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Kink Internal Modes and Kink Mobility in Klein-Gordon Lattices without Peierls-Nabarro Potential

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Conventional discretization of the Klein-Gordon field equation possesses the Peierls-Nabarro potential (PNp) which eventually traps moving kinks, at least in the regime of high discreteness. However, there exist two approaches to derive discrete Klein-Gordon models where kinks are PNp-free. We formulate a sufficient condition to obtain a discrete model with kinks free of PNp and demonstrate that the known models can be deduced from it. Using the ϕ^4 model as an example, the dynamical properties of kinks for the two known classes of PNp-free models are compared. The formulated necessary condition gives the possibility to construct new classes of PNp-free models.

1. Introduction

Generally speaking, the discrete Klein-Gordon equation supports a discrete set of equilibrium (static) topological solitons (kinks). For example, kink in classical discrete ϕ^4 model has two equilibrium positions, centered on a lattice cite (unstable equilibrium) and centered midway between two lattice cites (stable equilibrium). This can be contrasted to the continuum Klein-Gordon static kink which can be placed anywhere. However, it has been demonstrated that a nearest-neighbor discretization of the background forces makes it possible to remove the PNp [1-3] so that even highly-discrete kink can be at equilibrium at any position with respect to the lattice. Approach developed by Speight with co-workers [1] results in energy-conserving PNp-free model while the approach reported in [2] results in momentum-conserving PNp-free models. It has been demonstrated that energy-conserving and momentum-conserving models are mutually exclusive, i.e., if a model conserves energy then it cannot conserve momentum and vice versa [3].

In the present study we formulate a necessary condition to obtain a discrete PNp-free model which can result in energy- or momentum-conserving PNp-free models or models conserving neither energy, no momentum.

The paper is organized as follows. In Sec. 2, assuming that the background potential of the continuum Klein-Gordon field can be expanded in Taylor series we describe the general nearest-neighbor discrete model. In Sec. 3, the general expression for the energy-conserving discrete model is given. The main idea of the paper is expressed in Sec. 4, where we formulate a necessary condition to obtain a discrete PNp-free model. In Sec. 5, following the results of works [1] we present the energy-conserving PNp-free models. In Sec. 6, following the work [2] and a more recent work [3] we present the momentum-conserving PNp-free models. Section 7 is devoted to a particular example of Klein-Gordon model, namely to the ϕ^4 discrete model. Here we compare the kink internal modes and kink mobility in three models: momentum-conserving PNp-free, energy-conserving PNp-free, and energy-conserving classical discretizations. Section 8 concludes the paper.

2. General expression for the discrete Klein-Gordon model

We consider the Lagrangian of the Klein-Gordon field,

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

and the corresponding equation of motion,

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

Assuming that the background potential $V(\phi)$ can be expanded in Taylor series we write

$$V'(\phi)=\sum_{s=1}^{\infty}\sigma_s\phi^s. \tag{3}$$

For brevity, when possible, we will use the notations

$$\phi_{n-1}\equiv l, \qquad \phi_n\equiv m, \qquad \phi_{n+1}\equiv r. \tag{4}$$

We would like to construct a discrete analog to Eq. (2) of the form

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

where $C>0$ is a parameter and, in the continuum limit ($C\to\infty$), B is equal to V'. Note that, in the classical discretization, simply $B(l,m,r)=V'(m)$.

The most general choice for the function B in Eq. (5) is

$$B(l,m,r)=\sum_{s=1}^{\infty}B_s(l,m,r), \tag{6}$$

$$B_s(l,m,r)=\sum_{i=0}^{s}\sum_{j=i}^{s}b_{ij,s}r^i m^{j-i}l^{s-j}, \tag{7}$$

and

$$\sum_{i=0}^{s}\sum_{j=i}^{s}b_{ij,s}=\sigma_s. \tag{8}$$

In the continuum limit one has $l\to m$ and $r\to m$ and thus, under condition Eq. (8), the s-order term B_s reduces to $\sigma_s\phi_s$ and Eq. (6) has the desired limit, $V'(\phi)$. Furthermore, Eq. (7) takes into account all possible combinations of powers of $l,m,$ and r. Coefficients $b_{ij,s}$ make a triangular matrix of size $(s+1)\times(s+1)$. For example,

$$B_3(l,m,r)=\begin{array}{llll} b_{00,3}l^3 & +\ b_{01,3}ml^2 & +\ b_{02,3}m^2l & +\ b_{03,3}m^3 \\ & +\ b_{11,3}rl^2 & +\ b_{12,3}rml & +\ b_{13,3}rm^2 \\ & & +\ b_{22,3}r^2l & +\ b_{23,3}r^2m \\ & & & +\ b_{33,3}r^3 \end{array}. \tag{9}$$

Imposing different conditions on the coefficients $b_{ij,s}$ one can derive specific subclasses of discrete models having particular properties. Several subclasses are derived in the following.

3. Energy conserving models

Here we derive a general discrete model of the form of Eq. (5) for which a Lagrangian,

$$L=\sum_n\left[\frac{1}{2}\dot{\phi}_n^2-\frac{C}{2}(\phi_{n+1}-\phi_n)^2-\tilde{V}(\phi_{n+1},\phi_n)\right], \tag{10}$$

can be constructed. The most general polynomial form of $\tilde{V}(\phi_{n+1},\phi_n)$ can be presented as the sum of p-order terms

$$\tilde{V}(r,m)=\sum_{p=1}^{\infty}E_p(r,m), \qquad E_p(r,m)=\sum_{i=0}^{p-1}e_{i,p}r^i m^{p-i}. \tag{11}$$

Then, in the Euler-Lagrange equations of motion derived from Eq. (10) and Eq. (11), there will be

$$B_s(l,m,r)=\frac{\partial}{\partial m}\left[E_{s+1}(m,l)+E_{s+1}(r,m)\right]=\sum_{i=1}^{s}ie_{i,s+1}m^{i-1}l^{s+1-i}+\sum_{i=0}^{s}(s+1-i)e_{i,s+1}r^i m^{s-i}. \tag{12}$$

One can see that in the energy-conserving models $B(l,m,r)$ cannot contain the terms where powers of all three $l,m,$ and r appear simultaneously, i.e., $b_{ij,s}=0$ when both conditions, $i>0$ and $j<s$, are fulfilled. Coefficient $b_{0s,s}=(s+1)e_{0,s+1}$ is independent, while the other coefficients are dependent by pairs. If we denote $b_{0j,s}=(j+1)e_{j+1,s+1}$ for $j=0,...,s-1$, then $b_{is,s}=[(s+1-i)/i]b_{0(i-1),s}$ for $i=1,...,s$.

To summarize, the energy-conserving model of the form of Eqs. (5-8) is the one where (i) $b_{ij,s}=0$ when both conditions, $i>0$ and $j<s$, are fulfilled; (ii) $s+1$ coefficients $b_{0j,s}$ are independent ($j=0,...,s$); (iii) the other coefficients are related to the free coefficients as $b_{is,s}=[(s+1-i)/i]b_{0(i-1),s}$ for $i=1,...,s$; (iv) condition Eq. (8) must be taken into account to ensure the desired continuum limit and the number of independent coefficients in $B_s(l,m,r)$ becomes s.

For example, the terms $B_s(l,m,r)$ with $s=1,2,3$ have the following coefficients

$$b_{ij,1}=\begin{bmatrix} b_{00,1} & b_{01,1} \\ & b_{00,1}\end{bmatrix},\quad b_{ij,2}=\begin{bmatrix} b_{00,2} & b_{01,2} & b_{02,2} \\ & 0 & \frac{2}{1}b_{00,2} \\ & & \frac{1}{2}b_{01,2}\end{bmatrix},\quad b_{ij,3}=\begin{bmatrix} b_{00,3} & b_{01,3} & b_{02,3} & b_{03,3} \\ & 0 & 0 & \frac{3}{1}b_{00,3} \\ & & 0 & \frac{2}{2}b_{01,3} \\ & & & \frac{1}{3}b_{02,3}\end{bmatrix}. \tag{13}$$

Classical discretization is energy conserving one with all coefficients $b_{ij,s}=0$ except for $b_{0s,s}=\sigma_s$.

4. PNp-free models

To obtain a discrete Klein-Gordon model supporting PNp-free static kinks it is sufficient to demand that the static kink solution is obtainable from the discrete equation of the form

$$H(l,m) = A = const, \tag{14}$$

for arbitrary value of l (or m). Indeed, if this is so, one can obtain a continuous set of equilibrium kink solutions centered anywhere with respect to the lattice, which is different from the situation when there exists only a discrete set of equilibrium kink configurations.

With the sufficient condition Eq. (14), two classes of PNp-free models can be constructed.

The first class is the one where function $B(l,m,r)$ of Eq. (5) is taken in the form

$$\begin{aligned} B(l,m,r) = {} & \frac{C}{F_1(A)}(l-m)F_1\left(H(l,m)\right) - \frac{C}{F_1(A)}(m-r)F_1\left(H(m,r)\right) \\ & + F_2\left(H(l,m),l,m,r\right) - F_2\left(H(m,r),l,m,r\right), \end{aligned} \tag{15a}$$

or

$$\begin{aligned} B(l,m,r) = {} & \frac{C}{F_1(A)}(l-m)F_1\left(H(m,r)\right) - \frac{C}{F_1(A)}(m-r)F_1\left(H(l,m)\right) \\ & + F_2\left(H(l,m),l,m,r\right) - F_2\left(H(m,r),l,m,r\right), \end{aligned} \tag{15b}$$

where F_1 is arbitrary function $(F_1(A) \neq 0)$ and function F_2 is such that the continuum limit of $B(l,m,r)$ is $V'(\phi)$. With the choice Eq. (15a) or Eq. (15b), in view of Eq. (14), one has $B(l,m,r) = C(l+r-2m)$ and the static part of Eq. (5) is satisfied. In other words, any structure derived from iterative formula Eq. (14) is an equilibrium solution of Eq. (5).

In fact, Eq. (15a,b) can be written in a more general form taking the functions F_1 and F_2 dependent on both $H(l,m)$ and $H(m,r)$. We only demand that the two first terms as well as the two last terms in the right-hand side of Eq. (15a,b) do not cancel out but they cancel out after $H(l,m)$ and $H(m,r)$ are substituted with A.

The second class of PNp-free model was offered in [2] and later studied in [3]. Here we look for a function $D(l,m,r)$ such that

$$D(l,m,r)[C(l+r-2m) + B(l,m,r)] = H(l,m) - H(m,r). \tag{16}$$

If for the right-hand side of Eq. (5) the representation Eq. (16) is found then the static kink solution can be found from $H(l,m) = H(m,r)$, i.e., from Eq. (14), understanding that the constant value A can be determined for vacuum solution.

5. PNp-free energy conserving models

The models of this type were offered by Speight with co-authors [1] considering the discrete analog to Bogomol'nyi argument [4]. Their idea is to present the Lagrangian Eq. (10) in the form

$$L = \sum_n \left[\frac{1}{2}\dot{\phi}_n^2 - \frac{C}{2}(\phi_{n+1} - \phi_n)^2 - \left(\frac{G(r) - G(m)}{r - m} \right)^2 \right], \tag{17}$$

where

$$[G'(\phi)]^2 = V(\phi). \tag{18}$$

With function $G(\phi)$ given by Eq. (18) the continuum limit of Eq. (17) is Eq. (1). Besides, for the potential energy of the system one has

$$\begin{aligned} P &= \sum_n \left[\frac{C}{2}(\phi_{n+1}-\phi_n)^2 + \left(\frac{G(\phi_{n+1})-G(\phi_n)}{\phi_{n+1}-\phi_n} \right)^2 \right] \\ &= \sum_n \left[\sqrt{\frac{C}{2}}(\phi_{n+1}-\phi_n) - \frac{G(\phi_{n+1})-G(\phi_n)}{\phi_{n+1}-\phi_n} \right]^2 + \sum_n \sqrt{2C}\left[G(\phi_{n+1})-G(\phi_n)\right]. \end{aligned} \tag{19}$$

Let us now consider a static kink, i.e., the configuration with $\phi_n \to \phi_{-\infty}$ when $n \to -\infty$ and $\phi_n \to \phi_\infty$ when $n \to \infty$. Constants $\phi_{-\infty}$ and ϕ_∞ are the vacuums of the background potential, i.e., $V'(\phi_{-\infty}) = V'(\phi_\infty) = 0$, and $V''(\phi_{-\infty}) > 0$, $V''(\phi_\infty) > 0$. Background potential can have more than two vacuums and, in this case, for simplicity, we study the kink connecting two nearest vacuums.

Potential energy of the static kink must be minimal and, according to Eq. (19), minimum is achieved when

$$\frac{G(r)-G(m)}{(r-m)^2} = \sqrt{\frac{C}{2}}, \tag{20}$$

for any r and m and the energy of the kink is then

$$P_K = \sum_n \sqrt{2C}\left[G(\phi_{n+1})-G(\phi_n)\right] = \sqrt{2C}\left[G(\phi_\infty)-G(\phi_{-\infty})\right]. \tag{21}$$

Static kink solution can be found from Eq. (20) which has the form of Eq. (14).

When deriving the equations of motion from the Lagrangian Eq. (17) we come to Eq. (5) with

$$\begin{aligned} B(l,m,r) &= 2\frac{G(r)-G(m)}{(r-m)^3}\left[-G'(m)(r-m)+G(r)-G(m)\right] \\ &-2\frac{G(m)-G(l)}{(m-l)^3}\left[-G'(m)(m-l)+G(m)-G(l)\right]. \end{aligned} \tag{22}$$

One can easily check that, in view of Eq. (20), the static part of Eq. (5) with $B(l,m,r)$ given by Eq. (22) is equal to zero.

Thus, $B(l,m,r)$ given by Eq. (22) is a particular case of Eq. (15a) with $H(l,m) = [G(m)-G(l)]/(m-l)^2$, $F_1 = [H(l,m)]^2$, $F_2 = 2H(l,m)G'(m)$, $A = \sqrt{C/2}$.

6. PNp-free momentum conserving models

Let us construct the PNp-free models where the static part (right-hand side) of Eq. (5) is representable in the form of Eq. (16).

This problem will be solved in two steps. First, we find the functions $D(l,m,r)$ which can be used to symmetrize the linear coupling term $l+r-2m$ and then we check if they can symmetrize also the background force term $B(l,m,r)$. Thus, we need to obtain first

$$D(l,m,r)(l+r-2m) = Q(l,m)-Q(m,r). \tag{23}$$

One obvious solution to Eq. (22) is the zero-order polynomial function $D_0(l,m,r)\equiv 1$, for which $Q(l,m)=l-m$. We have also checked the k-order functions,

$$D_k(l,m,r)=\sum_{i=0}^{k}\sum_{j=i}^{k} d_{ij,k} r^i m^{j-i} l^{k-j}\,, \tag{24}$$

which contain all possible combinations of powers of l, m, and r. It is not difficult to prove that D_k with even k, except for $k=0$, cannot symmetrize the expression $l+r-2m$ to the form of Eq. (23). Symmetrization can be achieved for odd k, e.g., with $D_1=l-r$ and $D_3=(r-l)[r^2+l^2+2m(m-r-l)]$. At the second step we have checked the possibility to symmetrize the background force term $B(l,m,r)$ using the derived functions D_k, and we found that, for example, for $k=0,1,3,5$ the symmetrization can be achieved for particular relations between the coefficients $b_{ij,s}$. However, the coefficients $b_{ij,s}$ are such that only in the case $k=1$ the condition Eq. (8) can be met. This condition is important because it ensures the right continuum limit for the discrete model.

Thus, we could find only one function, namely, $D_1=l-r$, that can give the PNp-free discrete models of the considered type. Let us describe these models.

To achieve representation Eq. (16) for $B(l,m,r)$ with respect to $D_1=l-r$ we write

$$\begin{aligned}(r-l)B_s&=\sum_{i=0}^{s}\sum_{j=i}^{s} b_{ij,s} r^{i+1} m^{j-i} l^{s-j}\\&-\sum_{i=0}^{s}\sum_{j=i}^{s} b_{ij,s} r^{i} m^{j-i} l^{s-j+1}.\end{aligned} \tag{25}$$

Terms containing both l and r should be canceled out because they do not fit the representation of Eq. (16). This can be achieved by setting $b_{ij,s}=b_{(i+1)(j+1),s}$, i.e., coefficients in each diagonal of the triangular matrix must be equal. The simplified expression reads:

$$(r-l)B_s=\sum_{i=0}^{s} b_{is,s} r^{i+1} m^{s-i}-\sum_{i=0}^{s} b_{0i,s} m^i l^{s-i+1}\,. \tag{26}$$

To symmetrize the result, we add and subtract $b_{00,s}m^{s+1}$

$$\begin{aligned}(r-l)B_s&=b_{00,s}\left(r^{s+1}+m^{s+1}\right)-b_{00,s}\left(m^{s+1}+l^{s+1}\right)\\&+\sum_{i=1}^{s} b_{0(s-i+1),s} r^i m^{s-i+1}-\sum_{i=1}^{s} b_{0i,s} m^i l^{s-i+1},\end{aligned} \tag{27}$$

where we shifted the summation index by 1 in the first sum and also used the equality of the diagonal coefficients. The desired representation is obtained for arbitrary $b_{00,s}$ and arbitrary $b_{0i,s}=b_{0(s-i+1),s}$ for $i>0$.

Summing up, (i) the coefficients $b_{ij,s}$ within each diagonal are equal, (ii) the coefficients on the main diagonal can be chosen arbitrarily, and (iii) the terms on ith super-diagonal $(i>0)$ must have the same coefficients as the terms on $(s-i+1)$th diagonal (and these can also be chosen arbitrarily). For B_s the number of super-diagonals is s so that the number of free coefficients is $1+\langle s/2\rangle$, where $\langle x\rangle$ is lowest integer greater than or equal to x. We must also take into account the relation between coefficients Eq. (8) and the number of free coefficients becomes $\langle s/2 \rangle$.

For example, the terms $B_s(l,m,r)$ with $s=1,2,3$ have the following coefficients

$$b_{ij,1}=\begin{bmatrix} b_{00,1} & b_{01,1} \\ & b_{00,1} \end{bmatrix},\quad b_{ij,2}=\begin{bmatrix} b_{00,2} & b_{01,2} & b_{01,2} \\ & b_{00,2} & b_{01,2} \\ & & b_{00,2} \end{bmatrix},\quad b_{ij,3}=\begin{bmatrix} b_{00,3} & b_{01,3} & b_{02,3} & b_{01,3} \\ & b_{00,3} & b_{01,3} & b_{02,3} \\ & & b_{00,3} & b_{01,3} \\ & & & b_{00,3} \end{bmatrix}. \tag{28}$$

It has been demonstrated in [2] that the discrete model Eq. (5) with the static part representable in the form of Eq. (16) with $D(l,m,r)=l-r$ conserves linear momentum

$$M=\sum_{n=-\infty}^{\infty}\dot{\phi}_n\left(\phi_{n+1}-\phi_{n-1}\right). \tag{29}$$

Indeed, the equations of motion in this case are

$$\ddot{m}=\frac{H(l,m)-H(m,r)}{r-l}. \tag{30}$$

Then,

$$\frac{dM}{dt}=\sum_{n=-\infty}^{\infty}\ddot{\phi}_n\left(\phi_{n+1}-\phi_{n-1}\right)=\sum_{n=-\infty}^{\infty}\left[H(\phi_{n-1},\phi_n)-H(\phi_n,\phi_{n+1})\right]=0, \tag{31}$$

as telescopic sum.

Energy-conserving and momentum-conserving models are mutually exclusive, i.e., if a model of the form of Eq. (5) with a nonlinear function $B(l,m,r)$ conserves energy then it cannot conserve momentum and vice versa [3].

7. Application to ϕ^4 model

We now examine various models proposed as discretizations of the continuum field theory in the context of perhaps one of the most famous such examples, namely the double-well ϕ^4 model [5-7] (see also the review [8]).

The PNp-free discrete Klein-Gordon model conserving momentum is given by Eq. (5) with the nonlinear term Eqs. (6),(7) where the coefficients $b_{ij,s}$ are as described in Sec. 6. The continuum ϕ^4 model has the background potential $V(\phi)=(1-\phi^2)^2/4$, hence $V'(\phi)=-\phi+\phi^3$ so that in Eq. (3) all $\sigma_s=0$ except for $\sigma_1=-\sigma_3=-1$. The momentum-preserving PNp-free discretization then reads:

$$\begin{aligned}\ddot{m}=&\left(\frac{1}{h^2}+\alpha\right)(l+r-2m)+m-\beta(l^2+lr+r^2)+\beta m(l+r+m)\\&-\gamma(l^3+r^3+l^2r+lr^2)-\delta m(l^2+m^2+r^2+lr)-\frac{1}{2}(1-4\gamma-4\delta)m^2(l+r),\end{aligned} \tag{32}$$

where $\alpha=b_{00,1}$, $\beta=b_{00,2}$, $\gamma=b_{00,3}$, $\delta=b_{01,3}$ are free parameters and we did not include the terms with $s>3$.

The model of Eq. (32) will be compared to the energy-conserving PNp-free model obtained from Eq. (17) and Eq. (18) in ϕ^4 case. We have $G'(\phi)=(1-\phi^2)/2$, $G(\phi)=\phi(1-\phi^2/3)/2$, and, in view of Eq. (22), the equation of motion Eq. (5) is [1]

$$\ddot{m}=\left(\frac{1}{h^2}+\frac{1}{6}\right)(l+r-2m)+m-\frac{1}{18}\left[2m^3+(m+l)^3+(m+r)^3\right]. \tag{33}$$

We will also compare the above PNp-free models to the classical ϕ^4 discretization, i.e.,

$$\ddot{m}=\frac{1}{h^2}(l+r-2m)+m-m^3. \tag{34}$$

In Eqs. (32-34), $C=1/h^2$; h is the lattice spacing.

If in Eq. (32), $\alpha=\beta=\gamma=\delta=0$, then the models of Eq. (32) and Eq. (33) have the same linear vibration spectrum (i.e., dispersion relation $\omega=\omega(\kappa)$) for the vacuum solution $\phi_n=\pm 1$, namely $\omega^2=2+(4/h^2-2)\sin^2(\kappa/2)$. This can be compared to the spectrum of the vacuum of Eq. (34), $\omega^2=2+(4/h^2)\sin^2(\kappa/2)$.

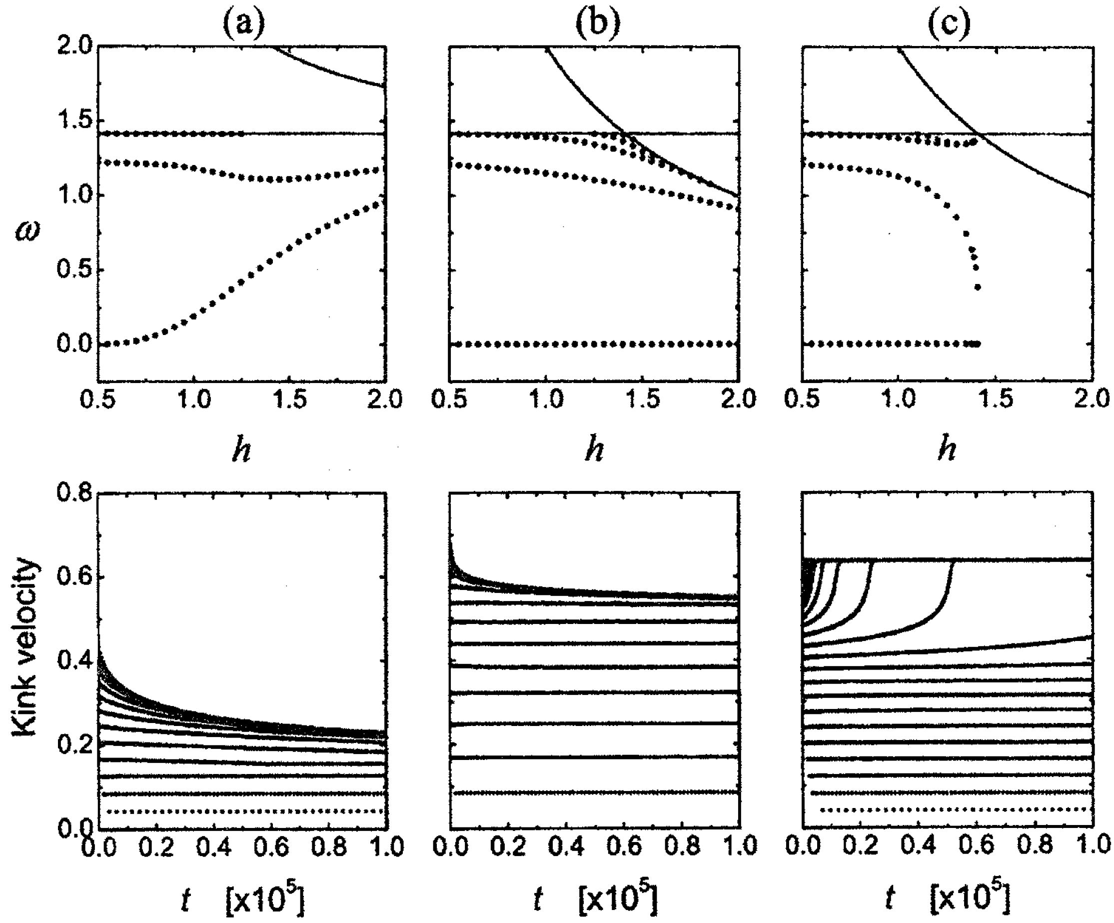

Fig. 1. Upper panels: boundaries of the linear spectrum of the vacuum (solid lines) and kink internal mode frequencies (dots) as functions of the lattice spacing h. Lower panels: time evolution of kink velocity for different initial velocities and $h=0.7$. The results are shown for (a) classical ϕ^4 model, Eq. (34), (b) PNp-free model conserving energy, Eq. (33), and (c) PNp-free model conserving momentum, Eq. (32), with $\alpha=\beta=\gamma=\delta=0$.

We analyze the kink internal modes (i.e., internal degrees of freedom [9]) for these three models. First, we determine the kink-like heteroclinic solution by means of relaxational dynamics. Then, the linearized equations are used in a lattice of $N = 200$ sites to obtain N eigenfrequencies and the corresponding eigenmodes. We are particularly interested in the eigenfrequencies which lie outside the linear vibration band of vacuum solution and thus are associated with the kink internal modes. It is worthwhile to notice that the eigenproblem for models conserving energy, Eq. (32) and Eq. (34), has a symmetric Hessian matrix while the non-self-adjoint problem for the momentum-conserving model Eq. (33) results in a non-symmetric matrix.

The top panels of Fig. 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 Eq. (34), (b) the PNp-free model of Eq. (33) conserving energy, and (c) the PNp-free model of Eq. (32) conserving momentum. In PNp-free models kinks possess a zero frequency, Goldstone translational mode similarly to the continuum ϕ^4 kink. Hence, the static kink can be centered anywhere on the lattice. The results presented in Fig. 1 are for the kink situated exactly between two lattice sites. This position is the stable position for the classical ϕ^4 discrete kink [9]. Since all three discrete models share the same continuum (ϕ^4) limit, their spectra are very close for small $h(< 0.5)$. We found that the model Eq. (32) may have kink internal modes lying *above* the spectrum of vacuum, e.g., for $\alpha = 1/2$, $\beta = 0$, $\gamma = 1/4$, and $\delta = 0$. Such modes are short-wavelength ones, with large amplitudes (energies) and they do not radiate because of the absence of coupling to the linear phonon spectrum.

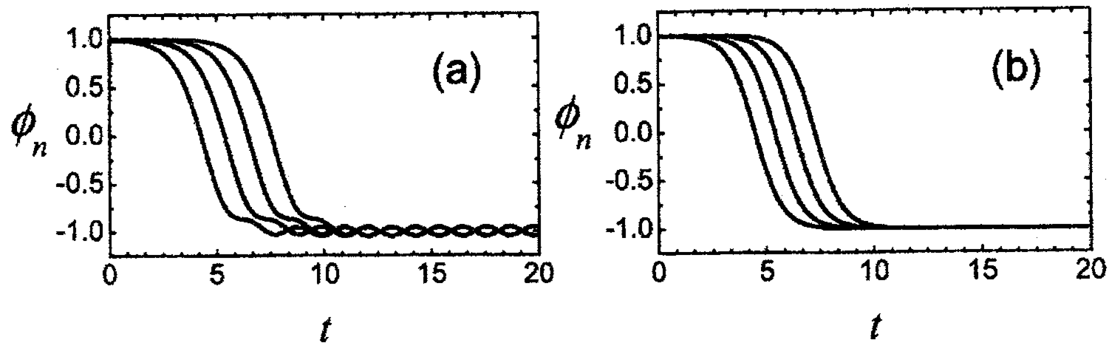

Fig. 2. Trajectories of particles (a) in the model of Eq. (32) with $h = 0.7$ when the kink moves with a steady velocity v^* (see Fig. 1(c), bottom panel) and (b) for the continuum ϕ^4 kink.

Perhaps more interesting are the implications of such discretizations on the mobility of kinks. In the PNp-free models, Eq. (32) and Eq. (33), the kink was launched using a perturbation along the Goldstone mode to provide the initial kick. In the classical model Eq. (34) for this purpose we employed the imaginary frequency (real eigenvalue) unstable eigenmode for a kink initialized at the unstable position (a site-centered kink). In all cases the amplitude of the mode is related to the initial velocity of the kink. In the bottom panels of Fig. 1 we present the time evolution of the kink velocity for different initial velocities and $h = 0.7$ for the three discretizations. The results suggest that the mobility of the kink in the classical ϕ^4 model presented in (a) is much smaller than in the PNp-free models, (b) and (c). Furthermore, a very interesting effect of kink *self-acceleration* can be observed in panel (c). Here there exists a selected kink velocity $v^* \approx 0.637$ and kinks launched with $v > v^*$, in a very short time (cannot be seen in the scale of the figure) adjust their velocities to v^*. More surprisingly, the velocity adjustment is observed even for kinks launched with $v < v^*$. In the steady-state regime, when the kink moves with $v = v^*$, it excites (in its tail) the short-wave oscillatory mode even though in front of the kink the vacuum is not perturbed.

These results generate the question of where the energy for the self-acceleration and vacuum excitation comes from. In Fig. 2(a) we show the trajectories of four neighboring particles when a kink moving with $v = v^*$ (see Fig. 1(c), bottom panel) moves through. For comparison, in (b) the trajectories for the classical ϕ^4 kink, $\phi_n(t) = \tanh[\rho(nh - vt)]$, where $\rho = 1/\sqrt{2-2v^2}$, are shown. In both cases the trajectories are identical and shifted with respect to each other by $t = h/v$, but in (b) they are the odd functions with respect the point $\phi_n = 0$ while in (a) they are not. The work done by the background forces, Eq. (5), to move the nth particle from one energy well to another is

$$W_n = -\int_{-\infty}^{\infty} \dot{m} B(l,m,r) dt . \tag{35}$$

For the ϕ^4 model Eq. (32) with $\beta = \gamma = \delta = 0$, the nonlinear part of $B(l,m,r)$ reduces to $B(l,m,r) = (1/2)m^2(l+r)$. It is straightforward to demonstrate that $W_n = 0$ for the classical ϕ^4 kink. However, if a term breaking odd symmetry, e.g., $\varepsilon \cosh^{-1}[\theta(nh - vt)]$, is added to the kink, the work becomes nonzero, $W_n = (\pi/2)\varepsilon(\varepsilon^2+1)[\cosh(\rho h) - 1]^3 / \sinh^4(\rho h)$, where we set for simplicity $\theta = \rho$. Numerically we found that W_n can be positive or negative depending on ρ, θ and the kink velocity, v. This simple analysis qualitatively explains the kink self-acceleration or deceleration and the vacuum excitation. The energy for this comes from the breaking of the odd symmetry of particle trajectories, which is possible in the case of path-dependent background forces. It is, thus, very interesting to highlight the distinctions between the regular discrete models, the PNp-free, energy conserving discrete models, and the PNp-free, momentum conserving discrete models. The first ones lead to rapid dissipation of the wave's kinetic energy due to the PN barrier. The second render the dissipation far slower in time. Finally the third may even sustain self-accelerating waves and locking to a particular speed due to the non-potential nature of the relevant model.

8. Discussion and conclusions

A sufficient condition to obtain a discrete Klein-Gordon model with static kinks free of Peierls-Nabarro potential was given (Sec. 4). The PNp-free models derived so far [1-3] can be extracted from this sufficient condition as particular cases.

A number of characteristic similarities and differences between energy- and momentum-conserving PNp-free discrete models were highlighted. The momentum conserving Klein-Gordon system with non-potential background forces discussed here differs from other path-dependent systems, e.g., having friction and/or AC drive, in the sense that the viscosity and external forces are not explicitly introduced. This makes the dynamics of the system peculiar, for example, as it was demonstrated, the existence, the intensity, and the sign of energy exchange with the surroundings depends on the symmetry and other characteristics of the motion.

It would be interesting to investigate if the sufficient condition of having no PNp formulated in Sec. 4 can be used to construct models conserving quantities other than energy and momentum.

Further investigation of the intriguing dynamic properties of such non-potential models is important, given the relevance of path-dependent forces in various applications such as, e.g., aerodynamic and hydrodynamic forces, the forces induced in automatic control systems and others. Such studies are in progress and will be reported in future publications.

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