Kinks in dipole chains

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Abstract

It is shown that the topological discrete sine-Gordon system introduced by Speight and Ward models the dynamics of an infinite uniform chain of electric dipoles constrained to rotate in a plane containing the chain. Such a chain admits a novel type of static kink solution which may occupy any position relative to the spatial lattice and experiences no Peierls–Nabarro barrier. Consequently the dynamics of a single kink is highly continuum-like, despite the strongly discrete nature of the model. Static multikinks and kink–antikink pairs are constructed, and it is shown that all such static solutions are unstable. Exact propagating kinks are sought numerically using the pseudo-spectral method, but it is found that none exist, except, perhaps, at very low speed.

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1. Introduction

Nonlinear Klein–Gordon kinks are found in many branches of theoretical physics. For applications in condensed matter and biophysics, the nonlinear Klein–Gordon equation is usually a continuum approximation of a more fundamental spatially discrete system: kinks really live on a lattice reflecting some crystalline or biomolecular structure. It has long been recognized that spatial discreteness introduces important new effects into the dynamics of kinks \cite{1}. Most notable is the Peierls–Nabarro (PN) barrier. Due to the loss of continuous translation symmetry, static kinks may generically be centred only on a lattice site or exactly half-way between lattice sites. The PN barrier is the energy difference between these two solutions. A kink moving with too little kinetic energy cannot surmount the PN barrier and becomes trapped. A kink moving with
high kinetic energy loses energy by emitting radiation and may also, eventually, become
trapped. So the dynamics of discrete kinks is much more complicated than their continuum
counterparts.

This rich behaviour has led mathematical physicists to study discrete Klein–Gordon
systems extensively for their own sake, independent of any physical application. In this
regard, there has been a recent resurgence of interest in so-called exceptional
discretizations of nonlinear Klein–Gordon models: those which, despite the loss of translation symmetry,
maintain a continuous family of static kink solutions, centred anywhere relative to the
lattice (loosely, a continuous translation orbit of static kinks). An early example of this
was the topological discrete sine-Gordon (TDSG) system [2], which eliminated the PN
barrier by preserving the Bogomol’nyi bound on kink energy. The idea was subsequently
applied to the $\phi^4$ model [3] and then generalized to all Klein–Gordon models [4]. A
rather different approach is to choose the continuous family of static kinks in advance, then
reverse-engineer a discrete Klein–Gordon system which supports them [5], the so-called
inverse method. Both this method and the topological discretization approach discretize
the Lagrangian of the system, so they preserve an energy conservation law. Kevrekidis
has given a method for constructing exceptional discretizations of the PDE itself, which
destroys the variational set-up but preserves a momentum conservation law [6]. Along with
the collaborators, he has recently shown that, if one discretizes the Laplacian in standard
fashion, it is impossible to preserve both energy and momentum conservation [7]. Note that
in the absence of a conserved energy it is not meaningful to speak of a PN potential. Most
recently, Barashenkov et al [8] have systematically constructed all polynomial exceptional
discretizations of the $\phi^4$ PDE with standard discrete Laplacian, finding families which
generalize the discrete $\phi^4$ systems of [3, 6]. The new exceptional discretizations they
find preserve neither energy nor momentum conservation. Moving outside the polynomial
class, Dmitriev et al have constructed yet more exceptional discrete Klein–Gordon models,
concentrating on the $\phi^4$ case, some of which conserve energy, some momentum, but none
both [9].

All these systems are theoretically interesting, but from a physical viewpoint they look
rather contrived, and it is hard to imagine a concrete physical system that they model. The
purpose of this paper is to point out that one of them does, in fact, model a simple physical
system: a uniform chain of electric dipoles. The kinks interpolate between the two vacuum
states where the dipoles are aligned uniformly forward and uniformly backward along the
chain. This system has three parameters: the dipole strength $d$, the inter-dipole separation $\delta$
and the dipole moment of inertia $I$. For all values of these parameters, this system can be
reduced to the TDSG system at a single fixed value of the lattice spacing ($h = \sqrt{12}$, it turns
out). This allows a concrete physical reinterpretation of much of the previous work on the
TDSG system [2, 10–12]. It also motivates us to investigate the TDSG system more deeply,
yielding some new results. We will construct static multikink and kink–antikink pair solutions
and prove that all static solutions apart from the kink, antikink and vacua are unstable. We will
also numerically seek exact propagating kinks using the pseudo-spectral method but will find
only nanopterons: travelling kinks with spatially oscillatory tails. The tail amplitude becomes
extremely small for low propagation speed, so that the possibility of exact propagating low
speed kinks cannot yet be discounted.

In section 2, we will introduce the dipole chain and demonstrate that it is modelled by
the TDSG system. In section 3 we will construct static solutions with an arbitrary winding
number and prove that all ‘non-Bogomol’nyi’ static solutions (that is, all solutions except
kinks, antikinks and vacua) are unstable. Section 4 presents our results on exact propagating
solutions, while section 5 contains some concluding remarks.
2. Dipole chains

If two electric dipoles of moments \( \mathbf{d}_1, \mathbf{d}_2 \) are held at positions \( \mathbf{r}_1, \mathbf{r}_2 \in \mathbb{R}^3 \), the potential energy due to their electrostatic interaction is

\[
\delta E = \frac{1}{4\pi \varepsilon_0} \frac{\mathbf{d}_1 \cdot \mathbf{d}_2 - 3(\mathbf{n} \cdot \mathbf{d}_1)(\mathbf{n} \cdot \mathbf{d}_2)}{|\mathbf{r}_1 - \mathbf{r}_2|^3},
\]

where \( \mathbf{n} = (\mathbf{r}_1 - \mathbf{r}_2)/|\mathbf{r}_1 - \mathbf{r}_2| \). Consider an infinite chain of equally spaced dipoles, all of equal strength, each free to rotate in some fixed plane containing the axis of the chain. Without loss of generality we can assume the chain is directed along the \( x \)-axis and the dipoles rotate in the \((x, y)\)-plane. Then the \( n \)th dipole is located at \( \mathbf{r}_n = (\delta n, 0, 0) \) and has moment \( \mathbf{d}_n = d(\cos \phi_n, \sin \phi_n, 0) \), where \( \delta \) is the inter-dipole spacing and \( \phi_n \) is the angle between \( \mathbf{d}_n \) and the \( x \)-axis. Hence, the potential energy of a neighbouring pair \( \mathbf{d}_n, \mathbf{d}_{n+1} \) is

\[
\delta E_n = \frac{d^2}{4\pi \varepsilon_0 \delta^3} \left[ \cos(\phi_{n+1} - \phi_n) - 3 \cos \phi_n \cos \phi_{n+1} \right]
\]

\[
= \frac{d^2}{4\pi \varepsilon_0 \delta^3} \left[ \sin^2 \frac{1}{2}(\phi_{n+1} - \phi_n) + 3 \sin^2 \frac{1}{2}(\phi_{n+1} + \phi_n) - 2 \right].
\]

It is convenient to add \( d^2/2\pi \varepsilon_0 \delta^3 \) to \( \delta E_n \) so that the minimum energy of a neighbouring pair is normalized to 0, occurring when \( \mathbf{d}_n = \mathbf{d}_{n+1} = (\pm d, 0, 0) \). The total potential energy of the chain, neglecting longer range interactions, is

\[
E_P = \frac{d^2}{4\pi \varepsilon_0 \delta^3} \sum_{n \in \mathbb{Z}} \left[ \sin^2 \frac{1}{2}(\phi_{n+1} - \phi_n) + 3 \sin^2 \frac{1}{2}(\phi_{n+1} + \phi_n) \right],
\]

while its total kinetic energy is

\[
E_K = \sum_{n \in \mathbb{Z}} \frac{1}{2} I \left( \frac{d\phi_n}{dt} \right)^2,
\]

where \( I \) is the moment of inertia of a dipole. The Lagrangian governing its time evolution is then \( L = E_K - E_P \).

If we define the natural units of energy and time to be \( E_0 = \sqrt{3}d^2/2\pi \varepsilon_0 \delta^3 \) and \( T_0 = (1/\sqrt{3}E_0)^{1/2} \), respectively, this Lagrangian coincides with that of the TDSG system [2] with lattice spacing \( \sqrt{12} \). More precisely, let us define the rescaled energy and time variables \( \hat{E}_K = E_K/E_0 \), \( \hat{E}_P = E_P/E_0 \) and \( \hat{t} = t/T_0 \). Then

\[
\hat{L} = \hat{E}_K - \hat{E}_P = \frac{h}{4} \sum_{n} \left[ \phi_n^2 \left( \frac{2}{h} \sin \frac{1}{2}(\phi_{n+1} - \phi_n) \right)^2 - 3 \sin^2 \frac{1}{2}(\phi_{n+1} + \phi_n) \right],
\]

where \( h = \sqrt{12} \) and \( \hat{f} := df/d\hat{t} \). This is precisely the TDSG Lagrangian. It is convenient to take \( \delta \) as the unit of length. Note that \( \delta, d, I \) affect the energy and length scales of the system but not its dynamical properties. These depend only on \( h \), which is fixed at \( \sqrt{12} \) for all dipole chains. Note also that the physical lattice spacing of the chain is \( \delta \), not \( h \). We shall henceforth use the rescaled variables exclusively and drop the \(^\ast\) superscripts.

The equation of motion of the TDSG system is

\[
\ddot{\phi}_n = \frac{4 - h^2}{4h^2} \cos \phi_n (\sin \phi_{n+1} + \sin \phi_{n-1}) - \frac{4 + h^2}{4h^2} \sin \phi_n (\cos \phi_{n+1} + \cos \phi_{n-1}).
\]

If \( 0 < h < 2 \), it supports static kink solutions

\[
\phi_n = 2 \tan^{-1} e^{a(n-b)}, \quad a = \log \left( \frac{2 + h}{2 - h} \right).
\]
centred anywhere on the lattice (the kink position $b$ may take any real value). All these kinks have energy 1, the minimum possible for a configuration with kink boundary behaviour ($\lim_{n \to \pm \infty} \phi_n = k \pm \pi$ with $|k_+ - k_-| = 1$). Thus they experience no PN barrier—this is an exceptional discretization of the continuum sine-Gordon model, which we recover in the limit $h \to 0$. Note that adding any integer multiple of $2\pi$ to a single $\phi_n$ preserves solutions of (2.6), so one should think of $\phi_n$ as an angular coordinate of period $2\pi$. The constant sequences $\phi_n = 0$ and $\phi_n = \pi$ are two distinct vacuum solutions, between which kink (2.7) interpolates. The dynamics of a single kink was studied in detail in [2]. It was found that kinks may propagate with arbitrarily low speed and never get pinned. Fast kinks on coarse lattices ($h$ close to 2) do excite significant radiation in their wake which causes them to decelerate appreciably, but this effect is far weaker than in the conventional discrete system with the same $h$. We shall return to the question of whether the system admits exact propagating kinks with constant speed in section 4, but in any case kinks are very highly mobile in this system. Kink–antikink collisions were studied numerically by Kotecha in [10], in the case where the kink and antikink are fired at one another with equal speed. Such collisions were found to be rather similar to continuum $\phi^4$ kink–antikink collisions. There is a critical speed $v_c$, depending on $h$, above which the kink and antikink pass through one another. Kotecha found that $v_c$, measured in lattice cells traversed per unit time, depends approximately linearly on $h$. Below $v_c$ there is a complicated (possibly fractal) structure of velocity windows in which the kink and antikink ‘bounce’ off one another $B \geq 1$ times, where a bounce consists of the kink passing through the antikink, then turning around and passing back through in the opposite direction. There seem to be windows with $B = \infty$, meaning that the kink–antikink pair settles into a breather-like oscillatory bound state. In fact, the TDSG system supports exact breather solutions [11], at least for $h$ close to 2, though these are all unstable [12].

In the case of the dipole chain, $h = \sqrt{12} > 2$, so the results of [2, 10–12] do not directly apply. To make use of them we must exploit a symmetry of (2.6): $\phi_n(t)$ is a solution of the spacing $h$ system if and only if

$$\psi_n(t) = (-1)^n \phi_n(2t/h)$$

is a solution of the spacing $h_\ast = 4/h$ system. Note that if $h > 2$ then $0 < h_\ast < 2$. We can thus identify the dipole chain with the TDSG system with lattice spacing $h_\ast = 4/\sqrt{12} = 2/\sqrt{3} < 2$; so the dipole chain supports a continuous translation orbit of ‘alternating’ kinks

$$\phi_n = (-1)^n 2 \tan^{-1} e^{a(n-b)}, \quad a = \log \left(\frac{\sqrt{3} + 1}{\sqrt{3} - 1}\right),$$

parametrized by $b \in \mathbb{R}$, all of which have energy 1. Note that $\phi_n$ still has kink boundary behaviour because $\phi_n$ is angular, so $\pi$ and $-\pi$ are identified. The kink experiences no PN barrier. These kinks are very highly discrete, in that their structure is spread over very few lattice sites. For example, 86.6% of the energy of the $b = 0$ kink resides in the $-1 \leq n \leq 1$ section of the chain. This kink is depicted in figure 1.

Since $h_\ast \approx 1.15$ is close to 1, the numerical results of [2] show that its propagation at modest speed is strongly continuum-like: radiative deceleration is weak and the kink speed

Figure 1. A site-centred dipole kink ($b = 0$).
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varies very little over a single lattice cell transit. Like their $h < 2$ counterparts, therefore, kinks in dipole chains are highly mobile. Radiative deceleration is essentially negligible if the frequency with which the kink centre hits the lattice sites is below the bottom edge of the phonon band of the lattice \[2\]. In the case of dipole kinks, this happens when

$$2\pi v < \frac{2}{\hbar} \iff v < \frac{1}{2\pi\sqrt{3}} \approx 0.092 \text{ sites/unit time.} \quad (2.10)$$

In 'laboratory' units, this becomes

$$v < \frac{d}{8\pi^2\varepsilon_0 I \delta}. \quad (2.11)$$

Turning to kink–antikink collisions, we can estimate the critical incidence speed, above which they pass through one another, for the spacing $h^* = 2/\sqrt{3}$ lattice, using Kotecha's linear fit:

$$v_c \approx 0.120 \text{ sites/unit time} \quad [10].$$

From (2.8) it then follows that the critical speed for dipole kink–antikink collisions is

$$v_c \approx 0.208 \text{ sites/unit time} \approx 0.144 \frac{d}{\sqrt{\varepsilon_0 I \delta}}. \quad (2.12)$$

The numerical results of [11] show that $h^*$ is too far from 2 for the dipole chain to support any breather solution constructed by continuation from the anti-continuum limit.

3. Static solutions

An important consequence of the PN potential in conventional discrete systems is that they can, in contrast to their continuum counterparts, support finite energy static multikink solutions. The point is that if two kinks are well separated, their mutual repulsion is too weak to overcome the pinning force due to the PN barrier. One can thus construct static solutions with arbitrarily many kinks and antikinks in stable equilibrium. Since the TDSG system has no PN barrier one might expect it to have no static multikinks either. However, this turns out to be false: one can construct static solutions with $\lim_{n \to \pm\infty} \phi_n = k\pm\pi$ for any integers $k, k_\pm$. Only the vacua and (anti)kink are however, stable. We shall assume $0 < h < 2$, so the results apply to the dipole chain if we choose $h = 2/\sqrt{3}$ and apply (2.8).

It is helpful to think of the static field equation as the variational equation for the functional $E_P$. To be precise, for any $k_-, k_+ \in \mathbb{Z}$, let

$$\ell^2_{k_-, k_+} := \left\{ \phi : \mathbb{Z} \to \mathbb{R} \mid \sum_{n=-\infty}^{\infty} (\phi_n - k_-\pi)^2 + \sum_{n=0}^{\infty} (\phi_n - k_+\pi)^2 < \infty \right\}. \quad (3.1)$$

Note that $\ell^2_{0,0} = \ell^2$, the Hilbert space of square summable sequences, and $\ell^2_{k, -k}$ is an affine space modelled on $\ell^2$, whose elements have boundary behaviour $\lim_{n \to \pm\infty} \phi_n = k\pm\pi$. It is straightforward to verify that $E_P : \ell^2_{k, -k} \to \mathbb{R}$ is $C^2$ and that $\phi$ is a critical point of $E_P$ if and only if each of its constituent triples $(\phi_{n-1}, \phi_n, \phi_{n+1})$ satisfies the static field equation:

$$\frac{\partial E_P}{\partial \phi_n} = -\frac{4 - \hbar^2}{8\hbar} \cos \phi_n (\sin \phi_{n+1} + \sin \phi_{n-1}) + \frac{4 + \hbar^2}{8\hbar} \sin \phi_n (\cos \phi_{n+1} + \cos \phi_{n-1}) = 0. \quad (3.2)$$

So critical points of $E_P$ on $\ell^2_{k, -k}$ are static solutions of the model with $\lim_{n \to \pm\infty} \phi_n = k\pm\pi$ and vice versa. Note that any triple with $\phi_{n+1} - \phi_{n-1} = \pi \mod 2\pi$ automatically satisfies (3.2) irrespective of its central value $\phi_n$, by $\pi$-antiperiodicity of cos and sin. Such triples turn out to be important for our analysis of static solutions, so we make the following definition.

**Definition 1.** A consecutive triple $(\phi_{n-1}, \phi_n, \phi_{n+1})$ in a sequence $\phi$ is called exceptional if $\phi_{n+1} - \phi_{n-1} = (2k + 1)\pi$ for some $k \in \mathbb{Z}$.
To discuss the stability of static solutions, we must introduce the second variation, or Hessian, of \( E_P \). Let \( \phi \) be a critical point of \( E_P \) and \( \phi^{s,t} \) be a two-parameter variation of it, that is, a smooth map \((-\epsilon, \epsilon) \times (-\epsilon, \epsilon) \rightarrow \mathbb{R}^k \), with \( \phi^{0,0} = \phi \). Let \( u = \partial_s \phi^{s,t} \big|_{(0,0)}, v = \partial_t \phi^{s,t} \big|_{(0,0)} \in \mathbb{R}^k \). Then the Hessian of \( E_P \) at \( \phi \) is the symmetric bilinear form \( \text{Hess}_\phi : \mathbb{R}^k \times \mathbb{R}^k \rightarrow \mathbb{R} \) defined by

\[
\text{Hess}_\phi(u, v) = \frac{\partial^2 E_P[\phi^{s,t}]}{\partial s \partial t} \bigg|_{s=t=0}.
\]

(3.3)

We say that \( \phi \) is stable if the associated quadratic form \( u \mapsto \text{Hess}_\phi(u, u) \) is positive semi-definite (i.e. \( \text{Hess}_\phi(u, u) \geq 0 \) for all \( u \)) and unstable otherwise. This definition is motivated by the analogy with a point particle moving in \( \mathbb{R}^3 \) under the influence of a potential \( V \), since then saddle points and maxima of \( V \) are clearly unstable equilibria. We will consider the linear stability criterion later in this section. By considering the variations \( \phi^{s,t} = \phi + (s + t)u \) and \( \phi^t = \phi + tu \), one sees that

\[
\text{Hess}_\phi(u, u) = \frac{d^2 E_P[\phi^t]}{dt^2} \bigg|_{t=0},
\]

(3.4)

so to prove instability it suffices to exhibit a one-parameter variation \( \phi^t \) of \( \phi \) such that \( \frac{d^2 E_P[\phi^t]}{dt^2} < 0 \) at \( t = 0 \).

Let us briefly recall the construction of the kink solutions of the model (2.7). The key idea is to write \( E_P \) in the form

\[
E_P[\phi] = -\frac{h}{4} \sum_n (D_n^2 + F_n^2), \quad D_n := \frac{2}{h} \sin \frac{1}{2} (\phi_{n+1} - \phi_n), \quad F_n := \sin \frac{1}{2} (\phi_{n+1} + \phi_n)
\]

(3.5)

and observe that \( D_n F_n = -\Delta \cos \phi_n \), where \( \Delta f_n := (f_{n+1} - f_n)/h \). Hence

\[
0 \leq -\frac{h}{4} \sum_n (D_n^2 - F_n^2)^2 = E_P + \frac{h}{2} \sum_n \Delta \cos \phi_n = E_P + \frac{1}{2} (\cos k_+ \pi - \cos k_- \pi).
\]

(3.6)

It follows that \( E_P \geq 1 \) on \( \ell^2_{0,1} \) and \( E_P = 1 \) if and only if \( D_n = F_n \) for all \( n \). This discrete Bogomol’nyi equation may be written as

\[
\tan \frac{\phi_{n+1}}{2} = \frac{2 + h}{2 - h} \tan \frac{\phi_n}{2}.
\]

(3.7)

and its general non-vacuum solution is (2.7). On \( \ell^2_{0,0} \), a similar argument beginning with summand \( (D_n + F_n)^2 \) shows that \( E_P \geq 1 \) and \( E_P = 1 \) if and only if \( D_n = -F_n \) for all \( n \), that is,

\[
\tan \frac{\phi_{n+1}}{2} = \frac{2 - h}{2 + h} \tan \frac{\phi_n}{2},
\]

(3.8)

whose general non-vacuum solution is

\[
\phi_n = 2 \tan^{-1} e^{-a(n-b)}.
\]

(3.9)

We shall refer to (2.7), (3.9) and the vacua as Bogomol’nyi solutions of the TDSG system. Since they globally minimize \( E_P \) within their boundary class, they are automatically critical points of \( E_P \) with non-negative Hessian and hence stable static solutions of the model.

To construct non-Bogomol’nyi static solutions, we exploit the possibility that \( \phi \) may have exceptional triples. An interesting fact about such a triple is that the potential energy contributed by its pair of constituent links is independent of the values of the triple.
Lemma 2. The potential energy contributed by any exceptional triple \((\phi_{n-1}, \phi_n, \phi_{n+1})\) is
\((4 + h^2)/4\).

Proof. Since \(\phi_{n+1} = \phi_{n-1} + (2k + 1)\pi\) for some \(k \in \mathbb{Z}\), the energy of the pair of links \((\phi_{n-1}, \phi_n), (\phi_n, \phi_{n+1})\) is
\[
\frac{h}{4} \left( D_{n-1}^2 + D_n^2 + F_{n-1}^2 + F_n^2 \right) = \frac{1}{h} \left[ \sin^2 \frac{1}{2} (\phi_n - \phi_{n-1}) + \sin^2 \frac{1}{2} (\phi_{n-1} + \pi - \phi_n) \right] \\
+ \frac{h}{4} \left[ \sin^2 \frac{1}{2} (\phi_n + \phi_{n-1}) + \sin^2 \frac{1}{2} (\phi_{n-1} + \pi + \phi_n) \right] = \frac{4 + h^2}{4h}.
\]

We now have the following proposition.

Proposition 3. Let \(\phi \in \ell_{k..k+1}^2\) be a static solution with energy \(E\) and let \(k\) be an integer. Then \(\bar{\phi} \in \ell_{k..k+1}^2 \) defined by
\[
\bar{\phi}_n = \begin{cases} 
\phi_n & n \leq k \\
\phi_{n-2} + \pi & n \geq k + 1
\end{cases}
\]
is also a static solution, with energy \(\bar{E} = E + (4 + h^2)/4h\).

Proof. Since \(\phi\) is a static solution, every triple \((\phi_{n-1}, \bar{\phi}_n, \bar{\phi}_{n+1})\) with \(n \not\in |k, k + 1|\) satisfies (3.2), while \(\bar{\phi}_{k+1} - \bar{\phi}_{k-1} = \bar{\phi}_{k+2} - \bar{\phi}_k = \pi\) by construction, so the triples centred on \(n = k\) and \(n = k + 1\) are exceptional. Hence \(\bar{\phi}\) is a static solution.

To compute the energy of \(\bar{\phi}\) note that \(D_n(\bar{\phi})^2 + F_n(\bar{\phi})^2 = D_n(\phi)^2 + F_n(\phi)^2\) for all \(n < k\) and \(D_n(\phi)^2 + F_n(\phi)^2 = D_{n-}\phi_{-2}(\phi)^2 + F_{n-}(\phi)^2\) for \(n > k + 1\). Hence \(E_P[\bar{\phi}] = E_P[\phi] + \delta E\), where \(\delta E\) is the energy of the pair of links forming the exceptional triple \((\phi_{k-1}, \bar{\phi}_k, \phi_{k+1})\). But \(\delta E = (4 + h^2)/4h\) by lemma 2, so
\[
E_P[\bar{\phi}] = E_P[\phi] + \frac{4 + h^2}{4h},
\]
as was to be proved.

If we choose \(\phi = 0\), the vacuum, in proposition 3, then \(\bar{\phi}\) is a step-function kink located at \(k\), of energy \((4 + h^2)/4h > 1\). If \(\phi\) is a kink, \(\bar{\phi}\) is a double kink whose energy exceeds 2, twice the energy of a single kink. If \(\phi\) is an antikink, \(\bar{\phi}\) is a (step) kink–antikink pair. Clearly we can iterate the procedure to generate non-Bogomol’nyi solutions with arbitrary boundary values. All solutions so constructed have higher energy than the minimum within \(\ell_{k..k}\) (1 if \(k = k_{\ast}\) is odd, 0 otherwise), leading one to expect them to be unstable. Also note that the energy of any such solution diverges as \(h \to 0\), as one would expect given that the continuum sine-Gordon model has no analogous static solutions. A static double kink, kink–antikink and triple kink are depicted in figure 2.

In fact, one can prove that all non-Bogomol’nyi static solutions are unstable, independent of any particular construction. Crucial to the argument is the fact that every finite energy static solution has Bogomol’nyi ‘tails’ as \(n \to \pm \infty\). More precisely, proposition 4 follows.

Proposition 4. Let \(\phi\) be a finite energy static solution. If \(\phi\) has no exceptional triples, it is either a vacuum, a kink or an antikink. If \(\phi\) has one or more exceptional triples, there exists \(N > 0\) such that \(D_n = F_n\) for all \(n > N\) or \(D_n = -F_n\) for all \(n < N\) and \(D_n = F_n\) for all \(n < -N\) or \(D_n = -F_n\) for all \(n < -N\). Hence, \(\phi\) coincides with a vacuum, a kink or an antikink for \(n > N\), and likewise for \(n < -N\).
Figure 2. Some non-Bogomol’nyi static solutions of the spacing $h = 2/\sqrt{3}$ TDSG system (left) and their corresponding dipole multikinks (right): a double kink (a), a kink–antikink (b) and a triple kink (c).

**Proof.** The proof rests on a pair of factorizations due to Ward [13]. First,

$$\frac{4}{\hbar} \frac{\partial E_P}{\partial \phi_n} = -\cos \frac{1}{2} (\phi_{n+1} - \phi_{n-1}) \left[ \frac{4}{\hbar^2} \sin \frac{1}{2} (\phi_{n+1} - 2\phi_n + \phi_{n-1}) - \sin \frac{1}{2} (\phi_{n+1} + 2\phi_n + \phi_{n-1}) \right],$$

so every unexceptional triple in the static solution $\phi$ satisfies

$$\frac{4}{\hbar^2} \sin \frac{1}{2} (\phi_{n+1} - 2\phi_n + \phi_{n-1}) - \sin \frac{1}{2} (\phi_{n+1} + 2\phi_n + \phi_{n-1}) = 0. \quad (3.12)$$

Second,

$$\Delta(D_n^2 - F_n^2) = \sin \frac{1}{2} (\phi_{n+1} - \phi_{n-1}) \times \left[ \frac{4}{\hbar^2} \sin \frac{1}{2} (\phi_{n+1} - 2\phi_n + \phi_{n-1}) - \sin \frac{1}{2} (\phi_{n+1} + 2\phi_n + \phi_{n-1}) \right]. \quad (3.13)$$

Now since $E_P[\phi]$ is finite, $\phi$ may have at most finitely many exceptional triples, by lemma 2, so there exists $N > 0$ such that no triple $(\phi_{n-1}, \phi_n, \phi_{n+1})$ is exceptional for $|n| > N$. But then for all $n > N$, (3.12) holds, so (3.13) implies that $D_n^2 - F_n^2 = C$, a constant. But $\sum_n (D_n^2 + F_n^2) < \infty$, so $D_n, F_n \to 0$ and we conclude that $D_n^2 = F_n^2$ for all $n > N$. Similarly, $D_n^2 = F_n^2$ for all $n < -N$. If $\phi$ has no exceptional triples, the same argument shows that $D_n^2 = F_n^2$ for all $n$.

It remains to rule out the possibility (for $n > N$) that $D_{n-1} = F_{n-1}$ while $D_n = -F_n$, or $D_{n-1} = -F_{n-1}$ while $D_n = F_n$, for we can then conclude that $\phi$ uniformly satisfies either (3.7) or (3.8) on its right tail. Assume the contrary. Then

$$\tan \frac{\phi_{n+1}}{2} = \tan \frac{\phi_{n-1}}{2}, \quad (3.14)$$

so $\phi_{n-1} = \phi_{n+1} \mod 2\pi$. But this contradicts (3.2), unless $\phi_{n-1} = \phi_{n+1} = 0$ or $\pi \mod 2\pi$. In this case, the right tail of $\phi$ is a vacuum since $0$ and $\pi$ are fixed points of both (3.7) and (3.8). Hence, either $\phi$ satisfies (3.7) for all $n > N$ or it satisfies (3.8) for all $n > N$ or both (the vacua). The left tail, $n < -N$, is handled similarly. Again, if $\phi$ has no exceptional triples then either $D_n = F_n$ for all $n$ or $D_n = -F_n$ for all $n$ so $\phi$ is a kink, antikink or vacuum. □
**Theorem 5.** Let \( \phi \) be a finite energy static solution other than the kink, antikink or vacuum. Then \( \phi \) is unstable, in the sense that there exists \( u \in \ell^2 \) such that \( \text{Hess}_\phi(u, u) < 0 \).

**Proof.** By proposition 4, \( \phi \) has at least one and at most finitely many exceptional triples. We may assume, without loss of generality, that the leftmost exceptional triple is \((\phi_{-1}, \phi_0, \phi_1)\), so that \( D_n^2 = F_n^2 \) for \( n \leq -1 \). Let \( \phi^{\alpha,t} \) be the 1-parameter family (parametrized by \( \alpha \)) of variations (parametrized by \( t \)) of \( \phi \), defined by

\[
\phi^{\alpha,t}_n = \begin{cases} 
\phi_n & n \neq \{-1, 0\}, \\
\phi_{-1} + \alpha t & n = -1, \\
\phi_0 + t & n = 0
\end{cases}
\]

(no note that \( \phi^{0,0} = \phi \) for all \( \alpha \)), and let \( u^\alpha = \tfrac{d\phi^{\alpha,t}}{dt}|_{t=0} \in \ell^2 \). We will show that there exists an \( \alpha_* \) such that

\[
\text{Hess}_{\phi}(u^{\alpha_*}, u^{\alpha_*}) = \frac{d^2}{dt^2} \bigg|_{t=0} E_P[\phi^{\alpha,t}] < 0.
\]

Note that \( u^\alpha = \alpha e_{-1} + e_0 \), where \( \{e_n | n \in \mathbb{Z}\} \) is the standard basis for \( \ell^2 \), so

\[
\text{Hess}_{\phi}(u^\alpha, u^\alpha) = a_0 + a_1 \alpha + a_2 \alpha^2 =: p_2(\alpha),
\]

some quadratic polynomial in \( \alpha \).

Now, \( \phi^{0,t} \) only varies \( \phi \) by changing \( \phi_0 \), which affects only the energies of the links \((\phi_{-1}, \phi_0, \phi_1) \) and \((\phi_0, \phi_{0}, \phi_{0}) \). But these two links constitute an exceptional triple for all \( t \), so the sum of their energies is \((4 + h^2)/4h\), independent of \( t \) by lemma 2. Hence \( E_P[\phi^{0,t}] = E_P[\phi] \) for all \( t \), so

\[
a_0 = \text{Hess}_{\phi}(u^0, u^0) = \frac{d^2}{dt^2} \bigg|_{t=0} E_P[\phi^{0,t}] = 0.
\]

and \( p_2(\alpha) = a_1 \alpha + a_2 \alpha^2 \). It thus suffices to show that \( p_2(-1) \neq p_2(1) \), since then \( a_1 \neq 0 \) so \( p_2(\alpha) \) takes negative values close to 0.

The variation \( \phi^{\alpha,t} \) changes only \( \phi_{-1} \) and \( \phi_0 \), so

\[
E_P[\phi^{\alpha,t}] = \text{const} - \frac{1}{2h} t \{ \cos(\phi_{-1} - \phi_{-2} + \alpha t) + \cos(\phi_0 - \phi_{-1} + (1 - \alpha) t) \\
- \cos(\phi_0 - \phi_{-1} + t) \} - \frac{h}{8} \{ \cos(\phi_{-1} + \phi_{-2} + \alpha t) + \cos(\phi_0 + \phi_{-1} + (1 + \alpha) t) \\
- \cos(\phi_0 + \phi_{-1} + t) \}
\]

\[
\Rightarrow p(1) = \frac{1}{2h} \{ \cos(\phi_{-1} - \phi_{-2}) - \cos(\phi_0 - \phi_{-1}) \} \\
+ \frac{h}{8} \{ \cos(\phi_{-1} + \phi_{-2}) + 3 \cos(\phi_0 + \phi_{-1}) \},
\]

\[
p(-1) = \frac{1}{2h} \{ \cos(\phi_{-1} - \phi_{-2}) + 3 \cos(\phi_0 - \phi_{-1}) \} \\
+ \frac{h}{8} \{ \cos(\phi_{-1} + \phi_{-2}) - \cos(\phi_0 + \phi_{-1}) \}
\]

\[
\Rightarrow 2a_1 = p(1) - p(-1) = -2 \frac{h}{h} \cos(\phi_0 - \phi_{-1}) + \frac{h}{2} \cos(\phi_0 + \phi_{-1}).
\]
But recall that $D^2 = F^2 - 1$, which implies that
\[ \cos(\phi_0 - \phi_{-1}) = 1 + \frac{h^2}{4}[\cos(\phi_0 + \phi_{-1}) - 1], \]  
and hence
\[ a_1 = \frac{4 - h^2}{4h} < 0. \]  
(3.21)

Thus $\text{Hess}_\phi(u^\alpha, u^\alpha) < 0$ for $\alpha$ sufficiently small and positive, so $\phi$ is unstable.

We will now deduce from theorem 5 that all non-Bogomol’nyi static solutions are linearly unstable. If the configuration space of our model were finite dimensional, this would follow immediately. However, in the infinite-dimensional case it is necessary to proceed carefully. Let $J^\phi : \ell^2 \rightarrow \ell^2$ be the Jacobi operator associated with the bilinear form $\text{Hess}_\phi$, that is, the unique linear map such that
\[ \langle u, J^\phi v \rangle_{\ell^2} \equiv \text{Hess}_\phi(u, v). \]  
(3.22)

Then the linearization of (2.6) about the static solution $\phi$ may be thought of as a second order linear ODE on $\ell^2$, namely,
\[ \frac{h^2}{2}\ddot{v} + J^\phi v = 0. \]  
(3.23)

We think of $v(t) \in \ell^2$ as a perturbation of $\phi$. If there exist perturbations which grow without bound (in $\ell^2$ norm), we say that $\phi$ is linearly unstable. Such a perturbation certainly exists if $J^\phi$ has a negative eigenvalue, since we can perturb in the direction of the corresponding eigenvector. It is not hard to show from theorem 5 that $\text{spec } J^\phi$ contains at least one negative real number. However, we cannot conclude immediately that this number is an eigenvalue, since in infinite dimensions it may lie in the continuous or residual part of $\text{spec } J^\phi$. A more detailed analysis of $\text{spec } J^\phi$ is required. We begin with two lemmas giving basic properties of $J^\phi$.

**Lemma 6.** $J^\phi$ is bounded and self-adjoint.

**Proof.** Clearly $J^\phi$ is symmetric by definition, so self-adjointness will follow from boundedness. As before, let $\{e_n | n \in \mathbb{Z}\}$ be the usual basis for $\ell^2$ and $J^\phi_{nm} := \langle e_n, J^\phi e_m \rangle$.

Then
\[ J^\phi_{nm} = \frac{\partial^2 E_P}{\partial \phi_n \partial \phi_m} \]
\[ = \frac{h}{8} \delta_{nm} \left[ \frac{4}{h^2} (\cos(\phi_m - \phi_{m-1}) + \cos(\phi_m - \phi_{m+1})) + \cos(\phi_m + \phi_{m-1}) + \cos(\phi_m + \phi_{m+1}) \right] \]
\[ + \left( \delta_{n,m-1} + \delta_{n,m+1} \right) \left[ - \frac{4}{h^2} \cos(\phi_m - \phi_n) + \cos(\phi_m + \phi_n) \right]. \]  
(3.24)

Hence, $(J^\phi v)_n = c_n v_n + d_{n-1} v_{n-1} + d_{n+1} v_{n+1}$, where $c_n$, $d_n$ are sequences bounded independent of $\phi$: $|c_n|, |d_n| \leq \left( 4 + \frac{h^2}{4} \right)/4h$. Thus
\[ ||J^\phi v||^2 = \sum_n (c_n v_n + d_{n-1} v_{n-1} + d_{n+1} v_{n+1})^2 \]
\[ \leq 3 \left( \frac{4 + \frac{h^2}{4} }{4h} \right)^2 \sum_n (v_n^2 + v_{n-1}^2 + v_{n+1}^2) = 9 \left( \frac{4 + \frac{h^2}{4} }{4h} \right)^2 ||v||^2, \]
as was to be proved.

It follows immediately from lemma 6 that $\text{spec } J^\phi$ is real, bounded and consists of eigenvalues and continuous spectrum only (there is no residual spectrum) [14].
Lemma 7 (Asymptotic positivity). Let $\phi$ be a finite energy static solution, and for each $N \in \mathbb{Z}^+$, let $V_N = \{ v \in \ell^2 | v_n = 0 \text{ for all } |n| > N \}$. Then for all $\varepsilon > 0$, there exists $N$ such that

$$\langle v, J^\phi v \rangle \geq \left( \frac{\hbar}{2} - \varepsilon \right) ||v||^2$$

for all $v \in V_N^\perp$.

**Proof.** By proposition 4, there exists $N_1 > 0$ such that $\phi$ coincides with a vacuum or (anti)kink located at $b_+$ for $n > N_1$ and a vacuum or (anti)kink located at $b_-$ for $n < -N_1$. Given the exponential decay properties of (anti)kinks (2.7), (3.9), it follows that

$$| \cos(\phi_n \pm 1) - 1 | < C e^{-2a|n|}$$

for all $|n| > N_1 + 1$, where $C > 0$ depends on $b_\pm$ and $\hbar$, but not $N_1$. (Recall that $a = \log((2 + \hbar)/(2 - \hbar))$. Let $J^0$ be the Jacobi operator of the vacuum,

$$J^0 v = \frac{4 + \hbar^2}{4\hbar} v - \frac{4 - \hbar^2}{8\hbar} (\tau_+ v + \tau_- v),$$

where $\tau_\pm$ are the unit shift maps, $(\tau_\pm v)_n = v_{n \pm 1}$, and $L = J^\phi - J^0$.

Choose $\varepsilon > 0$, and let $N$ be any integer exceeding both $N_1$ and $(1/2a) \log(2C/\hbar \varepsilon)$. Then for all $v \perp V_N$, $v_n = 0$ for $|n| \leq N$, so we see from (3.24) and (3.25) that

$$\langle v, L v \rangle \leq \sum_{m < -N} \left\{ \frac{4 + \hbar^2}{4\hbar} C e^{-2aN} v_m^2 + \frac{4 - \hbar^2}{4\hbar} |v_m v_{m-1}| \right\}$$

$$+ \sum_{m > N} \left\{ \frac{4 + \hbar^2}{4\hbar} C e^{-2aN} v_m^2 + \frac{4 - \hbar^2}{4\hbar} |v_m v_{m+1}| \right\}$$

$$= \left\{ \frac{4 + \hbar^2}{4\hbar} ||v||^2 + \frac{4 - \hbar^2}{4\hbar} \sum_{m \in \mathbb{Z}} |v_m v_{m+1}| \right\} C e^{-2aN}$$

$$\leq \frac{2}{\hbar} C e^{-2aN} ||v||^2 < \varepsilon ||v||^2$$

since $2|v_m v_{m+1}| \leq v_m^2 + v_{m+1}^2$. It follows, therefore, that

$$\langle v, J^\phi v \rangle = \langle v, J^0 v \rangle + \langle v, L v \rangle \geq \langle v, J^0 v \rangle - ||v, L v||$$

$$\geq \langle v, J^0 v \rangle - \varepsilon ||v||^2 = \frac{4 + \hbar^2}{4\hbar} ||v||^2 - \frac{4 - \hbar^2}{2\hbar} \langle v, \tau_+ v \rangle - \varepsilon ||v||^2$$

$$\geq \frac{\hbar}{2} ||v||^2 - \varepsilon ||v||^2$$

since $\tau_+^* = \tau_+, \langle v, \tau_+ \rangle \leq ||v|| ||\tau_+ v||$ by Cauchy-Schwarz and $\tau_+$ is an isometry. □

The key point is that $J^\phi$ is positive on a subspace of finite codimension (namely $V_N^\perp$), from which we will see that it can have no negative continuous spectrum. Therefore, if $J^\phi$ has some negative spectrum, as it does when $\phi$ is non-Bogomol’nyi, it must have at least one negative eigenvalue. We are now ready to state and prove the required spectral result.

**Theorem 8.** Let $\phi$ be a finite energy static solution other than the kink, antikink or vacuum. Then $J^\phi$ has a negative eigenvalue of finite multiplicity.
Proof. Since $J$ (we will drop the superscript) is bounded and self-adjoint, its spectrum is contained in the real interval $[Q_1, Q_2]$ where
\[ Q_1 := \inf_{v \neq 0} \frac{\langle v, Jv \rangle}{||v||^2}, \quad Q_2 := \sup_{v \neq 0} \frac{\langle v, Jv \rangle}{||v||^2}, \]
and, furthermore, contains $Q_1$ and $Q_2$ [15]. By theorem 5, $Q_1 < 0$, so it remains to show that $Q_1$ is an eigenvalue of finite multiplicity.

Choose $\varepsilon \in (0, h/2)$. Then by lemma 7, there exists $N > 0$ such that $\langle v, Jv \rangle \geq (\frac{h}{2} - \varepsilon)||v||^2$ for all $v \in V_N$. Let $P : \ell^2 \to \ell^2$ be orthogonal projection onto $V_N$, $P' := 1 - P$, $T := P'JP'$ and $A = P'JP + PJP + PJP$. Then $J = T + A$, both $T$ and $A$ are bounded and self-adjoint, and $T$ is, by construction, positive. Given any bounded sequence $u^i$ in $\ell^2$, $Au^i$ is bounded and takes values in a finite-dimensional subspace of $\ell^2$ (namely $V_N \oplus P'J(V_N)$), so it has a convergent subsequence by the Bolzano–Weierstrass theorem. Thus $A$ is compact and hence trivially $T$-relatively compact [16, p 194]. Thus $\text{spec}_e J$, the essential spectrum of $J = T + A$, coincides with the essential spectrum of $T$ [16, p 244], which is bounded below by $(h/2) - \varepsilon$ [15]. Hence $Q_1$ is not in $\text{spec}_e J$. But $J$ is self-adjoint, so $\text{spec} J \setminus \text{spec}_e J$ contains only eigenvalues of finite multiplicity [16, p 518]. Hence, $Q_1$ is a negative eigenvalue of finite multiplicity, as was to be proved.

We note in passing that, since $\varepsilon$ could be chosen freely in the above argument, we get the extra information that the continuous spectrum of $J$ is bounded below by $2/h$.

Corollary 9 (Linear instability). Let $\phi$ be a finite energy static solution other than the kink, antikink or vacuum. Then the linearized TDSG flow about $\phi$ supports solutions which grow unbounded exponentially fast.

Proof. Let $u \in \ell^2$ be the eigenvector associated with the negative eigenvalue $Q_1 = -v^2$. Then (3.23) supports the solution
\[ v(t) = u \exp \left( \sqrt{\frac{v^2}{h}} t \right), \]
which grows unbounded exponentially fast.

We close this section by noting that there is a two parameter family of static solutions for which every triple is exceptional:
\[ \phi_n = \begin{cases} 
\alpha & n = 0 \mod 4, \\
\beta & n = 1 \mod 4, \\
\alpha + \pi & n = 2 \mod 4, \\
\beta + \pi & n = 3 \mod 4.
\end{cases} \]
These stand at the opposite extreme from the Bogomol’nyi solutions. Clearly they have infinite energy.

4. Exact propagating kinks

An important question is whether there exist moving kink solutions that propagate with constant velocity. In other words, in this section we are going to look for solutions that satisfy the following condition:
\[ \phi_n(t) = \phi(n - st) \equiv \phi(z), \quad z = n - st. \]
Figure 3. Profiles of the nanopteron solution $u(z)$ of (4.2) for $s = 0.2$ and $s = 0.5$ (with larger oscillating tail). The inset shows details of the tail of the solution for $s = 0.2$. In both cases $h = 1.3$.

Substituting this ansatz into (2.6), we see that the profile $\phi$ satisfies a nonlinear advance-delay ODE, namely

$$s^2 \phi''(z) = \frac{4 - h^2}{4h^2} \cos \phi(z)[\sin \phi(z + 1) + \sin \phi(z - 1)]$$

$$- \frac{4 + h^2}{4h^2} \sin \phi(z)[\cos \phi(z + 1) + \cos \phi(z - 1)].$$

(4.2)

It is very hard to prove rigorous results on the solutions of such ODEs, and comparatively little is known in general. Friesecke and Wattis [17] have proved the existence of propagating pulses in FPU chains with superquadratic intersite potential. Somewhat closer to the current situation, Iooss and Kirchgässner [18] have proved the existence, in linearly coupled oscillator chains, of small amplitude travelling pulses with small oscillatory tails. Neither method developed in these papers applies directly to the travelling kink problem we seek to address.

We will approach the problem numerically by seeking kink solutions of (4.2) using the pseudo-spectral method, a highly effective tool for finding travelling-wave solutions in lattices, which has been developed in a number of papers [19–21]. The idea is to write $\phi$ as a basic kink (for example, $2 \tan^{-1} e^{-az}$) plus a small correction $\delta \phi(z)$, write down a truncated Fourier series for $\delta \phi(z)$ and hence reduce (4.2) to a large algebraic system for the unknown Fourier coefficients, which can be solved using the Newton method. For technical details see [20,21]. We stress that this method is based not on lattice simulations but on iterative techniques and it enables us to find travelling-wave solutions with any given precision.

Straightforward application of the pseudo-spectral method to the TDSG system shows that, as for conventional discretizations, moving kink solutions with oscillating tails, or so-called nanopterons, appear. Two such nanopterons are depicted in figure 3. The amplitude $A$ of the oscillating tail depends on speed $s$ and lattice spacing $h$. If $A(s, h) = 0$, one has a genuine travelling kink, since $\phi$ satisfies kink boundary conditions. Such solutions usually have codimension 1 in the $s, h$ parameter space, so they occur at isolated values of $s$ if $h$ is fixed and vice versa. A heuristic explanation of this was provided by Aigner et al [22]. They think of the travelling kink profile $\phi$ as a heteroclinic orbit from 0 to $\pi$ and informally compute the dimensions of the stable and unstable manifolds of these fixed points by considering the
linearization of (4.2) about them. Every independent oscillatory solution of the linearization cuts the dimension of each of these manifolds by 1 and increases the codimension of the space of travelling kinks by 1. Applying their argument to the TDSG system leads one to expect that the codimension equals the number of non-negative solutions $k$ of equation

$$s^2 k^2 = 1 + \frac{4 - h^2}{h^2} \sin^2 \frac{k}{2},$$

obtained by demanding that $\phi = \cos k\tau$ be a solution of the linearization of (4.2). For fixed $h$, this number is 1 for $s$ large, but grows without bound as $s \to 0$, suggesting that travelling kinks, if they exist at all, should disappear in the low speed limit. On the other hand, the $s \to 0$ limit of the TDSG system is clearly very un-generic, since the system supports a continuous orbit of static kinks, so it remains possible that the arguments of [22] are misleading in this case.

To resolve this issue, we have systematically computed the nanopteron tail amplitude $A$ as a function of $s$ for various values of $h$ (see figure 4). In no case do we see zeros of $A$, isolated or otherwise, at large $s$, so we actually find no travelling kinks in the portion of parameter space where they are expected to arise with codimension 1. The small $s$ regime is more interesting. As $s \to 0$, the amplitude drops monotonically to a value so small as to be 0 to within numerical tolerance. Certainly $A(0) = 0$ since there is no PN barrier, and $\phi(\tau) = 2 \tan^{-1} e^{iz}$ solves (4.2) at $s = 0$. This small $s$ behaviour is very different from that of the conventional discrete sine-Gordon (DSG) system,

$$\phi_n = \phi_{n+1} - \frac{2\phi_n + \phi_{n-1}}{h^2} - \sin \phi_n,$$

included in figure 3 for comparison: $A(s)$ clearly remains bounded away from 0 for this system. For the TDSG system, it is possible that $A(s)$ really does attain the value 0 on some narrow interval $[0, s_*(h)]$, so that exact travelling kinks exist for all speeds not exceeding $s_*(h)$. More
likely $A(s)$ rises immediately from 0. This would be consistent with some formal asymptotics of Oxtoby et al computed in the context of exceptional discretizations of the $\phi^4$ system [23]. However, the question is numerically inaccessible. All we can say is that the tail amplitude goes rapidly to zero as $s \to 0$, and that this is reflected in a high degree of practical kink mobility, as demonstrated in previous studies [2–4], and by our own simulations, described below.

In order to check the dynamics of the TDSG and DSG systems, we performed numerical simulations of (2.6) and (4.4). The initial conditions were chosen by assuming translational invariance of the solution. In the case of the TDSG, we substitute $b = st$ in (2.7) and compute $\phi_n(0), \dot{\phi}_n(0)$:

$$\phi_n(0) = 2 \tan^{-1} e^{a(n-n_0)},$$

$$\dot{\phi}_n(0) = \frac{d}{dt} \phi_n(t)|_{t=0} = -as / \cosh[a(n-n_0)].$$

In the case of the conventional DSG, due to the absence of an explicit stationary solution, we take its continuum approximation $\phi_n(t) = 4 \tan^{-1} e^{b(n-n_0-st)}$ and compute $\phi_n(0), \dot{\phi}_n(0)$. Both equations have been simulated using the 4th order Runge–Kutta method on a finite lattice of size $N$. The position of the kink’s centre of mass, defined as

$$X_c(t) = \frac{\sum_{n=1}^N n(\phi_{n+1} - \phi_{n-1})}{2(\phi_N - \phi_1)},$$

has been plotted as a function of time in figure 5.

One can clearly see from this figure the difference between the two discretizations. In the TDSG case the kink moves freely along the lattice even when kicked with very small initial velocities (lines 1, 2 and 3). By inspecting this figure it is easy to see that, for small initial velocities, the actual velocity of propagation almost coincides with the initial velocity, so that the kink suffers practically no radiative deceleration. The figure also shows the existence of a velocity threshold above which radiative deceleration becomes important: the kink given an
initial velocity $s = 0.5$ quickly slows down to approximately $s = 0.1$ (line 4). In contrast, line 5 corresponds to the kink of the conventional DSG, kicked with an initial velocity $s = 0.1$. The kink propagates several sites and then finds itself trapped by the lattice. The same happens for smaller values of the initial velocity $s$. Thus, in the dynamical picture, the absence of the PN barrier for the TDSG manifests itself in the possibility, for all practical purposes, of free propagation of kinks with an arbitrarily small velocity.

5. Conclusion

We have shown that there is a concrete physical system modelled by an exceptional discretization of the sine-Gordon model, namely a uniform chain of electric dipoles, modelled by the TDSG system. Previous work [2] shows that such a chain admits a continuous translation orbit of static kinks, with no PN barrier, and that these kinks are highly mobile and exhibit strongly continuum-like behaviour (no trapping, low radiative deceleration, etc), despite being inherently very highly discrete. We have constructed static multikink solutions of the system and proved that all finite energy non-Bogomol’nyi static solutions (i.e. all except the kink, antikink and vacua) are unstable.

A key step in the analysis of static solutions was the observation that, while the solution has no exceptional triple, it ‘conserves’ the two-point function $D_n^2 - F_n^2$ as $n$ ‘evolves’ along the lattice. This is strongly reminiscent of Kevrekidis’s method [6], so one might ask whether the TDSG system conserves both energy and momentum (it falls outside the class of models considered in [7]). The answer appears, unfortunately, to be no. From (2.6), (3.11) and (3.13) it follows that

$$\sum_n \phi_n \tan \frac{1}{2} (\phi_{n+1} - \phi_{n-1}) = 0 \quad (5.1)$$

for any finite energy solution, but there is no obvious way to write this as a total time derivative.

We have investigated the possibility that the TDSG system admits exact constant-speed propagating kinks, finding only nanopterons, that is, kinks with spatially oscillatory tails. This is in contrast to the results of Oxtoby et al on exceptional discrete $\phi^4$ systems, who found isolated velocities for which the tail amplitude vanishes exactly so that exact propagating kinks exist [23]. In the TDSG case, the tail amplitude vanishes rapidly in the zero velocity limit and may, in fact, remain exactly zero on a small velocity interval, but the resolution of this issue is beyond the capability of our numerics. If so, the travelling kinks would form a codimension 0 family in a regime where, if they exist at all, they should be isolated, in contradiction to the heuristic barrier of Aigner et al [22]. This is perhaps unlikely [23] but should not be discounted altogether given the other highly ungeneric features of the system. Whether or not exact propagating solutions exist, numerical simulations confirm that the kink can move freely with arbitrarily small velocity, so that kinks enjoy a high degree of practical mobility, in marked contrast to the conventional DSG. It is possible that exact travelling kinks with a structure more complicated than that accommodated by the ansatz (4.1) exist. This problem requires a separate investigation.

To our knowledge, this is the first known example of an exceptional discrete system which models a genuine physical system. One could object that the model takes into account only the interactions between nearest neighbour dipoles. This is true, although this is a standard approximation made when modelling lattice systems. Including longer range inter-dipole forces will presumably destroy the exact continuous translation orbit of static kinks and introduce a small PN barrier. Since longer range forces are much weaker (note the $|r|^{-3}$ in
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(2.1)) one would hope that the PN barrier is so small as to be negligible in practice. To estimate how small, we have added the energy due to next-to-nearest neighbour dipole pairs to $E_P$,

$$E'_P = \frac{1}{8} \frac{\hbar}{4} \sum_n \left\{ \frac{4}{h^2} \sin^2 \frac{1}{2} (\phi_{n+1} - \phi_{n-1}) + \sin^2 \frac{1}{2} (\phi_{n+1} + \phi_{n-1}) \right\}, \quad h := \sqrt{12}, \quad (5.2)$$

in natural units, and numerically minimized $E_P + E'_P$ for site-centred and link-centred alternating kinks using a gradient flow method. We find that site-centred kinks now have very slightly lower energy. The PN barrier

$$\frac{E(b = 1/2) - E(b = 0)}{E(b = 0)} < 0.009\%.$$ \quad (5.3)

This is absolutely tiny in comparison with conventional discrete systems and strongly suggests that the inclusion of only nearest-neighbour interactions in the model is a sensible approximation.

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