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Standard Nearest Neighbor Discretizations of Klein-Gordon Models Cannot Preserve Both Energy and Linear Momentum

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We consider nonlinear Klein-Gordon wave equations and illustrate that standard discretizations thereof (involving nearest neighbors) may preserve either standardly defined linear momentum or total energy but not both. This has a variety of intriguing implications for the “non-potential” discretizations that preserve only the linear momentum, such as the self-accelerating or self-decelerating motion of coherent structures such as discrete kinks in these nonlinear lattices.

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Introduction. In the last two decades, the interplay of nonlinearity and spatial discreteness has been increasingly recognized as vital for the understanding of a variety of physical systems [1]. Such contexts range from calcium waves in living cells [2] to the propagation of action potentials through the cardiac tissue [3] and from chains of chemical reactions [4] to applications in superconductivity and Josephson junctions [5], nonlinear optics and fiber/waveguide arrays [6], complex electronic materials [7], Bose-Einstein condensates [8] or the local denaturation of the DNA double strand [9].

On the other hand, spatially discrete systems (of coupled nonlinear ordinary differential equations) are also relevant as discretizations and computational implementations of the corresponding continuum field theories that are applicable to a variety of contexts such as statistical mechanics [10], solid state physics [11], fluid mechanics [12] and particle physics [13] (see also references therein). Nonlinear Klein-Gordon type equations are a prototypical example among such wave models and their variants span a variety of applications including Josephson junctions in superconductivity, cosmic domain walls in cosmology, elementary particles in particle physics and denaturation bubbles in the DNA, among others.

In this communication, we examine some of the key properties that ensue when discretizing nonlinear Klein-Gordon (KG) equations, using nearest neighbor approximations (which are the most standard ones implemented in the literature; see e.g., [1]). In particular, we focus on the physically relevant invariances of the continuum equation (more specifically, the conservation of the linear momentum and of the total energy of the system) and illustrate the surprising result that if we demand that the energy be conserved, then the momentum cannot be conserved, while if we demand that the momentum be conserved then the energy cannot be conserved (resulting in a so-called non-potential model [14]). Our presentation will be structured as follows. First, we will provide the general mathematical setting of KG equations and study their discretizations that conserve linear momentum and energy, comparing and constructing the properties of the two. Then, we are going to give an application of our

considerations to the physically relevant ϕ^4 model, i.e., the ubiquitous double well potential. Finally, we will summarize our conclusions and discuss future directions.

Setup and Analytical Results. We consider the Lagrangian of the Klein-Gordon field,

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

and the corresponding equation of motion,

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

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

$$V'(\phi) = \sum_{s=0}^{\infty} \sigma_s \phi^s. \quad (3)$$

For brevity, when possible, we will use the notations

$$\phi_{n-1} \equiv l, \quad \phi_n \equiv m, \quad \phi_{n+1} \equiv r. \quad (4)$$

We start with a general proof of our main statement, namely that discretizations that preserve linear momentum and energy are mutually exclusive for nearest neighbor discretizations. As was shown in [15], the standard discretization of Eq. (2) that preserves the discrete analog of the linear momentum, defined in a standard way,

$$M = \sum_{n=-\infty}^{\infty} \dot{\phi}_n (\phi_{n+1} - \phi_{n-1}), \quad (5)$$

is one of the form:

$$\ddot{m} = C(l+r-2m) - \frac{F(r,m) - F(m,l)}{r-l}, \quad (6)$$

where $C = 1/h^2$, where h is the lattice spacing, and the derivative of F is equal to V in the continuum limit ($C \rightarrow \infty$). Then,

$$\begin{aligned} \frac{dM}{dt} &= \sum_n \ddot{\phi}_n (\phi_{n+1} - \phi_{n-1}) \\ &= \sum_n [H(\phi_{n+1}, \phi_n) - H(\phi_n, \phi_{n-1})] = 0, \end{aligned} \quad (7)$$

where $H(r, m) = C(r^2 + m^2 - 2mr) - F(r, m)$, and the terms $\dot{\phi}_n(\dot{\phi}_{n+1} - \dot{\phi}_{n-1})$ cancel out as the telescopic sum.

However, if the model is potential, for nearest neighbor discretizations the nonlinear term will be of the form $\tilde{V}(r, m)$ such that the Lagrangian can be written as:

$$L = \sum_n \left[\frac{1}{2} \dot{\phi}_n^2 - \frac{C}{2} (\phi_{n+1} - \phi_n)^2 - \tilde{V}(\phi_{n+1}, \phi_n) \right], \quad (8)$$

where the first term gives the kinetic energy, \mathcal{K} , and the two other terms give negative potential energy, $-\mathcal{P}$, so that the total energy is $E = \mathcal{K} + \mathcal{P}$. However, then a model that would enforce both energy and momentum conservation would have to satisfy:

$$\frac{F(r, m) - F(m, l)}{r - l} = \frac{\partial}{\partial m} [\tilde{V}(r, m) + \tilde{V}(m, l)]. \quad (9)$$

After multiplying with $r - l$, this, in turn, implies that the cross terms involving all 3 of r, m and l should be presentable in the form

$$r \frac{\partial \tilde{V}(m, l)}{\partial m} - l \frac{\partial \tilde{V}(r, m)}{\partial m} = P(r, m) - P(m, l). \quad (10)$$

This is satisfied only if $\tilde{V}(x, y)$ is a (symmetric) quadratic function in its arguments. However, this is incompatible with the nonlinear nature of the model. Hence, it is not possible to satisfy both conservation laws at once.

Let us now derive the general discrete Klein-Gordon model of the form of Eq. (6) conserving momentum. For the polynomial background forces Eq. (3), the nonlinear term of Eq. (6) can be presented as the sum of s -order terms

$$B(l, m, r) = \frac{F(r, m) - F(m, l)}{r - l} = \sum_{s=0}^{\infty} B_s(l, m, r), \quad (11)$$

with

$$B_s = \sum_{i=0}^s \sum_{j=i}^s b_{ij,s} r^i m^{j-i} l^{s-j}, \quad (12)$$

where

$$\sum_{i=0}^s \sum_{j=i}^s b_{ij,s} = \sigma_s. \quad (13)$$

In the continuum limit one has $l \rightarrow m$ and $r \rightarrow m$ and thus, Eq. (11) together with Eq. (13) ensure the desired limit, $V'(\phi)$. Furthermore, Eq. (12) takes into account all possible combinations of powers of l, m , and r . Coefficients $b_{ij,s}$ make a triangular matrix of size $(s+1) \times (s+1)$. Let us find the coefficients $b_{ij,s}$ to satisfy Eq. (11). We write

$$(r - l)B_s = \sum_{i=0}^s \sum_{j=i}^s b_{ij,s} r^{i+1} m^{j-i} l^{s-j} - \sum_{i=0}^s \sum_{j=i}^s b_{ij,s} r^i m^{j-i} l^{s-j+1}. \quad (14)$$

Terms containing both l and r should be canceled out because they do not fit the representation of Eq. (11). 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:

$$(r - l)B_s = \sum_{i=0}^s b_{i,s} r^{i+1} m^{s-i} - \sum_{i=0}^s b_{0i,s} m^i l^{s-i+1}. \quad (15)$$

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

$$(r - l)B_s = b_{00,s}(r^{s+1} + m^{s+1}) - b_{00,s}(m^{s+1} + l^{s+1}) + \sum_{i=1}^s b_{0(s-i+1),s} r^i m^{s-i+1} - \sum_{i=1}^s b_{0i,s} m^i l^{s-i+1} \quad (16)$$

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 i th 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 $1 + \lceil s/2 \rceil$, where $\lceil x \rceil$ is lowest integer greater than or equal to x . We must also take into account the relation between coefficients Eq. (13) and the number of free coefficients becomes $\lceil s/2 \rceil$.

For example, the coefficients of B_3 are

$$b_{ij,3} = \begin{bmatrix} b_{00,3} & b_{01,3} & b_{02,3} & b_{01,3} \\ & b_{00,3} & b_{01,3} & b_{02,3} \\ & & b_{00,3} & b_{01,3} \\ & & & b_{00,3} \end{bmatrix}, \quad (17)$$

$$4b_{00,3} + 4b_{01,3} + 2b_{02,3} = \sigma_3.$$

Since the model Eq. (6) is translationally invariant, the static kink is free of the Peierls-Nabarro potential (PNP) [15], i.e., the periodic potential that nonlinear waves have to overcome to move by one lattice site [16] (see also references therein). This is an important qualitative difference with respect to the conventional discretization when, in Eq. (1), $V(\phi)$ is substituted with $V(\phi_n)$ and thus, in the equation of motion Eq. (2), $V'(\phi)$ becomes $V'(\phi_n)$.

Another class of Klein-Gordon models which support energy conservation and sustain static kinks but which are free of PNP has been derived by Speight and collaborators [17]. In such models the background potential term of Eq. (1), $P = \int V(\phi) dx$, should be discretized as

$$P = \sum_n \left(\frac{G(\phi_{n+1}) - G(\phi_n)}{\phi_{n+1} - \phi_n} \right)^2, \quad \text{with } [G'(\phi)]^2 = V(\phi). \quad (18)$$

Numerical Results/Model Comparison. 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 [10, 11, 13] (see also the review [18]).

The discrete Klein-Gordon model conserving momentum is given by Eq. (6) with the nonlinear term Eq. (11) where the coefficients $b_{ij,s}$ are as described in the previous section. 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 discretization then reads:

$$\begin{aligned} \ddot{m} = & (C + \alpha)(l + r - 2m) + m \\ & - \beta(l^2 + lr + r^2) + \beta m(l + r + m) \\ & - \gamma(l^3 + r^3 + l^2r + lr^2) - \delta m(l^2 + m^2 + r^2 + lr) \\ & - \frac{1}{2}(1 - 4\gamma - 4\delta)m^2(l + r), \end{aligned} \quad (19)$$

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. (19) will be compared to the model obtained from Eq. (18) in ϕ^4 case [17], namely

$$\begin{aligned} \ddot{m} = & \left(C + \frac{1}{6}\right)(l + r - 2m) + m \\ & - \frac{1}{18} [2m^3 + (m + l)^3 + (m + r)^3], \end{aligned} \quad (20)$$

and also to the “standard” ϕ^4 discretization, i.e.,

$$\ddot{m} = C(l + r - 2m) + m - m^3. \quad (21)$$

If in Eq. (19), $\alpha = \beta = \gamma = \delta = 0$, then the models of Eq. (19) and Eq. (20) have the same linear vibration spectrum (i.e., dispersion relation $\omega = \omega(\kappa)$) for the vacuum solution $\phi_n = \pm 1$, namely $\omega^2 = 2 + (4C - 2)\sin^2(\kappa/2)$. This can be compared to the spectrum of the vacuum of Eq. (21), $\omega^2 = 2 + 4C\sin^2(\kappa/2)$.

We analyze the kink internal modes (i.e., internal degrees of freedom [19]) 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. (20) and Eq. (21), has a symmetric Hessian matrix while the non-self-adjoint problem for the momentum conserving model Eq. (19) 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. (21), (b) the PNP-free model of Eq. (20) conserving energy, and (c) the PNP-free model of Eq. (19) 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

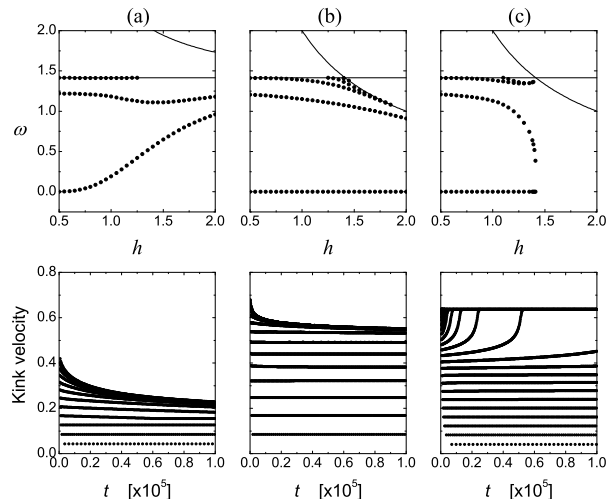


FIG. 1: Upper panels: boundaries of the linear spectrum of the vacuum (solid lines) and kink internal mode frequencies (dots) as functions of the lattice spacing $h = 1/\sqrt{C}$. Lower panels: time evolution of kink velocity for different initial velocities and $h = 0.7$. The results are shown for (a) classical ϕ^4 model, Eq. (21), (b) PNP-free model conserving energy, Eq. (20), and (c) PNP-free model conserving momentum, Eq. (19), with $\alpha = \beta = \gamma = \delta = 0$.

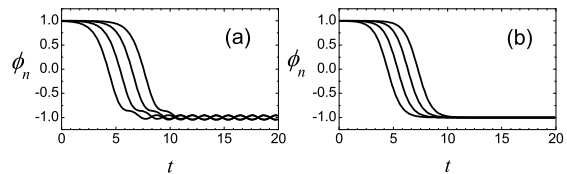


FIG. 2: Trajectories of particles (a) in the model of Eq. (19) with $h = 0.7$ when the kink moves with a steady velocity v^* (see Fig. 1(c), bottom panel) and (b) for the continuum ϕ^4 kink.

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 [19]. Since all 3 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. (19) 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.

Perhaps more interesting are the implications of such discretizations on the mobility of these localized coherent structures. In the PNP-free models, Eq. (19) and

Eq. (20), the kink was launched using a perturbation along the Goldstone mode to provide the initial kick. In the classical model Eq. (21) 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 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 $\rho = [2 - 2v^2]^{-1/2}$, 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. (11), to move the n th particle from one energy well to another is $W_n = -\int_{-\infty}^{\infty} \dot{m}B(l, m, r)dt$. For the ϕ^4 model Eq. (19) 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, $W_n = \frac{\pi}{2}\varepsilon(\varepsilon^2 + 1)[\cosh(\rho h) - 1]^3/\sinh^4(\rho h)$, 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.

Conclusions and Future Challenges. The statement that Klein-Gordon discrete model cannot conserve energy and momentum simultaneously was proved for the case of standard nearest-neighbor discretizations. This raises the issue of how to gauge the “adequacy” of a discretization scheme with respect to the continuum model dynamics. In view of this question, a number of characteristic similarities and differences between energy- and momentum-conserving 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. 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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