or $q = u + \sum_{n>1} A_n h^{n-1} u^n$ with constant A_n, etc. Then,

$$\frac{1}{2}\frac{\mathrm{d}q}{\mathrm{d}\phi}\left(\frac{\mathrm{d}q}{\mathrm{d}u}\right)^{-1} = D(x). \tag{14}$$

Discretizing the left-hand side of equation (14) we obtain

$$D_2 = \frac{1}{2}\frac{q(u_m, h) - q(u_l, h)}{r - l}\left[\frac{1}{q'(u_l)} + \frac{1}{q'(u_m)}\right]. \tag{15}$$

Inspired by [8], we note that, in the continuum limit,

$$\frac{v(m, r)}{r - m} - \frac{v(l, m)}{m - l} \rightarrow \frac{\mathrm{d}v}{\mathrm{d}\phi} - v\frac{\phi_{xx}}{\phi_x^2}, \tag{16}$$

and find

$$\begin{aligned} D_3 &\equiv \frac{u_m}{r - m} - \frac{u_l}{m - l} + \sqrt{2V(l, m, r)}\left(\frac{\sqrt{C(r - m)^2 - u_m}}{r - m} - \frac{\sqrt{C(m - l)^2 - u_l}}{m - l}\right) \\ &\rightarrow \frac{\mathrm{d}u}{\mathrm{d}\phi} - u\frac{\phi_{xx}}{\phi_x^2} + \sqrt{2V}\left(\frac{\mathrm{d}\sqrt{2V}}{\mathrm{d}\phi} - \sqrt{2V}\frac{\phi_{xx}}{\phi_x^2}\right) \\ &= D(x). \end{aligned} \tag{17}$$

Since the expressions for $D_i(l, m, r)$ given by equations (13), (15) and (17) tend to $D(x)$ in the continuum limit, one can write the following discrete analogue to the Klein–Gordon equation (2)

$$\ddot{m} = \sum_i b_i D_i(l, m, r), \qquad \text{where} \quad \sum_i b_i = 1. \tag{18}$$

Then, by construction, any structure derived from the two-site problem of equation (11) is a static solution of equation (18) and hence, the latter is the static PNp-free discrete model.

The model of equation (18) can be generalized in a number of ways. For example, equation (17) can be modified choosing different functions $V(l, m, r)$ to discretize $V(\phi)$. Then, the modified $\tilde{D}_3$ can be added to the linear combination on the right-hand side of equation (18).

The model of equation (18) can also be generalized by appending terms which disappear in the continuum limit and ones that vanish upon substituting $u_l = 0$ and $u_m = 0$. For example, the derivative $\mathrm{d}f(u)/\mathrm{d}\phi$ can be discretized as $2[f(u_m) - f(u_l)]/(r - l)$ or as $2f'(u_l/2 + u_m/2)(u_m - u_l)/(r - l)$. If we have a difference of such terms in the equation of motion, then in the continuum limit they will cancel out.

Any term on the right-hand side of equation (18) can be further modified by multiplying by a continuous function $e(C, l, m, r)$, whose continuum limit is unity (see e.g. [16] for such an example, also discussed in more detail below).

Generally speaking, the discrete PNp-free Klein–Gordon models derived here do not conserve either an energy, or a momentum-like quantity. However, as will be demonstrated below, they contain energy-conserving and momentum-conserving subclasses.

4. Connection with previously reported models

One energy-conserving PNp-free Klein–Gordon model has been derived by Speight with co-workers [8] with the use of the Bogomol'nyi argument [17]. Their model can be written in the form of equation (2), with the Lagrangian

$$L = \frac{1}{2}\sum_n \dot{\phi}_n^2 - \frac{C}{2}\sum_n (\phi_n - \phi_{n-1})^2 - \sum_n \left(\frac{G(\phi_n) - G(\phi_{n-1})}{\phi_n - \phi_{n-1}}\right)^2, \quad \text{where} \quad G'(\phi) = \sqrt{V(\phi)}. \tag{19}$$

The static kink solution can then be derived from the lattice Bogomol'nyi equation [8], which can be taken in the form

$$U(l, m) = C(m - l)^2 - 2\left(\frac{G(m) - G(l)}{m - l}\right)^2 = 0, \tag{20}$$

which is a particular case of equation (11). The equation of motion derived from equation (19), written in terms of equation (20), is

$$\ddot{m} = \frac{U_m}{r - m} - \frac{U_l}{m - l} + \sqrt{2V(m)}\left(\frac{\sqrt{C(r - m)^2 - U_m}}{r - m} - \frac{\sqrt{C(m - l)^2 - U_l}}{m - l}\right). \tag{21}$$

The right-hand side of equation (21) is a particular case of $D_3(l, m, r)$ given by equation (17) with $V(l, m, r) = V(m)$.

Momentum-conserving PNp-free models were proposed in [9] and further studied in [18]. They are the non-Hamiltonian models of the form

$$\ddot{m} = D_1(l, m, r), \tag{22}$$

where D_1 is given by equation (13). Note that equation (22) can be mapped into the formulation of equation (7). Static kink solutions in this model can be found from equation (11).

If equation (11) is taken in the particular form of equation (20), then the momentum-conserving PNp-free model equation, (22), and the energy-conserving PNp-free model equation, (21), have exactly the same static kink solutions. It has been proved that a standard nearest-neighbour discrete Klein–Gordon model, conserving both an energy and the momentum of equation (6), does not exist [18].

5. Application to the ϕ^4 model

As an example, we will discretize the well-known ϕ^4 field theory with the potential

$$V(\phi) = \tfrac{1}{4}(1-\phi^2)^2. \tag{23}$$

By construction, the PNp-free models derived above are written in singular form. In this form, the equations are inconvenient in practical simulations and one may wish to find such particular cases when singularities disappear.

For example, for the energy-conserving PNp-free model expressed by equations (19)–(21), singularity always disappears when $G(\phi)$ is polynomial [8]. Particularly, for the ϕ^4 model with the potential equation (23), one obtains from equation (21) the following energy-conserving PNp-free discretization derived in [8]

$$\ddot{m} = \left(C+\tfrac{1}{6}\right)(l+r-2m) + m - \tfrac{1}{18}[2m^3 + (m+l)^3 + (m+r)^3], \tag{24}$$

whose static kink solution can be found from equation (20), which, for the ϕ^4 potential, obtains the form

$$3\sqrt{2C}(m-l) + m^2 + lm + l^2 - 3 = 0. \tag{25}$$

Now let us turn to the momentum-conserving model. Substituting equation (11) into equation (22) we obtain

$$\ddot{m} = C(r-2m+l) - 2\frac{V(m,r)-V(l,m)}{r-l}. \tag{26}$$

To remove the singularity, $V(l,m)$ should be taken in the symmetric form $V(l,m) = V(m,l)$, e.g., as

$$\begin{aligned} V(l,m) = {} & (1/4) - (\alpha/2)(m^2+l^2) + (\alpha - 1/2)ml + (\beta/2)(m^3+l^3) - (\beta/2)ml(m+l) \\ & + (\gamma/2)(m^4+l^4) + (\delta/2)ml(m^2+l^2) - (\gamma+\delta-1/4)m^2l^2, \end{aligned} \tag{27}$$

with free parameters α, β, γ and δ. In the continuum limit, when $l \to m$ and $r \to m$, equation (27) reduces to $V(\phi)$. Substituting equation (27) into equation (26), we obtain the following momentum-conserving PNp-free ϕ^4 model derived in [18]

$$\begin{aligned} \ddot{m} = {} & (C+\alpha)(l-2m+r) + m - \beta(l^2+lr+r^2) + \beta m(l+r+m) - \gamma(l^3+r^3+l^2r+lr^2) \\ & - \delta m(l^2+m^2+r^2+lr) + (2\gamma+2\delta-1/2)m^2(l+r). \end{aligned} \tag{28}$$

The momentum-conserving model equation (28) with $\alpha = \beta = \gamma = \delta = 0$ can be written in the form

$$\ddot{m} = \left(1 - \frac{m^2}{2C}\right)C(l-2m+r) + m - m^3. \tag{29}$$

The following energy-conserving model, studied in [16],

$$\ddot{m} = C(l - 2m + r) + \frac{m - m^3}{1 - m^2/(2C)}, \tag{30}$$

has the same continuum limit as model equation (29). Furthermore, it can be derived from equation (29) by multiplication with a factor $e(C, l, m, r) = 1/(1 - m^2/(2C))$, which possesses a unit continuum limit. The model equation (29) is PNp-free and thus, model equation (30) is also PNp-free since they have the same static solutions derivable from $C(m - l)^2 - (1 - ml)^2/2 = 0$. Thus, we have another example when energy-conserving and momentum-conserving PNp-free models have exactly the same static kink solutions.

It is interesting to note that the energy-conserving model of equation (30) cannot be constructed by the method reported in [8], where discretization of the anharmonic term always involves ϕ_{n-1} and ϕ_{n+1}. More generally than it is done in [8], the problem of finding the energy-conserving PNp-free models can be formulated as follows. We need to discretize the potential energy of the Lagrangian equation (1) in a way that the corresponding equation of static equilibrium is satisfied when a two-point discretization of equation (9) is satisfied. Both energy-conserving models discussed above are the solutions of this problem.

As an example of a model conserving neither energy nor momentum we take equation (15) for the case of $q(u, h) = u + Ahu^2$ with constant A and obtain

$$\ddot{m} = \frac{u_m - u_l}{r - l} \frac{(1 + Ahu_l + Ahu_m)^2}{(1 + 2Ahu_l)(1 + 2Ahu_m)}. \tag{31}$$

This model can be obtained from the momentum-conserving model defined by equation (13) by multiplying by another function that reduces to unity in the continuum limit ($h \to 0$). Obviously, model equation (31) has the same static kink solutions as the original momentum-conserving model (at $A = 0$). It can also be demonstrated that the spectra of small amplitude vibrations in the vicinity of vacuum solution and frequencies of kink internal modes in the model equation (31) are A-independent.

6. Numerics

In our recent work [18], some properties of kinks were compared for the 'standard' energy-conserving ϕ^4 discretization having PNp,

$$\ddot{m} = C(l + r - 2m) + m - m^3, \tag{32}$$

with the PNp-free models conserving energy equation (24) and momentum equation (29).

It was found that the mobility of kinks in the PNp-free models is higher and also that in the momentum-conserving, PNp-free models, a kink self-acceleration effect may be observed. The origin of the effect is the non-conservative (non-self-adjoint) nature of the model which, however, can be noted only for asymmetric trajectories of particles when the kink traverses then [18]. If the trajectories are symmetric, there is no energy exchange with the surroundings and the kink dynamics is the same as in energy-conserving models, e.g., the kink self-acceleration effect disappears. Kinks in some of the momentum-conserving models were found to have internal modes with frequencies above the phonon spectrum. Such modes do not radiate and they can have large amplitudes storing a considerable amount of energy.

Here, we present/compare results for the energy-conserving PNp-free model equation (30) and the PNp-free model of equation (31), generally speaking, conserving neither energy nor momentum. For the latter model, we take u_l in the form of equation (11), where the ϕ^4 potential is discretized according to equation (27) and, for the sake of simplicity, we set

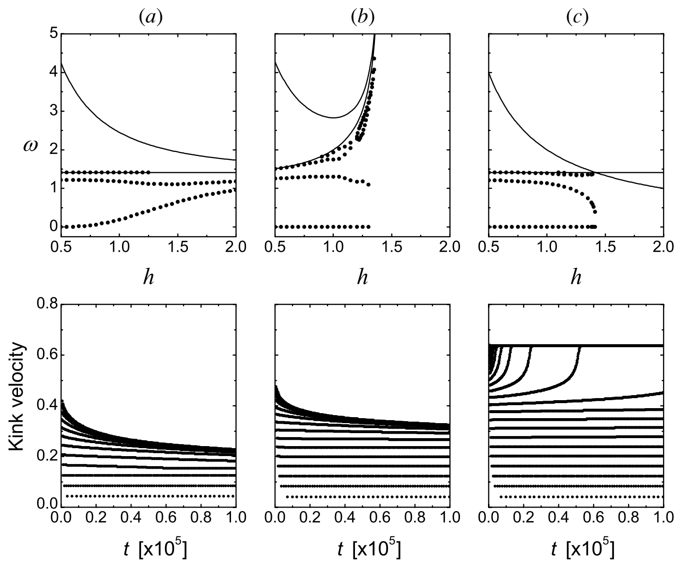

Figure 1. Upper panels: boundaries of the linear spectrum of the vacuum (solid lines) and kink internal mode frequencies (dots) as functions of the lattice spacing $h = 1/\sqrt{C}$. Lower panels: time evolution of kink velocity for different initial velocities and $h = 0.7$. The results are shown for (*a*) classical ϕ^4 model, equation (32), (*b*) PNp-free model conserving energy, equation (30) and (*c*) PNp-free model conserving momentum, equation (33) at $A = 0$.

$\alpha = \beta = \gamma = \delta = 0$. We obtain

$$\ddot{m} = \left[\left(1 - \frac{m^2}{2C}\right) C(l - 2m + r) + m - m^3\right] \frac{(1 + Ahu_l + Ahu_m)^2}{(1 + 2Ahu_l)(1 + 2Ahu_m)},$$
$$\text{where} \quad u_l = C(m - l)^2 - (1 - ml)^2/2. \tag{33}$$

For $A = 0$, equation (33) coincides with the momentum-conserving model equation (29).

As was already mentioned for a more general case of equation (31), in the model equation (33), the static kink solutions, phonon spectra and frequencies of kink internal modes are A-independent. The energy-conserving model, equation (30), has the same static kink solutions as model equation (33) but their spectra are different. The linear vibration spectrum of the vacuum for equation (33) is $\omega^2 = 2 + (4C - 2)\sin^2(\kappa/2)$ and that for equation (30) is $\omega^2 = 4C/(2C - 1) + 4C\sin^2(\kappa/2)$, while the one for the classical model equation (32) is $\omega^2 = 2 + 4C\sin^2(\kappa/2)$.

The top panels of figure 1 present the boundaries of the linear vibration spectrum of the vacuum (solid lines) and the kink internal modes (dots) as the functions of lattice spacing h for (*a*) the classical ϕ^4 model of equation (32), (*b*) the PNp-free model of equation (30) conserving energy and (*c*) the PNp-free model of equation (33) at $A = 0$ conserving momentum. In PNp-free models kinks possess a zero frequency, Goldstone translational mode. Since all models presented in figure 1 share the same continuum ϕ^4 limit, their spectra are very close for small h (<0.5).

The bottom panels of figure 1 show the time evolution of kink velocity for the corresponding models at $h = 0.7$ for kinks launched with different initial velocities. To boost the kink, we used the semi-analytical solution for the normalized Goldstone mode, whose amplitude serves as a measure of the initial kink velocity. One can see that the mobility of kinks in the PNp-free models shown in (*b*) and (*c*) is higher than in the classical

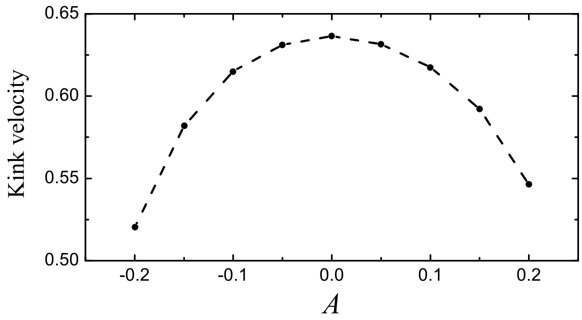

Figure 2. The kink velocity in the regime of steady motion (see bottom panel in figure 1(c)) for the PNp-free ϕ^4 model, equation (33), is shown as a function of parameter A. For $|A| > 0.2$, the kink self-acceleration effect disappears.

model having PNp and shown in (a). In the energy-conserving models shown in (a) and (b), the kink velocity decreases monotonically due to the energy radiation. Non-Hamiltonian momentum-conserving model in (c) shows the effect of kink self-acceleration discussed in [18].

With respect to the self-acceleration effect, it is important to note that we do not address in detail here special terms describing external fields, i.e., in the continuum limit, model equation (33) reduces to the classical ϕ^4 equation. Thus, the very peculiar kink self-acceleration effect, which is due to the fact that equation (33) describes an open system [18], has no relation with the well-studied problem of acceleration of kinks by external field.

When a discrete Klein–Gordon kink propagates, particles are moved, one after another, from one energy well into another. For a system with potential background forces, energy spent to raise a particle to the top of (symmetric) energy barrier is exactly equal to the energy release in the particle motion down to the bottom of the neighbouring energy well and both these energies are path independent. As was demonstrated in [18], for the non-potential model equation (33) with $A = 0$, these energies are, generally speaking, path dependent. However, if the particle trajectories have odd symmetry, the energy increments for 'up' and 'down' motions exactly compensate each other, and, if the odd symmetry is broken, they are not equal. In our simulations, we boost the kinks along the Goldstone mode with particle trajectories having odd symmetry. Our numerical results suggest that (see the bottom panel of figure 1(c)), slow kinks move with constant velocities (<0.3) preserving the odd symmetry of particle trajectories. For faster kinks, this type of motion appears to be unstable. In this case, the odd symmetry of particle trajectories is broken and the particles gain some extra energy after being moved from one potential well to another. This energy accelerates the kink and excites the vacuum (see figure 2 in [18]). Energy lost for vacuum excitation increases with increase in kink velocity and, at a particular value of velocity, a steady motion is achieved.

It is interesting to study what happens when the parameter A in equation (33) deviates from zero and the conservation law of the model (momentum conservation) disappears. We found that the effect of kink self-acceleration, which can be seen in the bottom panel of figure 1(c) for $A = 0$, remains for $|A| < 0.2$ but the value of the kink velocity in the steady motion regime decreases with increase in $|A|$ as it is presented in figure 2. For $|A| > 0.2$ kink self-acceleration effect disappears and kink velocity gradually decreases with time. From the above, we infer that properties such as the self-acceleration (for momentum-conserving models) or the Bogomol'nyi bounds (for energy-conserving discretizations) render such models rather special within the broader class of PNp-free models. However, the critical ingredient for the more general feature of (*static*) PN absence exists in the form of a reduction of the second-order problem into a first order.

7. Conclusions

A general procedure for deriving discrete Klein–Gordon models whose static kinks can be placed anywhere with respect to the underlying lattice was described. Such models are called *static* PNp-free models. It was demonstrated that the models of this kind derived earlier [8, 9, 16, 18] are special cases of the wider family of models derived here.

Static kink solutions for the PNp-free models can be found from the nonlinear algebraic equation of the form $u(l, m) = 0$, which is a discrete analogue of the first integral of the static continuum Klein–Gordon equation of motion. This ensures the existence of static kink solutions at least for the regime of sufficiently weak discreteness and smooth background potential. The range of the discreteness parameter supporting stable static kinks varies according to the specific properties of the model.

In this paper, we have discussed only nearest-neighbour discretizations. However, one can easily write a PNp-free model involving more distant neighbours by replacing equation (18) with higher-order finite difference operators approximating equation (2), keeping the two-point approximation, equation (11), for the first integral of equation (10).

Discrete kinks in the static PNp-free models possess the zero-frequency translational Goldstone mode and they can (almost) freely move with at least infinitesimally small velocity. Such kinks are not trapped by the lattice and they can be accelerated by even weak external fields.

As a topic for future studies, it would be interesting to find any possible relation between models constructed here and models that support travelling kink solutions for finite kink velocity. Such connections are apparently under intense investigation [14] and should provide a framework for understanding travelling in dispersive lattice systems.

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