A discrete $\phi^4$ system without Peierls-Nabarro barrier

J.M. Speight
Department of Mathematics
University of Texas at Austin
Austin, Texas 78712, U.S.A.

Abstract

A discrete $\phi^4$ system is proposed which preserves the topological lower bound on the kink energy. Existence of static kink solutions saturating this lower bound and occupying any position relative to the lattice is proved. Consequently, kinks of the model experience no Peierls-Nabarro barrier, and can move freely through the lattice without being pinned. Numerical simulations reveal that kink dynamics in this system is significantly less dissipative than that of the conventional discrete $\phi^4$ system, so that even on extremely coarse lattices the kink behaves much like its continuum counterpart. It is argued, therefore, that this is a natural discretization for the purpose of numerically studying soliton dynamics in the continuum $\phi^4$ model.

1 Introduction

Solitons have diverse applications in many branches of physics. Those with applications in high energy physics are topological solitons which arise almost exclusively in non-integrable Lagrangian field theories (integrability appears incompatible with Lorentz invariance in spacetimes of realistic dimension). In the absence of integrability, there is no hope of solving the multisoliton initial value problem exactly. One approach to the study of soliton dynamics is to perform numerical simulations of the field equations. In so doing one is forced to discretize space in some way, and this inevitably introduces fictitious discretization effects into the dynamics, which one should seek to minimize.

The standard discretization of a field theory is obtained by replacing spatial partial derivatives by simple difference operators, leaving it otherwise unchanged, so that one is really studying a large network of oscillators, each moving in an identical substrate potential, with nearest neighbour couplings. Such systems are intrinsically interesting (they have applications in condensed matter and biophysics) and have been extensively studied in recent years [1,2,3]. One discretization effect is that static solitons can no longer be centred on any point in space: they must lie in the centre of a lattice cell, or exactly on a lattice site, and the energies of these two types of static solution are different. So there is an energy barrier, called the Peierls-Nabarro (PN) potential resisting the propagation of a soliton from cell to cell. As a soliton moves through the lattice, its periodic motion in and out of the PN potential excites small amplitude travelling waves (radiation) which travel in its wake, draining its kinetic energy. The soliton decelerates under this dissipation until it no longer has sufficient energy to surmount the PN barrier. It is then pinned to a lattice cell.

If one is to use the standard discretization to simulate continuum soliton dynamics, these extraneous discretization effects must be rendered insignificant by using a very fine spatial lattice, with spacing $h$ of order (soliton width)/20. This works well, but is computationally expensive, especially in high dimensions. In this paper we consider an alternative approach, originated by Richard Ward, in the case of $\phi^4$ theory in $1+1$ dimensions. Exploiting the non-uniqueness of the discretization process, one can find a discrete $\phi^4$ system which has no PN barrier. One would expect kink dynamics in such a system to be much simpler and more continuum-like than in the conventional discrete
system, even on relatively coarse lattices. This expectation has been confirmed for a similar discrete sine-Gordon system \[4\]. The rest of the paper is organized as follows: in section \[2\] we define the discrete \(\phi^4\) system, in section \[3\] we prove that it has no PN barrier, in section \[4\] we present numerical simulations of the system, and compare its performance with that of the conventional discrete system, and finally section \[5\] presents some concluding remarks.

2 A topological discrete \(\phi^4\) system

The continuum \(\phi^4\) model consists of a real valued scalar field \(\phi : \mathbb{R}^{1+1} \to \mathbb{R}\) whose time evolution is governed by the Lagrangian \(L = E_K - E_P\), the kinetic and potential energy functionals being, respectively,

\[
E_K = \int_{-\infty}^{\infty} dx \frac{1}{2} \dot{\phi}^2 \tag{1}
\]

\[
E_P = \int_{-\infty}^{\infty} dx \left[ \frac{1}{2} \left( \frac{\partial \phi}{\partial x} \right)^2 + \frac{1}{8} (1 - \phi^2)^2 \right]. \tag{2}
\]

To ensure that \(\phi\) has finite energy, one imposes that \(\phi \to \pm 1\) as \(|x| \to \infty\). The trivial solutions \(\phi(x,t) = \pm 1\) are the vacua of the model, while a solution interpolating between \(-1\) and \(1\) (\(1\) and \(-1\)) is a kink (antikink). Static kinks are minimals of \(E_P[\phi]\) and can be found by means of a Bogomol’nyi argument \[5\]. Namely, if \(\lim_{x \to \pm \infty} \phi = \pm 1\), then

\[
0 \leq \frac{1}{2} \int_{-\infty}^{\infty} dx \left[ \frac{d\phi}{dx} \frac{1}{2} (1 - \phi^2) \right]^2 = E_P - \frac{1}{2} \int_{-\infty}^{\infty} dx \frac{d\phi}{dx} (1 - \phi^2)
\]

\[
= E_P - \frac{1}{2} \left[ \phi - \frac{1}{3} \phi^3 \right]_{-1}^1 = E_P - \frac{2}{3} \tag{3}
\]

So \(E_P \geq \frac{2}{3}\) in the kink sector, with equality if and only if

\[
\frac{d\phi}{dx} = \frac{1}{2} (1 - \phi^2). \tag{4}
\]

Equation \[4\] is called the Bogomol’nyi equation. Note that it is a first order o.d.e., unlike the static field equation which is second order. It is easily solved, yielding

\[
\phi(x) = \tanh \frac{1}{2} (x - b) \tag{5}
\]

where the constant of integration \(b\) is identified as the position of the kink centre.

Upon discretization, \(x\) takes values in \(h\mathbb{Z} = \{0, \pm h, \pm 2h, \ldots\}\), where \(h\) is the lattice spacing. It is convenient to introduce the notation \(f_+(x) = f(x + h)\) and \(f_-(x) = f(x - h)\) for forward and backward shifted versions of any function \(f\), and \(\Delta f = h^{-1}(f_+ - f)\) for the forward difference operator. Ward’s idea is to seek a discrete version of the potential energy of the form

\[
E_P = h \sum_x \left( \frac{1}{2} D^2 + \frac{1}{8} F^2 \right) \tag{6}
\]

where \(D \to \partial \phi / \partial x\) and \(F \to (1 - \phi^2)\) in the continuum limit \(h \to 0\), and \(D\) and \(F\) have the product

\[
DF = -\Delta \left( \frac{\phi^3}{3} - \phi \right) \tag{7}
\]
Such a lattice potential energy clearly has the correct continuum limit. The crucial point is that, given (7), the discrete system has a Bogomol’nyi argument exactly analogous to its continuum counterpart. Let \( \phi : h\mathbb{Z} \to \mathbb{R} \) have kink boundary conditions. Then

\[
0 \leq \frac{h}{2} \sum_x \left( D - \frac{1}{2} F \right)^2 = E_P - \frac{h}{2} \sum_x DF
\]

\[
= E_P + \frac{h}{2} \sum_x \Delta \left( \frac{1}{3} \phi^3 - \phi \right) = E_P - \frac{2}{3},
\]

using the boundary conditions \( \phi \to \pm 1 \) as \( x \to \pm \infty \). It follows that \( E_P \geq \frac{2}{3} \) with equality if and only if \( \phi \) satisfies the lattice Bogomol’nyi equation,

\[ D = \frac{1}{2} F. \tag{9} \]

The most natural choice of \( D \) and \( F \) seems to be \[ D = \Delta \phi \]

\[ F = 1 - \frac{1}{3} (\phi_+^2 + \phi_+ \phi + \phi^2), \tag{10} \]

which clearly have the correct continuum limits, and are easily shown to satisfy equation (9). Note that the lattice Bogomol’nyi equation (9) is a first order difference equation, while the static field equation,

\[ \frac{\partial E_P}{\partial \phi} = 0 \tag{11} \]

is a second order difference equation. We have shown that if a solution of (9) exists with kink boundary conditions then it is a global minimal of \( E_P \) (within the kink sector) with energy \( \frac{2}{3} \), and hence a static kink solution. The next section is devoted to proving the existence of such solutions.

We will refer to this lattice system as the topological discrete \( \phi^4 \) system (TD\( \phi^4 \)S) since it preserves the topological lower bound on kink energy. The conventional discrete \( \phi^4 \) system also has a potential energy of the form (6), but while \( D \) is the same (a standard forward difference), \( F \) is chosen to be the same as in the continuum model, \( F = 1 - \phi^2 \). In this case, the Bogomo’nyi argument is lost. So the essential difference here is that we have “distributed” the double well substrate potential over pairs of nearest neighbour lattice sites. In both discrete systems, one completes the dynamics by defining the obvious kinetic energy functional,

\[ E_K = \frac{h}{2} \sum_x \dot{\phi}^2. \tag{12} \]

Other interesting choices can be made [4], but this is the simplest.

### 3 The kink moduli space

We start with a definition: a two-sided sequence \( \phi : h\mathbb{Z} \to \mathbb{R} \) is a static kink if it is a solution of the Bogomol’nyi equation (9), is monotonic and converges to 1 at \( \infty \) and \(-1 \) at \(-\infty \). The space of all static kinks is called the kink moduli space, denoted, for a particular value of \( h \), by \( M_h \).

Given that discretization has broken the continuous translation symmetry of the continuum model to symmetry under integer translations by \( h \), one would expect \( M_h \) to be discrete. This is indeed true for conventional discrete systems, where kinks must lie halfway between or exactly on top of lattice sites, the difference in energy between these two types of static solution being the origin of
the PN barrier, which so complicates the kink dynamics. However, the TDφ4S, remarkably, has a continuous moduli space: static kinks may take any position relative to the lattice. All such kinks saturate the Bogomol’nyi bound on energy, so there is no PN barrier resisting their propagation through the lattice. Specifically, we will prove,

**Proposition 1** If \( h \in (0, 2] \) then for all \( \phi_0 \in (-1, 1) \) there exists a unique static kink with \( \phi(0) = \phi_0 \).

Note that a continuous translation orbit of kinks can equally well be parametrized by kink position \( b \in \mathbb{R} \) (defined, for example by linear interpolation) or by the value of the field at \( x = 0 \), \( \phi(0) \in (-1, 1) \). So proposition 1 could be rephrased: for all \( h \in (0, 2] \), \( M_h = \mathbb{R} \). This is the important result for our purposes. It is also interesting to consider what happens to the kink moduli space for \( h > 2 \). In fact, except for some special values of \( h \in (2, 3] \), \( M_h = \emptyset \). However, for an infinite discrete subset of \((2, 3], M_h = h\mathbb{Z} \). Precisely,

**Proposition 2** For \( h > 3 \) there exist no static kinks. There exists a strictly decreasing sequence \( h_n \) with \( h_0 = 3 \) and \( \lim_{n \to \infty} h_n = 2 \) such that if \( h = h_n \) there exists exactly one static kink (modulo lattice translations). This kink is symmetric about its central site(s) and has exactly \( n + 1 \) sites different from \( \pm 1 \).

**Proof of proposition 1**: Since the Bogomol’nyi equation,

\[
\frac{\phi_{+}^{2}}{6} + \left( \frac{6}{h} + \phi \right) \phi_{+} + \left( \phi^{2} - \frac{6}{h} \phi - 3 \right) = 0
\]

is forward backward symmetric, that is, invariant under \((\phi_{+}, \phi) \mapsto (-\phi, -\phi_{+})\), it suffices to prove that for any \( h \in (0, 2] \) the right hand sequence converges to 1 for all \( \phi(0) \in (-1, 1) \). Note that given \( \phi \in (-1, 1) \), equation (13) does not uniquely determine \( \phi_{+} \) since both roots are real. However, the lower root is always less than \( \phi \), and we seek monotonic solutions, so we can discard the lower root at each iteration. It follows that if a static kink with \( \phi(0) = \phi_0 \in (-1, 1) \) exists, it is unique.

It remains to prove convergence to 1 of the sequence

\[
\phi(nh) = f^n(\phi_0)
\]

generated by iterating upper root of equation (13), starting at any value \( \phi_0 \in (-1, 1) \) and assuming that \( 0 < h \leq 2 \). Here \( f^n \) denotes the \( n \)-th composition of \( f \) (so \( f^0 = \text{Id} \)), and

\[
f(q) = \frac{1}{2} \left[ - \left( \frac{6}{h} + q \right) + \sqrt{\left( \frac{6}{h} + q \right)^2 - 4 \left( q^2 - \frac{6}{h} q - 3 \right)} \right]
\]

A straightforward calculation shows that on \([-1, 1], f(q) \geq q \), the only fixed points being \( \pm 1 \). Furthermore, \( f(q) > 1 \) if and only if \( q \in I_h \), this being the interval \((\gamma - |\gamma - 1|, \gamma + |\gamma - 1|)\) where \( \gamma = 3h^{-1} - 2^{-1} \). Since \( I_h \cap [-1, 1] = \emptyset \) if \( h \leq 2 \), we find that \( f \) is bounded above by 1 on \([-1, 1] \). So the sequence \( f^n(\phi_0) \) is monotonic and bounded, and hence, by the monotone convergence theorem, convergent. Call its limit \( L \). We have established that \( f : [-1, 1] \to [-1, 1] \), so the sequence \( f^n(\phi_0) \) lies in the interval \([-1, 1] \). Either there exists \( N \in \mathbb{N} \) such that \( f^n(\phi_0) = L \) for all \( n \geq N \) or \( L \) is an accumulation point of \([-1, 1] \). In either case \( L \in [-1, 1] \) since \([-1, 1] \) is closed. Consider then the image of the sequence \( f^n(\phi_0) \) under \( f \). Since \( f \) is continuous, \( f(f^n(\phi_0)) \to f(L) \). But \( f(f^n(\phi_0)) \) is a subsequence of \( f^n(\phi_0) \), so converges to \( L \). Hence \( L \) is a fixed point of \( f \), and since \( L \) cannot be \(-1 \), it follows that \( \phi(nh) \to 1 \). \( \square \)

It is interesting to compare the situation with that of the topological discrete sine-Gordon (TDSG) system [4]. There, one is fortunate enough to have an explicit formula for the static kink
solution, obtained by slightly modifying the continuum kink. One finds that \( M_h = \mathbb{R} \) for all \( h < 2 \), but the “proof” of this fact rests on the observation that the explicit formula has a continuous real-valued parameter in it. Unfortunately, no continuum-inspired ansatz seems to work for the TD\( \phi^4 \)S Bogomol’nyi equation, so we are forced to give a less constructive proof. Note that in both systems the kink moduli space degenerates at \( h = 2 \). This may seem an artificial coincidence which would be lost if different normalizations were used, but in fact the TD\( \phi^4 \)S was normalized specifically so that the minimum phonon frequency (the angular frequency of small amplitude travelling waves) is unity, as in the TDSG system. One then finds that both systems have the same phonon dispersion relation,

\[
\omega^2 = \frac{4 + h^2}{4h^2} - \frac{4 - h^2}{2h^2} \cos kh
\]

obtained by substituting a travelling wave ansatz \( \cos(kx - \omega t) \) with frequency \( \omega \) and wavenumber \( k \) into the linearized equation of motion (linearized about the vacuum \( \phi = 1 \), not \( \phi = 0 \)). So in both systems \( M_h \) degenerates precisely where the phonon dispersion relation collapses to a flat line. Since there is no obvious relation between the existence of kinks, a nonlinear phenomenon, and the radiation of the system, a linear phenomenon, this coincidence is rather strange. One difference between the two systems is that, whereas there are no kinks for \( h > 2 \) in the TDSG system, there are kinks in the TD\( \phi^4 \)S for certain discrete values of \( h \) in \( (2, 3] \), as stated in proposition 2, to whose proof we now turn.

**Proof of proposition 2:** We adopt the definitions and notation used in the proof of proposition 1. As stated above, \( f(q) > 1 \) if \( q \in I_h \), so a static kink must have \( \phi(0) \notin I_h \). Consider the backwards iteration \( \phi_- = f(\phi) \). By forward-backward symmetry, \( f(q) < -1 \) if \( q \in \bar{I}_h = (-\gamma - |\gamma - 1|, -\gamma - |\gamma - 1|) \), where \( \gamma \) was defined above. So any static kink must also have \( \phi(0) \notin \bar{I}_h \). If \( h > 3 \) then \((-1, 1) \subset I_h \cup \bar{I}_h \). Hence there exists no static kink for \( h > 3 \).

Let \( h \in (2, 3] \) and \( \phi(x) \) be a static kink. Since \( \lim_{x \to \pm \infty} \phi = \pm 1 \), either \( \phi(\pm x) = \pm 1 \) for all \( x > Nh \) for some \( N \in \mathbb{Z}^+ \), or either \( 1 \) or \( -1 \) is an accumulation point of the sequence. The latter cannot be the case since \( \phi \) is bounded away from \( 1 \) and \( -1 \) by the intrusion of \( I_h \) and \( \bar{I}_h \) into \([-1, 1]\) respectively (see figure 1). So the static kink must be constant away from its centre. This is possible if and only if there exists \( n \in \mathbb{N} \) such that

\[
f^n(-\gamma + |\gamma - 1|) = \gamma - |\gamma - 1| \tag{17}
\]

where \( f^n \) again denotes the \( n \)-th composition of \( f \). For then if \( \phi(0) = -\gamma + |\gamma - 1| \), the backward sequence jumps immediately to \(-1\), which is a fixed point, and the forward sequence leads, after \( n \) iterations to \( \gamma - |\gamma - 1| \), which is subsequently mapped to the fixed point 1. Clearly such a kink is unique modulo lattice translations, is symmetric and has \( n + 1 \) sites different from \( \pm 1 \). For example, if \( h = 3 \) then \(-\gamma + |\gamma - 1| = 0 \) so there is a static kink with \( \phi(0) = 0 \) and \( \phi(x) = x/|x| \) elsewhere. The only other static kinks are obtained by lattice translation of this one.

So for each \( n \in \mathbb{N} \) there is an \( n + 1 \) site kink in the system with spacing \( h = h_n \) where \( h_n \) is a solution of equation (17); \( h_0 = 3 \) is a solution with \( n = 0 \). We seek to prove the existence of a decreasing sequence of such solutions, \((h_n)_n\), converging to 2. Let \( \chi = \gamma - |\gamma - 1| \), so \( h \in [2, 3] \Rightarrow \chi \in [0, 1] \), and define \( g(\chi) = -f(-\chi) \), a graph of which is presented in figure 2. Then the condition (17) for the existence of a static kink can be rewritten

\[
g^n(\chi) = -\chi \tag{18}
\]

Note that \( g(0) = -1, g(1) = 1 \) and \( g \) is continuous, so \( g \) has a root, call it \( r_1 \), between 0 and 1, and so there exists a solution \( \chi_1 \) of \( g(\chi) = -\chi \) in \((0, r_1)\). Now, if \( g^n \) has a root \( r_n \in (0, 1) \), then \( g^{n+1} \) has a root \( r_{n+1} \in (r_n, 1) \) since \( g^{n+1}(r_n) = -1 \) and \( g^{n+1}(1) = 1 \). Hence, by induction, for each
Having established that kinks of the TD$^4$S experience no PN barrier, the question arises whether the resulting kink dynamics is consequently simpler than that customarily observed in discrete systems. We address this question by performing numerical simulations of the lattice equation of motion. This involves approximately solving the following system of coupled nonlinear o.d.e’s,

$$\ddot{\phi} = \frac{1}{\hbar^2} (\phi_+ - 2\phi + \phi_-) + \frac{1}{12} \left[ (2\phi + \phi_-) \left( 1 - \frac{1}{3} (\phi^2 + \phi_\phi - + \phi_\phi^2) \right) + (2\phi + \phi_+) \left( 1 - \frac{1}{3} (\phi^2 + \phi_\phi + + \phi_\phi^2) \right) \right]$$

(20)

on a large (but finite) lattice, with a Lorentz boosted continuum kink solution as initial data. (Although it would be straightforward to generate a genuine discrete static kink for the initial profile, there is no obvious way to boost it, without an explicit formula. In any case, the point of the endeavour is to simulate continuum kink dynamics.) Simulations were performed with a variety of lattice spacings and initial kink velocities. The solutions were generated using a simple fourth order Runge-Kutta scheme.

In every case it was found that the kink moves freely through the lattice, without being pinned (see figure 4), exciting small amplitude travelling waves which propagate backwards in its wake. To reduce reflexion of this radiation from the fixed left hand boundary during long simulations, the first few lattice sites were damped. Figure 5 presents plots of velocity against time for several
long duration simulations. (The thickness of the curve is due to velocity oscillations as the kink passes from cell to cell. This dynamical wobble is not caused by any PN type potential, but can be understood in terms of geodesic motion on the moduli space $M_h$ with respect to a periodic metric. After an initial drop in velocity as the kink relaxes to a profile more suited to the discrete system, subsequent kink deceleration is very modest, even at high speed ($v = 0.6$) and on coarse lattices.

This behaviour should be contrasted with that of the standard discrete system, whose equation of motion,

$$\ddot{\phi} = \frac{1}{h^2}(\phi_+ - 2\phi + \phi_-) + \frac{1}{2}\phi(1 - \phi^2)$$

(21)

was solved using the same algorithm and initial data, for purposes of comparison (also figure 5). These results are similar to those obtained by Combs and Yip in their work on the conventional discrete $\phi^4$ system. One sees that at every value of $h$, kink dynamics in the TD$\phi^4S$ is far less dissipative, the difference being more pronounced for larger $h$. Indeed, a kink set off with a speed $v = 0.6$ on a lattice with $h = 1.8$ quickly becomes trapped in the conventional system (figure 6), but remains free (apparently) indefinitely in the TD$\phi^4S$.

5 Concluding remarks

In this paper we have shown that by choosing a discretization which preserves the Bogomol'nyi bound on kink energy, one can find a discrete $\phi^4$ system which has no Peierls-Nabarro potential. The resulting kink dynamics is much simpler than one expects of a discrete system, even on coarse lattices. The kinks are never pinned, and suffer only modest radiative deceleration. So the TD$\phi^4S$ is an efficient and natural choice of discretization for numerical study of the continuum $\phi^4$ model.

In higher dimensional field theories with topological solitons (the $O(3)$ sigma, Skyrme and abelian Higgs models for example) the reduction in computational cost would be quite significant if similarly natural discretizations could be found. Here, however, there is an extra concern: solitons on high dimensional lattices tend to be unstable because they can unwind and "fall through" a single plaquette. One way to preserve the stability of the continuum model is again to preserve the Bogomol'nyi bound on soliton energy, an approach pursued by Ward for two planar field theories. In this case it seems impossible to eliminate the PN barrier entirely, although one can attempt to reduce it as much as possible. It would be interesting to see to what extent these discrete systems have continuum-like soliton dynamics, as has been found here for $\phi^4$ kinks, and elsewhere for sine-Gordon kinks.

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Figure captions

Figure 1: The shaded region, excluding boundaries, represents $\phi$ values which get mapped outside the interval $[-1, 1]$ under either forward or backward iteration of the Bogomol’nyi equation. The intersection of any vertical line with this region is $I_h \cup \tilde{I}_h$.

Figure 2: The function $g(\chi)$ of the proof of proposition 2.

Figure 3: A static kink of the model with $h = 1.5$. Circles represent the kink profile itself, while the solid line represents its energy distribution, which should be regarded as residing in the links between lattice sites. Note the extreme discreteness of this structure: over 99% of the kink’s energy is carried by the 4 central links.

Figure 4: Propagation of a kink through the lattice of spacing $h = 1$, with an initial speed $v = 0.2$. Note the apparent lack of radiation in the kink’s wake.

Figure 5: Comparison of the motion of fast kinks (initial velocity $v = 0.6$) in the TD$\phi^4$S with that in the conventional discrete system, for lattices of spacing $h = 1.0, h = 1.4$ and $h = 1.8$. In each case velocity is plotted against time for both systems on the same graph, the upper curve showing the TD$\phi^4$S data and the lower curve showing the conventional system data. The difference is particularly striking for $h = 1.8$, since the kink quickly becomes pinned in the conventional system, while it remains free indefinitely in the TD$\phi^4$S.

Figure 6: Kink pinning in the conventional system with $h = 1.8$. Set off at a speed of 0.6, the kink manages to travel through only 8 lattice cells before being trapped by the PN barrier. This should be compared with the dynamics of a TD$\phi^4$S kink on the $h = 1.8$ lattice, which remains free indefinitely and after 3000 time units has decelerated by less than 17%. 

8
$h = 1.5$
h=1.8
The graph shows the kink position over time with $h=1.8$. The x-axis represents time $t$ and the y-axis represents the kink position.