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Abstract

A spatially discrete version of the general kink-bearing nonlinear Klein-Gordon model in $(1+1)$ dimensions is constructed which preserves the topological lower bound on kink energy. It is proved that, provided the lattice spacing h is sufficiently small, there exist static kink solutions attaining this lower bound centred anywhere relative to the spatial lattice. Hence there is no Peierls-Nabarro barrier impeding the propagation of kinks in this discrete system. An upper bound on h is derived and given a physical interpretation in terms of the radiation of the system. The construction, which works most naturally when the nonlinear Klein-Gordon model has a squared polynomial interaction potential, is applied to a recently proposed continuum model of polymer twistons. Numerical simulations are presented which demonstrate that kink pinning is eliminated, and radiative kink deceleration greatly reduced in comparison with the conventional discrete system. So even on a very coarse lattice, kinks behave much as they do in the continuum. It is argued, therefore, that the construction provides a natural means of numerically simulating kink dynamics in nonlinear Klein-Gordon models of this type. The construction is compared with the inverse method of Flach, Zolotaryuk and Kladko. Using the latter method, alternative spatial discretizations of the twiston and sine-Gordon models are obtained which are also free of the Peierls-Nabarro barrier.

1 Introduction

A major difficulty in the study of soliton dynamics in the context of high energy physics is that the requirement of Lorentz invariance appears incompatible with integrability, at least for Lagrangian field theories in spacetimes of realistic dimension. The PDEs of most interest, therefore, are nonintegrable, and there is no prospect of finding interesting exact solutions of multisoliton initial value problems. This is why numerical simulation is a popular and important tool. In performing numerical simulations one is forced to discretize space in some way, and this inevitably introduces fictitious discretization effects, which one should seek to minimize.

The standard discretization of a field equation (in which spatial partial derivatives are replaced by simple difference operators, nothing else being changed) replaces it with an infinite system of coupled ODEs, representing a network of identical oscillators, nearest neighbours being coupled by springs. Such networks have been extensively studied in recent years [1, 2, 3], primarily because of their condensed matter and biophysical applications. The crucial discretization effect encountered is that static solutions may no longer be centred at an arbitrary position in space, but must lie exactly on a lattice site, or at the centre of a lattice cell. These two types of static solution have different energies (one is a saddle point, the other a minimum), so there is an energy barrier, called the Peierls-Nabarro (PN) barrier, resisting the free propagation of solitons from cell to cell. As a soliton moves through the lattice, its motion in and out of the PN potential excites small amplitude traveling waves in its wake (radiation, or phonons) which drain its kinetic energy, causing it to decelerate. Sometimes the kink slows down so much that it has insufficient energy to surmount the PN barrier, whereupon it becomes pinned to a lattice cell.

Clearly, this behaviour is very different from soliton dynamics in the continuum, so if the standard discretization is to be used the height of the PN barrier must be made negligible by using a very fine spatial lattice, with spacing h of order (soliton width)/20, say. This is computationally expensive. An alternative approach, due to Richard Ward, is to exploit the non-uniqueness of the discretization process to find a discretization with no PN barrier at all. The hope would then be that the discrete soliton dynamics would closely mimic its continuum counterpart even on very coarse lattices, with say h of order soliton width.

How does one find such a discretization? Ward's idea is to construct a discrete system which naturally preserves the “Bogomol'nyi” properties of its continuum counterpart, that is, a topological lower bound on soliton energy which is attained by solutions of some sort of first order self-duality equation. Of course, the continuum system one starts with must be of Bogomol'nyi type, but most systems of interest in particle theory are (e.g. BPS monopoles, instantons, sigma model lumps, vortices, kinks). The idea has proved very successful in the cases of sine-Gordon and ϕ^4 kink dynamics [4, 5]; that is, it was found that kink pinning was eliminated, and radiative deceleration greatly reduced in comparison with the standard discretizations. Unfortunately, work on higher dimensional systems (where the benefit of a coarse lattice would be greatest) has been less encouraging [6]. It is possible to find discretizations of some planar models which preserve the Bogomol'nyi bound on soliton energy (and this ensures that the solitons are more stable than they would otherwise be), but the bound is unattainable, and there is no discrete self-duality equation. So the PN barrier persists, although it is reduced to some extent. Alternatively, by imposing rotational symmetry one can find discretizations with saturable Bogomol'nyi bounds [7, 8] but then, of course, the system is effectively one-dimensional.

The purpose of this paper is to demonstrate that Ward's idea works completely generally for relativistic one-dimensional kinks. More precisely, we will construct a “topological” discretization of a general nonlinear Klein-Gordon theory in \mathbb{R}^{1+1} . This will, by construction, preserve the familiar Bogomol'nyi bound on kink energy. We will then prove that there exist static kinks saturating this bound centred *anywhere* relative to the lattice, so that there is no PN barrier in this discretization. The construction is a generalization of the topological discrete ϕ^4 system previously mentioned [5]. As an extra example, we apply the construction to a recently proposed continuum model of polymer twistons [9], and again find that elimination of the PN barrier leads to continuum-like dynamics deep within the discrete regime.

2 Relativistic kinks

The nonlinear Klein-Gordon system consists of a scalar field $\phi : \mathbb{R}^{1+1} \rightarrow \mathbb{R}$ whose dynamics is governed by the Lagrangian $L = E_K - E_P$, the kinetic and potential energy functionals being, respectively,

$$\begin{aligned} E_K &= \frac{1}{2} \int_{-\infty}^{\infty} dx \dot{\phi}^2, \\ E_P &= \frac{1}{2} \int_{-\infty}^{\infty} dx \left[\left(\frac{\partial \phi}{\partial x} \right)^2 + F_c(\phi)^2 \right]. \end{aligned} \quad (1)$$

The field equation is the Euler-Lagrange equation obtained by demanding that ϕ be a local extremal of the action $S = \int dt L$. The following restrictions are made on F_c so as to ensure that kink solutions exist: $F_c \in C^1(\mathbb{R}, \mathbb{R})$, $2 \leq \text{card}(F_c^{-1}(0)) \leq \aleph_0$, and for all $u \in F_c^{-1}(0)$, $F'_c(u) \neq 0$. So the model has at least 2 and at most countably many degenerate zero vacua, which we label so that $F_c^{-1}(0) = \{u_i : i \in J\}$ where $J \subseteq \mathbb{Z}$ is a (perhaps unbounded) set of consecutive integers, $0 \in J$, and $i > j \Rightarrow u_i > u_j$. Given these restrictions, F_c must change sign at every u_i . It is convenient to label the vacua so that F_c is positive on (u_i, u_{i+1}) whenever i is even (hence negative when i is odd). For any pair $i, j \in J$, $|i - j| = 1$, by a type (i, j) kink we mean any finite energy solution of the field equation with the boundary behaviour

$$\phi(x, t) \rightarrow \begin{cases} u_i & x \rightarrow -\infty \\ u_j & x \rightarrow \infty, \end{cases} \quad (2)$$

for all t . It would be conventional to call these “antikinks” in the case where i is odd, but the distinction is rather cumbersome for our purposes, and will not be made.

Static type (i, j) kinks may be obtained by a Bogomol'nyi argument [10]. To this end, let

$$G(\phi) := \int_0^\phi d\psi F_c(\psi). \quad (3)$$

Clearly, $G \in C^2(\mathbb{R}, \mathbb{R})$ and $G' = F_c$. Stable static solutions are local minimals of $E_P[\phi]$. Assuming $\phi : \mathbb{R} \rightarrow \mathbb{R}$ has boundary behaviour (2), we have,

$$E_P[\phi] = \frac{1}{2} \int_{-\infty}^{\infty} dx \left[\frac{d\phi}{dx} - (-1)^i F_c(\phi) \right]^2 + (-1)^i \int_{-\infty}^{\infty} dx \frac{d\phi}{dx} F_c(\phi)$$

$$\begin{aligned}
&\geq (-1)^i \int_{u_i}^{u_j} d\phi F_c(\phi) \\
&= |G(u_j) - G(u_i)|.
\end{aligned} \tag{4}$$

The factor $(-1)^i$ is included to ensure an optimal bound whether i is even or odd. So, assuming type (i, j) boundary behaviour, $E_P \geq |G(u_j) - G(u_i)|$, with equality if and only if the Bogomol'nyi equation,

$$\frac{d\phi}{dx} = (-1)^i F_c(\phi), \tag{5}$$

holds. This first order ODE is readily reduced to quadratures. Let I_{ij} be the open interval between u_i and u_j . Then, for each $\phi_0 \in I_{ij}$, there exists a unique solution of (5) with boundary behaviour (2) and $\phi(0) = \phi_0$. The set of such solutions constitutes a translation orbit of any one of them, since for each fixed x , $\phi(x)$ is a monotonic function of ϕ_0 . So we may parametrize the moduli space of static (i, j) kinks, M_{ij}^c , by $\phi_0 \in I_{ij}$, just as well as by kink position, defined for example by $b = \phi^{-1}(\frac{1}{2}(u_i + u_j))$. The former parametrization generalizes more naturally to discrete systems than does the latter.

For purposes of comparison with the discrete case, we remark that the full field equation is

$$\ddot{\phi} = \frac{\partial^2 \phi}{\partial x^2} - F'_c(\phi) F_c(\phi). \tag{6}$$

Note that the static field equation is a second order ODE, while the Bogomol'nyi equation (5) is first order.

3 Topological discretization

From now on, x takes values in a lattice of spacing $h > 0$, so $x \in h\mathbb{Z} = \{0, \pm h, \pm 2h, \dots\}$. We introduce the notation f_+ and f_- for forward and backward shifted versions of any function $f : h\mathbb{Z} \rightarrow \mathbb{R}$, that is $f_{\pm}(x) := f(x \pm h)$. Also, we denote by Δ the forward difference operator: $\Delta f := h^{-1}(f_+ - f)$. Discretization of the nonlinear Klein-Gordon system proceeds by defining discrete versions of E_K and E_P . These take the form

$$\begin{aligned}
E_K &= \frac{h}{2} \sum_{x \in h\mathbb{Z}} \dot{\phi}^2, \\
E_P &= \frac{h}{2} \sum_{x \in h\mathbb{Z}} [(\Delta\phi)^2 + F^2],
\end{aligned} \tag{7}$$

where F is a function of ϕ, ϕ_+ which will be defined below. This will have the correct continuum limit provided that $\lim_{\phi_+ \rightarrow \phi} F(\phi, \phi_+) = F_c(\phi)$.

We shall choose F as follows:

$$F(\phi, \phi_+) = \begin{cases} \frac{G(\phi_+) - G(\phi)}{\phi_+ - \phi} & \phi \neq \phi_+ \\ F_c(\phi) & \phi = \phi_+. \end{cases} \tag{8}$$

This looks singular when $\phi = \phi_+$, but in fact $F : \mathbb{R}^2 \rightarrow \mathbb{R}$ is C^1 as may be shown by using local compactness of \mathbb{R} and Taylor's Theorem. (The practicalities of evaluating F in a computer algorithm will be discussed in section 5.) The important point is that for all ϕ, ϕ_+ ,

$$(\Delta\phi)F = \Delta G, \tag{9}$$

and this allows one to make a Bogomol'nyi argument analogous to that in section 2. Namely, assuming that ϕ has type (i, j) boundary behaviour,

$$\begin{aligned}
E_P[\phi] &= \frac{h}{2} \sum_{x \in h\mathbb{Z}} [\Delta\phi - (-1)^i F]^2 + (-1)^i h \sum_{x \in h\mathbb{Z}} (\Delta\phi)F \\
&\geq (-1)^i h \sum_{x \in h\mathbb{Z}} \Delta G \\
&= |G(u_j) - G(u_i)|,
\end{aligned} \tag{10}$$

so this gives a lower bound on type (i, j) kink energy, which is attained if and only if

$$\Delta\phi = (-1)^i F, \quad (11)$$

which will henceforth be called the discrete Bogomol'nyi equation (DBE).

What this argument shows is that *if* solutions of the DBE exist with the correct boundary behaviour, then they are minimals of E_P within their class, and hence static solutions of the model. Existence of such solutions centred *anywhere* relative to the lattice will be proved in section 4. Since all such solutions have energy $|G(u_j) - G(u_i)|$, the kinks experience no PN barrier.

The discrete field equation is again the Euler-Lagrange equation for the action $S = \int dt (E_K - E_P)$:

$$\ddot{\phi} = \frac{\phi_+ - 2\phi + \phi_-}{h^2} - F(\phi, \phi_+)F_1(\phi, \phi_+) - F(\phi, \phi_-)F_1(\phi, \phi_-), \quad (12)$$

where F_1 is the partial derivative of $F : \mathbb{R} \times \mathbb{R} \rightarrow \mathbb{R}$ with respect to the first factor, and symmetry of F (under $\phi \leftrightarrow \phi_+$) has been used. The static field equation is a second order nonlinear difference equation, in contrast with the DBE (11) which is first order.

The system should be compared with the standard discrete nonlinear Klein-Gordon system whose kinetic energy is the same, but whose potential energy is

$$E_P = \frac{h}{2} [(\Delta\phi)^2 + F_c(\phi)^2]. \quad (13)$$

So the topological discretization differs only in that its “substrate” potential has been symmetrically distributed over pairs of nearest neighbours. In the standard discrete system, the Bogomol'nyi argument is lost. The discrete field equation is

$$\ddot{\phi} = \frac{\phi_+ - 2\phi + \phi_-}{h^2} - F_c(\phi)F'_c(\phi). \quad (14)$$

4 Continuity of the kink moduli space

It is convenient to make the following definition: a type (i, j) static kink (where $|i - j| = 1$, as before) is a monotonic mapping $\phi : h\mathbb{Z} \rightarrow \mathbb{R}$ having (i, j) boundary behaviour (2) and satisfying the DBE (11) everywhere. Since the continuous translation symmetry of the continuum model has been broken to symmetry under integer translations by h , there is no reason to expect *a priori*, the existence of a continuous “translation orbit” of static kink solutions. Indeed, in conventional discretizations, the (i, j) kink moduli space (that is, the set of type (i, j) static kink solutions) is $M_{ij}(h) = \frac{h}{2}\mathbb{Z}$, the PN barrier being the difference in E_P between “odd” and “even” members of this set. By contrast, we will prove that the topological discrete system defined in section 3 has static kinks centred anywhere relative to the lattice, so $M_{ij}(h) = \mathbb{R}$, at least for h sufficiently small.

The idea behind the proof, which will be presented only for the case of even i (the odd i case follows *mutatis mutandis*), is that any pair (ϕ, ϕ_+) satisfying the DBE (11) may be associated with a point on the intersection curve of the plane $\phi - \phi_+ + hz = 0$ with the surface $z = F(\phi, \phi_+)$ in (ϕ, ϕ_+, z) space. If $h = 0$, the plane is vertical, and the vertical projection of this curve onto the (ϕ, ϕ_+) plane is clearly the graph of a function g interpolating between (u_i, u_i) and (u_j, u_j) (namely, $g = \text{Id}$). If $h > 0$, but very small, the plane tilts slightly away from the vertical, but one may show that such a function persists, and the sequence generated by iteration of g on any $\phi_0 \in I_{ij}$, a solution of the DBE by construction, has the required convergence properties.

Theorem For any pair $i, j \in J$ such that $|i - j| = 1$, there exists $h_* > 0$ such that for all $h \in (0, h_*)$ and for all $\phi_0 \in I_{ij}$ there exists a type (i, j) static kink with $\phi(0) = \phi_0$.

Proof: Let i be even. Given any C^1 function $m : \mathbb{R}^n \rightarrow \mathbb{R}$, m_p denotes its partial derivative with respect to the p -th factor. Also, any bounded open interval $(z - \epsilon, z + \epsilon)$ will be denoted $B_\epsilon(z)$. We first note that the only fixed points of the DBE

$$\frac{\phi_+ - \phi}{h} = F(\phi, \phi_+) \quad (15)$$

are the vacua, since $\phi_+ = \phi \Rightarrow F(\phi, \phi) = F_c(\phi) = 0$. Now, one may regard a pair (ϕ, ϕ_+) satisfying (15) as a zero of the C^1 function $f : \mathbb{R}^3 \rightarrow \mathbb{R}$

$$f(\phi_+, \phi, h) = \phi_+ - \phi - hF(\phi, \phi_+). \quad (16)$$

Note that for any $\psi \in \mathbb{R}$, $f(\psi, \psi, 0) = 0$ and $f_1(\psi, \psi, 0) = 1 \neq 0$, so by the Implicit Function Theorem, for every $\psi \in \mathbb{R}$ there exists $\epsilon_\psi > 0$ and a C^1 function $g : B_{\epsilon_\psi}(\psi) \times B_{\epsilon_\psi}(0) \rightarrow \mathbb{R}$ such that $\phi_+ = g_\psi(\phi, h)$ is the unique solution of $f(\phi_+, \phi, h) = 0$ in $B_{\epsilon_\psi}(\psi)$ for any $(\phi, h) \in \text{dom} g_\psi$. Consider any closed bounded interval $I \subset \mathbb{R}$. Since I is compact, the open covering $\{B_{\epsilon_\psi}(\psi) : \psi \in I\}$ has a finite subcovering, $\{B_{\epsilon_n}(\psi_n) : n = 1, 2, \dots, N\}$, which can be used to construct a C^1 function $g : I \times B_\epsilon(0) \rightarrow \mathbb{R}$ where $\epsilon = \inf_n \epsilon_n > 0$. Namely,

$$g(\phi, h) = g_{\psi_n}(\phi, h) \quad \text{if } \phi \in (\psi_n - \epsilon_n, \psi_n + \epsilon_n). \quad (17)$$

This is well defined by the local uniqueness of each g_{ψ_n} . For each $(\phi, h) \in I \times (-\epsilon, \epsilon)$, $\phi_+ = g(\phi, h)$ is the locally unique solution of (15).

Consider the case $I = \overline{I}_{ij}$, the closure of the interval I_{ij} . We claim that there exists $h_* \in (0, \epsilon)$ such that for every $h \in [0, h_*)$, $g(\cdot, h) : \overline{I}_{ij} \rightarrow \mathbb{R}$ is strictly increasing. To see this, note that $g(\cdot, 0) = \text{Id}$, so $g_1(\phi, 0) = 1 > 0$. Now g_1 is uniformly continuous on, say, $\overline{I}_{ij} \times [-\frac{\epsilon}{2}, \frac{\epsilon}{2}]$, so there exists $h_* \in (0, \frac{\epsilon}{2}]$ such that for all $h \in [0, h_*)$ $g_1(\cdot, h) : \overline{I}_{ij} \rightarrow \mathbb{R}$ is bounded away from 0.

Since the endpoints u_i, u_j are fixed points of g , an immediate consequence is that for all $h \in (0, h_*)$, $g(\cdot, h)$ is an increasing C^1 mapping $\overline{I}_{ij} \rightarrow \overline{I}_{ij}$, which we denote by simply g for the rest of this proof. Hence, for any $\phi_0 \in I_{ij}$ the double-sided iteration sequence $\phi(nh) = g^n(\phi_0)$ exists and is a solution of the DBE (15) ($g^0 := \text{Id}$ and for $n < 0$, $g^n := (g^{-1})^{|n|}$, the existence of the inverse being guaranteed since g is increasing). By monotonicity of g , for fixed $n \in \mathbb{Z}$, $\phi(nh)$ is an increasing function of ϕ_0 . There can be no fixed points of g other than the endpoints (because $|i - j| = 1$), so either

$$\begin{aligned} \text{case A:} \quad & g(\phi) > \phi \quad \forall \phi \in I_{ij} \\ \text{or case B:} \quad & g(\phi) < \phi \quad \forall \phi \in I_{ij}. \end{aligned}$$

Given our definition of F_c , case A occurs when $i < j$ and case B when $i > j$ (recall we have assumed that i is even).

Case A: the iteration sequence is increasing, bounded above by u_j and below by u_i and hence both left and right convergent. Since \overline{I}_{ij} is closed, it contains L, R , the left and right limits. Consider the image of the forward sequence $\phi(nh)$, $n \geq 1$ under g . Since g is continuous, $g(\phi(nh)) \rightarrow g(R)$. But $g(\phi(nh))$ is a subsequence of $\phi(nh)$ and hence converges to R . Hence R is a fixed point of g , and so $R = u_j$. Similarly, considering the image of the sequence $\phi(-nh)$, $n \geq 1$, under g^{-1} one concludes that $L = u_i$. Hence ϕ has the correct limiting behaviour.

Case B: now the iteration sequence is decreasing and bounded above by u_i and below by u_j . A similar argument shows that $\phi(nh) \rightarrow u_i$ as $n \rightarrow -\infty$ and $\phi(nh) \rightarrow u_j$ as $n \rightarrow \infty$. This completes the proof. \square

An important point to note is that h_* , the upper bound on lattice spacing up to which $M_{ij}(h)$ is continuous (henceforth assumed to be optimal), depends in general on (i, j) . If $F_c^{-1}(0)$ is finite, a global upper bound on h may be found, namely,

$$h_*^g := \inf\{h_*(i, j) : i, j \in J, |i - j| = 1\} > 0 \quad (18)$$

so that the topological discretization with $0 < h < h_*^g$ has continuous moduli spaces for all types of kink. This is not necessarily true if $F_c^{-1}(0)$ is infinite (for then it is possible that $h_*^g = 0$). For any particular (i, j) , one can find an upper bound on h_* however, meaning that in no case does continuity of $M_{ij}(h)$ persist for all $h > 0$.

The upper bound is obtained by again thinking of the graph of the function $g(\cdot, h)$, whose existence was proved above, as the vertical projection of the intersection of the plane $\phi - \phi_+ + (-1)^i h z = 0$ with the surface $z = F(\phi, \phi_+)$. Recall that this graph always passes through (u_k, u_k) , where $k = i, j$. Consider the behaviour of the tangent to the graph at (u_k, u_k) . As h grows large, this tangent passes either through the horizontal or through the vertical (depending on whether i is odd or even, and whether $k = i$ or $k = j$). In either case, from this point on (i.e. for larger h) either monotonicity or existence of $g(\cdot, h)$ is lost, and so the existence or correct

limiting behaviour of the iteration sequence $\phi(nh) = g^n(\phi_0, h)$ is generically lost. This will be explained in more detail shortly.

The gradient of the tangent through (u_k, u_k) may be calculated by demanding that $(\phi, \phi_+) = (u_k + \delta, u_k + \delta_+)$ remains a solution of the DBE (11) to leading order in $\|\delta\| = [\delta^2 + \delta_+^2]^{\frac{1}{2}}$. Using Taylor's Theorem for G ,

$$G(u_k + \delta) = G(u_k) + \frac{\delta^2}{2} F'_c(u_k) + o(\delta^2), \quad (19)$$

one finds that

$$\frac{\delta_+}{\delta} = \frac{2 + (-1)^i h F'_c(u_k)}{2 - (-1)^i h F'_c(u_k)} + o(\|\delta\|). \quad (20)$$

So if i is even, meaning that $F'_c(u_i) > 0$ and $F'_c(u_j) < 0$, the tangent through (u_i, u_i) is vertical when $h = 2/F'_c(u_i)$, and the tangent through (u_j, u_j) is horizontal when $h = 2/|F'_c(u_j)|$. On the other hand, if i is odd, then $F'_c(u_i) < 0$ and $F'_c(u_j) > 0$, so the tangent through (u_i, u_i) is horizontal when $h = 2/|F'_c(u_i)|$, and the tangent through (u_j, u_j) is vertical when $h = 2/F'_c(u_j)$. In either case, we obtain the same upper bound on h_* , namely

$$h_* \leq h_1 := \inf \left\{ \frac{2}{|F'_c(u_i)|}, \frac{2}{|F'_c(u_j)|} \right\}. \quad (21)$$

One may similarly define

$$h_2 := \sup \left\{ \frac{2}{|F'_c(u_i)|}, \frac{2}{|F'_c(u_j)|} \right\}, \quad (22)$$

which will prove useful below.

A typical situation is depicted graphically in figure 1. Here, $h_1 = 2/|F'_c(u_1)|$, $h_2 = 2/|F'_c(u_0)|$ and $h_1 < h < h_2$, so the tangent through (u_1, u_1) has passed through the horizontal. It is impossible for $\phi(nh)$ to converge *monotonically* to u_1 with u_1 as a cluster point of the sequence: the sequence must overshoot u_1 as $\phi(nh)$ exceeds φ_h . The only possibility for a $(0, 1)$ kink to exist for this value of h , therefore, is that ϕ has a constant right hand tail, that is, there exists $N \in \mathbb{Z}$ such that $\phi(nh) = u_1$ for all $n \geq N$. This, in turn, is possible only if $\phi(0) = \varphi_h$, or one of its preimages under the iteration. One can restate this condition as $\phi(0) \in \Phi_h$ where

$$\Phi_h := \{\gamma_h^n(\varphi_h) : n = 0, 1, 2, \dots\}, \quad (23)$$

γ_h being the partial inverse of $g(\cdot, h)$, with $\gamma_h : [u_0, u_1] \rightarrow [u_0, \varphi_h]$. The set Φ_h parametrizes a discrete moduli space of kinks $M_{01}(h)$, all identical modulo lattice translations. Note that the left hand boundary behaviour of ϕ remains good for all $\phi(0) \in (u_0, u_1)$ in this situation.

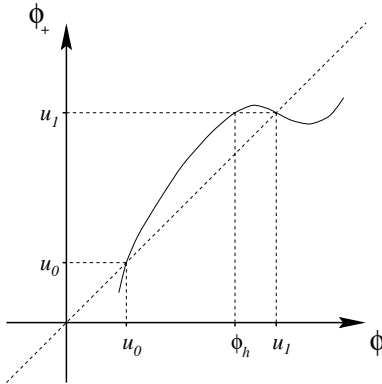


Figure 1: A section of the curve $\Delta\phi = F$, with $h_1 < h < h_2$.

In figure 2, h has been increased further, so that $h > h_2$, and now the sequence ϕ behaves badly at both ends. In order for $\phi(nh) \rightarrow u_0$ monotonically as $n \rightarrow -\infty$, ϕ must have a constant left tail, so one must have $\phi(0) \in \tilde{\Phi}_h$, where

$$\tilde{\Phi}_h := \{\tilde{\gamma}_h^n(\tilde{\varphi}_h) : n = 0, 1, 2, \dots\}, \quad (24)$$

and $\tilde{\gamma}_h : [u_0, \varphi_h] \rightarrow [\tilde{\varphi}_h, u_1]$ is defined by the curve shown. In this case, for ϕ to satisfy the definition of a static kink, both the left and right tails must be constant, which can only happen if $\tilde{\Phi}_h = \Phi_h$. One expects this to occur only for a discrete set of h values, which accumulate towards h_2 . When h becomes very large, one expects the projected intersection curve to pass outside the open square $(u_0, u_1) \times (u_0, u_1)$ completely, so that no static kink solutions are possible.

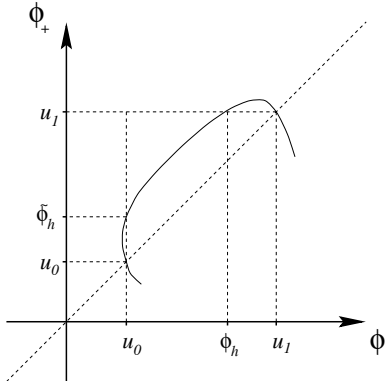


Figure 2: A section of the curve $\Delta\phi = F$, with $h > h_2$.

We are led, therefore, to the following conjecture for the generic behaviour of $M_{ij}(h)$ as h varies: for $h \in (0, h_1]$, $M_{ij}(h)$ is continuous, \mathbb{R} ; for $h \in (h_1, h_2]$, $M_{ij}(h)$ is discrete, $h\mathbb{Z}$; for almost all $h \in (h_2, \infty)$ $M_{ij}(h) = \emptyset$, but there exists a bounded countable set $H \subset (h_2, \infty)$ with $\inf H = h_2$ such that $M_{ij}(h) = h\mathbb{Z}$ for all $h \in H$. The conjecture is represented schematically in figure 3. It matches the observed behaviour for the topological discrete sine-Gordon [4] and ϕ^4 [5] systems. In both these cases $h_1 = h_2$ because the kinks interpolate between identical vacua, so the middle band is missing, and for the sine-Gordon model $H = \emptyset$. The example of twistons, discussed in section 5 produces the full generic behaviour, with all three bands. It is probably possible to construct a function F_c such that this conjectured behaviour fails (by making $F_c(\frac{1}{2}(u_i + u_j))$ very close to zero, for example), but such a system is rather contrived. One should note that the onset of discreteness in the kink moduli space is due to the requirement that kinks should be monotonic (after all, they are supposed to model continuum kinks, which always are), rather than the appearance of some kind of PN barrier.

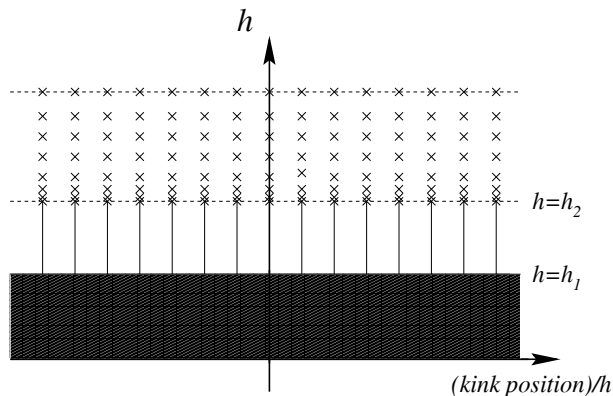


Figure 3: Schematic picture of the generic structure of the kink moduli space $M_{ij}(h)$ as h varies. Horizontal sections represent the moduli spaces for each specific value of h .

The upper bound $h_* \leq h_1$ has a remarkable physical interpretation in terms of the radiation of the system. Just as different pairs of vacua u_i, u_j have different types of kink interpolating between them, so each different vacuum u_k has its own type of radiation. In each case, the dispersion relation for this radiation may be obtained by substituting a traveling wave ansatz, $\cos(kx - \omega t)$, into the discrete field equation linearized about

$\phi = u_k$. Noting that $F_1(u_k, u_k) = \frac{1}{2}F'_c(u_k)$, one finds that ω and k must be related by

$$\omega^2 = [F'_c(u_k)]^2 + \left[\frac{4}{h^2} - (F'_c(u_k))^2 \right] \sin^2 \left(\frac{kh}{2} \right). \quad (25)$$

Note that this sinusoidal dispersion relation collapses to a flat line when $h = 2/|F'_c(u_k)|$, and that for larger h , the curve has a maximum instead of a minimum at $k = 0$. For $h \geq 2/|F'_c(u_k)|$, then, the discrete system fails to model accurately the radiation of the continuum system (which obeys the relativistic energy-momentum relation $\omega^2 = [F'_c(u_k)]^2 + k^2$) even in the long wavelength limit. So the upper bound on h_* derived above is precisely that value of h for which radiation about one or other of the vacua between which the kinks interpolate starts to behave badly.

5 Twistons

The original motivation for the construction in section 3 was to provide an efficient and natural means of simulating soliton dynamics numerically, on a computer. In this light, two substantial objections to the discretization procedure can be raised. First, even if F_c is known in closed form, its anti-derivative G may not be. In this case, every evaluation of F in the computer program would require the approximate evaluation of two definite integrals ($G(\phi)$ and $G(\phi_+)$). Clearly this cannot be computationally efficient. Second, the piecewise definition of F is highly inconvenient for numerical purposes. That is, even if an explicit formula for G exists, evaluation of F for ϕ close to ϕ_+ would be subject to significant rounding errors, unless (for example) a polynomial approximation to F were used in a narrow strip containing the diagonal $\phi = \phi_+$. Again, this is complicated and inefficient. There is, however, a large class of potentials F_c^2 for which both objections are avoided, namely those where F_c is polynomial. In this case, G is also polynomial (hence available in closed form) and, by the remainder theorem, so is $[G(\phi_+) - G(\phi)]/(\phi_+ - \phi)$, which may obviously be extended to the whole (ϕ, ϕ_+) plane to give a global, rather than piecewise, definition of F .

One example of such a polynomial discrete system has already been investigated [5]. To illustrate the construction further, we shall investigate the topological discretization of a recently proposed continuum model of so-called twistons in crystalline polyethylene [9]. We emphasise that the aim here is *not* to propose a physically realistic discrete model of such polymer twistons, but rather to demonstrate that our discrete system performs favourably in comparison with the conventional discretization when simulating soliton dynamics in the *continuum* model.

The continuum system has interaction potential F_c^2 , where

$$F_c(\phi) = \phi(1 - \phi^2). \quad (26)$$

We have normalized F_c differently from [9], and absorbed a coupling constant. So, there are three zero vacua, $u_0 = -1$, $u_1 = 0$ and $u_2 = 1$, and four different types of kink. Actually, all four types are trivially related to one another by reflexions in space and/or the codomain, and so we shall consider only type $(0, 1)$ kinks. The static profiles of these may be found explicitly using the Bogomol'nyi argument outlined in section 2, namely,

$$\phi(x) = -\sqrt{\frac{1}{2}(1 - \tanh(x - b))}. \quad (27)$$

Turning now to the topological discretization of this model (so now $x \in h\mathbb{Z}$), we find that $G(\phi) = \phi^2(\phi^2 - 2)/4$, and

$$F(\phi, \phi_+) = \frac{G(\phi_+) - G(\phi)}{\phi_+ - \phi} = \frac{1}{4}(\phi_+^2 + \phi^2 - 2)(\phi_+ + \phi). \quad (28)$$

As remarked above, F has a simple closed form, and its evaluation presents no problems for a computer program. By the general existence theorem of section 4, there exists $h_* > 0$ such that for all $h \in (0, h_*)$ there is a continuum of $(0, 1)$ kink solutions $M_{01}(h)$ of the DBE,

$$\frac{\phi_+ - \phi}{h} = \frac{1}{4}(\phi_+^2 + \phi^2 - 2)(\phi_+ + \phi), \quad (29)$$

parametrized by $\phi(0) \in (-1, 0)$. All such solutions have energy $E_P = |G(0) - G(-1)| = \frac{1}{4}$, so there is no PN barrier. Recall that, in general, one has an upper bound h_1 on h_* . In the present case, $F'_c(-1) = -2$ and $F'_c(0) = 1$, so $h_1 = 1$ and $h_2 = 2$.

We do not propose to prove rigorously that $h_* = h_1 = 1$ for this model. Rather, by plotting the zero contours of the function

$$f(\phi_+, \phi, h) = \phi_+ - \phi - \frac{h}{4}(\phi_+^2 + \phi^2 - 2)(\phi_+ + \phi) \quad (30)$$

for various values of h we will demonstrate that the generic behaviour of $M_{ij}(h)$ described in section 4 is highly plausible. Recall, from the proof in that section that this contour contains, at least for small h , the graph of the function $g(\cdot, h)$ which one iterates to generate the static kink. Zero contours of f for $h = 0.5, 1.0, 1.5, 2.0, 2.5$ and 4, found using the contourplot utility of Maple, are shown in figure 4. While $h < 1$, the contour contains the graph of a continuous increasing function $g(\cdot, h) : [-1, 0] \rightarrow [-1, 0]$, so that $M_{01}(h)$ is continuous. However, when $h = 1$, the tangent to the contour at $(-1, -1)$ passes through the vertical, so for $h > 1$ only kinks with a constant left tail can exist, which can only happen for nongeneric $\phi(0)$, and $M_{ij}(h)$ is discrete. When $h = 2$, the tangent to the contour at $(0, 0)$ passes through the horizontal. For $h > 2$ kinks must also have a constant right hand tail, so they may only exist for nongeneric $\phi(0)$ and h . This situation continues until $h \geq 4$, when the contour passes outside the open square $(-1, 0) \times (-1, 0)$. Indeed, at $h = 4$, the DBE supports only “step function” kinks,

$$\phi(x) = \begin{cases} -1 & x < Nh \\ 0 & x \geq Nh, \end{cases} \quad (31)$$

as may be shown by explicit calculation.

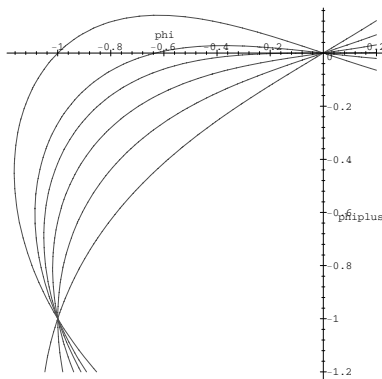


Figure 4: Zero contours of $\phi_+ - \phi - hF(\phi, \phi_+)$ for the values $h = 0.5, 1.0, 1.5, 2.0, 2.5$ and 4, from least to most curved.

Since the DBE (29) is a cubic polynomial equation, it is possible in principle to solve for ϕ_+ in terms of ϕ (or *vice versa*) and hence generate exact static kink solutions, although it appears that no closed formula for $\phi(x)$ exists (in particular, a continuum-inspired ansatz does not seem to work). In general, if F_c is a degree p polynomial, the DBE is a degree p polynomial equation for $\phi_+(\phi)$, so for $p \geq 5$ such an approach would not work. Even for $p = 3, 4$, implementation would be complicated. Instead, one may solve the DBE approximately with some kind of root-finding algorithm. In figure 5 we present a kink solution found by solving (29) with $h = 0.8$ using the bisection method. Note that the kink structure is spread over very few lattice sites, so the system is deep in the discrete regime.

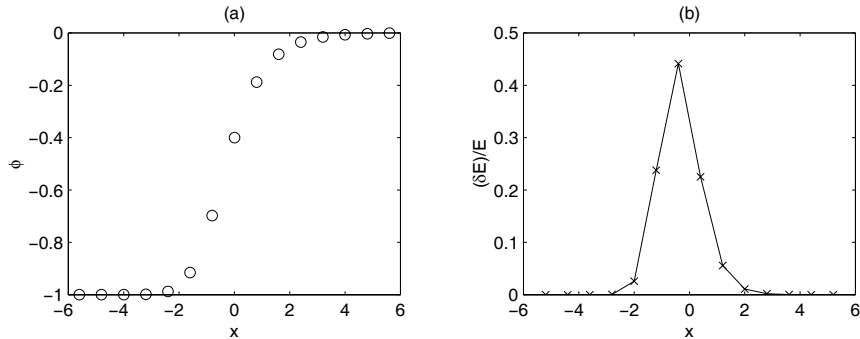


Figure 5: Example of a static kink solution on a lattice of spacing $h = 0.8$ obtained by approximate solution of the DBE using the bisection method. Plot (a) shows the field ϕ . Plot (b) shows the energy distribution of the kink. The energy should be thought of as located in the links between pairs of lattice sites. This plot shows the energy in each link as a fraction of the total energy.

6 Numerical simulations

So far, we have considered only the static model. In this section we will discuss numerical simulations of the full, time-dependent discrete field equation, that is, numerical solutions of the coupled set of ODEs (12). In solving these ODEs one must also discretize *time* in some way. It should be regarded as a strength of our approach that there is great freedom in precisely how one does this, since one may choose a method specifically adapted to the dynamics one seeks to simulate. For example, in kink-antikink interactions, the solitons usually spend a long time well separated, then experience a brief, but very violent interaction when they finally become close. In this situation a variable time step (rather than a fixed, rectangular space-time mesh) is clearly sensible. For other problems it may be desirable to preserve the symplectomorphicity of the phase space flow (both (6) and (12) are Hamiltonian dynamical systems), so that a symplectic integrator with fixed time step would be more appropriate.

Since the aim here is to test our discretization's performance, we shall consider a simple and clear-cut dynamical problem, for which the continuum behaviour is easily understood: single $(0,1)$ kink motion at constant speed. The continuum field equation (6) is Lorentz invariant, so there exist Lorentz boosted kinks moving with any speed $v \in [0,1)$. These provide the initial data, sampled on the discrete lattice $h\mathbb{Z}$, for our simulations. The lattice spacing was chosen to be $h = 0.8$, so that the kink width is comparable to h . Recall that a major departure of conventional discrete systems from their continuum counterparts is that solitons suffer radiative deceleration, and possibly pinning, in the highly discrete regime. An important test of the topological discretization, therefore, is to monitor kink velocity $v(t)$ over simulations of long duration (3000 time units in this case), to see to what extent radiative deceleration is present. One certainly expects moving kinks to excite some radiation. For a type (i, j) kink, this will move with a maximum group velocity of

$$v_g^{\max} := \left. \frac{d\omega}{dk} \right|_{\max} = 1 - \frac{h}{2} |F'_c(u_k)| \quad (32)$$

where $k = i$ if $v > 0$ or $k = j$ if $v < 0$, since phonons are excited behind the kink, and hence are small oscillations about its trailing vacuum [11]. So for right moving $(0,1)$ kinks, $v_g^{\max} = 0.2$, while for left moving $(0,1)$ kinks, $v_g^{\max} = 0.6$. In either case, one wishes to avoid radiation being reflected from the fixed boundaries and interfering with the kink's motion, so the first few sites at either end of the (finite) lattice are damped. This adds a non-Hamiltonian piece to the flow, so a symplectic integrator is not appropriate, and we choose to use a fourth order Runge-Kutta method with fixed time step $\delta t = 0.01$. The algorithm, and the checks made on its accuracy and stability (energy conservation etc.) have been described previously [5].

Simulations were performed for various initial velocities, and in all cases it was found that kink pinning was eliminated, as one would expect: kinks propagate freely, indefinitely. Figure 6 shows plots of $v(t)$ for right-moving kinks with initial velocities $v(0) = 0.2, 0.4, 0.6$ and 0.8 . Figure 7 presents similar graphs for left moving

kinks, with $v(0) = -0.2, -0.4, -0.6$ and -0.8 . In every case, the upper curve shows $v(t)$ for the topological discretization (12), while the lower curve shows $v(t)$ for the same initial value problem for the conventional discretization (14), solved using the same numerical scheme. The thickness of the curves is due to velocity oscillations as the kink moves from cell to cell through the lattice. These are partly an artifact of the way we define kink position (linear interpolation in this case), and partly dynamical. In both systems one may regard the effective kink mass as depending periodically on the kink position, and in the conventional (but not the topological) discretization, the kink velocity oscillates as it moves up and down in the PN potential. As found previously for sine-Gordon and ϕ^4 kinks, radiative deceleration is drastically cut using the topological discretization.

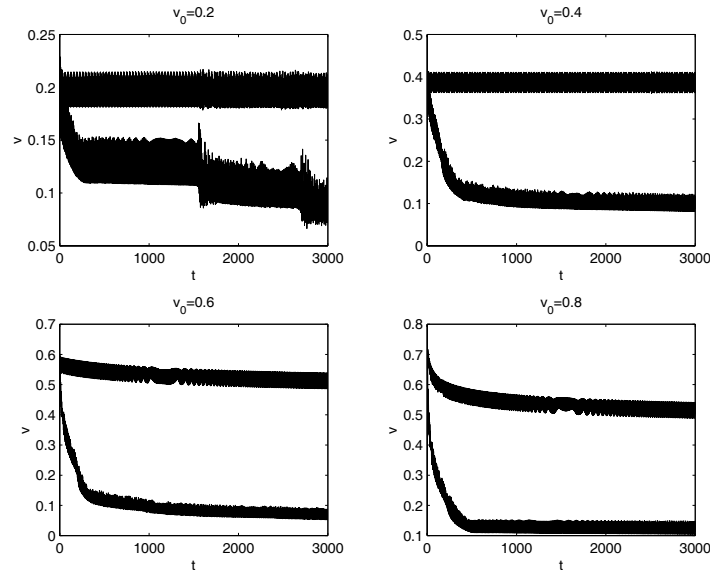


Figure 6: Comparison of the motion of right-moving kinks in the topological discrete twiston system with that in the conventional discretization, for various initial velocities. The lattice spacing is $h = 0.8$. In each case, velocity is plotted against time for both systems on the same graph, the lower curve showing the data for the conventional discrete system.

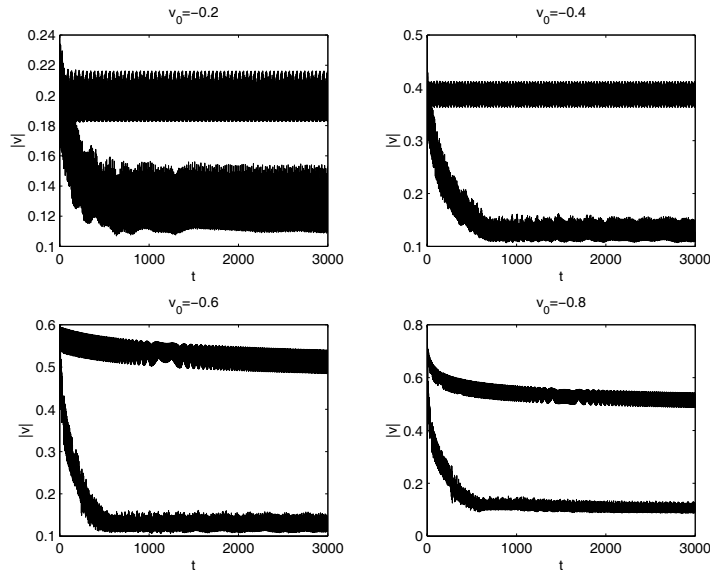


Figure 6: Comparison of the motion of left-moving kinks in the topological and conventional discrete twiston systems, with lattice spacing $h = 0.8$. Speed is plotted against time for both systems on the same graph, the lower curve showing the data for the conventional discrete system. As with right-moving kinks, radiative deceleration is much less pronounced in the topological discretization.

7 Other methods

The discretization method outlined in section 3 is not the only way to arrive at discrete systems without a Peierls-Nabarro barrier. Having performed the construction, one is always free to replace $\Delta\phi$ by $D = X\Delta\phi$ and F by $\tilde{F} = F/X$ where X is any function of (ϕ, ϕ_+, h) which reduces to unity in the continuum limit, $h \rightarrow 0$, $\phi_+ = \phi + O(h)$. Since $D\tilde{F} = \Delta G$, the potential energy functional

$$E_P = \frac{h}{2} \sum_{x \in h\mathbb{Z}} (D^2 + \tilde{F}^2) \quad (33)$$

is again subject to the Bogomol'nyi argument, yielding the same lower bound on type (i, j) kink energy, but the DBE is now different: $D = \pm\tilde{F}$. For example, the sine-Gordon model has $F_c = \sin$, and hence its topological discretization has

$$F(\phi, \phi_+) = \begin{cases} -\frac{\cos \phi_+ - \cos \phi}{\phi_+ - \phi} & \phi_+ \neq \phi \\ \sin \phi & \phi_+ = \phi. \end{cases} \quad (34)$$

If one chooses $X = \text{sinc } \frac{1}{2}(\phi_+ - \phi)$, (where $\text{sinc } x := x^{-1} \sin x$ when $x \neq 0$ and $\text{sinc } 0 := 1$), then defining $D = X\Delta\phi$ and $\tilde{F} = F/X$ one recovers the original topological discrete sine-Gordon system [4], namely

$$\begin{aligned} D &= \frac{2}{h} \sin \frac{1}{2}(\phi_+ - \phi) \\ \tilde{F} &= \sin \frac{1}{2}(\phi_+ + \phi). \end{aligned} \quad (35)$$

In general, the kind of analysis carried out in section 4 should still work for the new DBE (and certainly does in the specific case of the sine-Gordon system outlined above), although the geometric picture of a plane intersecting a surface no longer applies. Using this trick, one may be able to avoid a piecewise definition of \tilde{F} even when F_c is not polynomial. However, no systematic method for choosing X suggests itself.

Finally, we wish to describe briefly a completely different approach due to Flach, Kladko and Zolotaryuk, called the inverse method. The following is a somewhat reinterpreted version of the method outlined in [12] (the authors of which were primarily concerned with exact *moving* discrete solitons, rather than the Peierls-Nabarro barrier). The idea is that, given a continuum nonlinear Klein-Gordon model possessing a type (i, j) kink with static profile ϕ_K , one seeks a one-site substrate potential $V_h(\phi)$ such that the discrete field equation

$$\ddot{\phi} = \frac{\phi_+ - 2\phi + \phi_-}{h^2} - V'_h(\phi) \quad (36)$$

preserves the one parameter family of static solutions $\phi(nh) = \phi_K(nh - b)$. Clearly, one needs

$$V'_h(\phi_K(z)) = \frac{1}{h^2}[\phi_K(z+h) - 2\phi_K(z) + \phi_K(z-h)] \quad (37)$$

for all $z \in \mathbb{R}$. This uniquely determines $V'_h : I_{ij} \rightarrow \mathbb{R}$ by monotonicity of ϕ_K . Note that, by construction, in the limit $h \rightarrow 0$, the right hand side of (37) becomes ϕ_K'' so, given that ϕ_K satisfies the static continuum field equation (6), $V'_h(\phi)$ must have the correct continuum limit ($\lim_{h \rightarrow 0} V'_h = F_c F'_c$). Since this is a continuous family of static solutions, they must all have the same energy. Indeed, equation (37) may be interpreted as the condition

$$\frac{d}{db} E_P[\phi_K(nh - b)] = 0, \quad (38)$$

where the potential energy is

$$E_P[\phi] = h \sum_{x \in h\mathbb{Z}} \left[\frac{1}{2}(\Delta\phi)^2 + V_h(\phi) \right]. \quad (39)$$

Hence there is no PN barrier resisting the propagation of kinks in this discrete system. If ϕ_K is analytic, $V'_h(\phi)$ can be written as a power series in ϕ , although there may exist no closed formula for V'_h . This may be a significant drawback of the inverse method, in comparison with the topological discretization approach, which works very explicitly, at least for all polynomial F_c .

In some special cases, V'_h can be obtained in closed form: one example is ϕ^4 theory, where $\phi_K = \tanh$ and an explicit formula for V_h has been known for some time [13]. As a new example, one could consider the continuum twiston model defined in section 5, whose $(2, 1)$ kink has profile $\phi_K(x) = [\frac{1}{2}(1 - \tanh x)]^{\frac{1}{2}}$. In this case, $\phi_K(z \pm h)$ can be written in terms of $\phi_K(z)$ using hyperbolic trigonometric identities, so one finds,

$$V_h(\phi) = \frac{\phi}{h^2} \left\{ \sqrt{\frac{1 - \tanh h}{1 + (1 - 2\phi^2) \tanh h}} + \sqrt{\frac{1 + \tanh h}{1 - (1 - 2\phi^2) \tanh h}} - 2 \right\}, \quad (40)$$

which has $V'_h(\pm 1) = V'_h(0) = 0$, as expected. It is unclear how “special” F_c must be in order for the V'_h obtained by this inverse method to be expressible in closed form – perhaps this happens whenever F_c is polynomial. If so, one would expect the expressions involved to become extremely complicated as the degree of F_c grows. The inverse method also works explicitly when applied to the sine-Gordon kink profile, $\phi_K(x) = 2 \tan^{-1} e^x$, so generating yet another discrete sine-Gordon system with no PN barrier (see also [14]). In this case,

$$V'_h(\phi) = \frac{2}{h^2} \left[\tan^{-1} \left(e^h \tan \frac{\phi}{2} \right) + \tan^{-1} \left(e^{-h} \tan \frac{\phi}{2} \right) - \phi \right]. \quad (41)$$

Equations (40) and (41) can be integrated to give explicit formulae for V_h , and hence E_P , for these models, although the formulae are rather complicated. This is little practical disadvantage, since only V'_h appears in the discrete field equation. The strength of this method is that one has an explicit formula for the family of static discrete kinks, instead of an abstract existence theorem. It certainly merits further investigation.

Acknowledgments

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