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Translationally invariant discrete kinks from one-dimensional maps

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For most discretizations of the ϕ^4 theory, the stationary kink can only be centered either on a lattice site or midway between two adjacent sites. We search for exceptional discretizations that allow stationary kinks to be centered anywhere between the sites. We show that this translational invariance of the kink implies the existence of an underlying one-dimensional map $\phi_{n+1}=F(\phi_n)$. A simple algorithm based on this observation generates three families of exceptional discretizations.

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Since the early 1960s, the ϕ^4 equation,

$$\phi_{tt}=\phi_{xx}+\tfrac{1}{2}\phi(1-\phi^2), \tag{1}$$

has been one of the workhorses of statistical mechanics [1] and quantum-field theory [2]. Its kink solution,

$$\phi(x,t)=\tanh\frac{x-ct-x^{(0)}}{2\sqrt{1-c^2}}, \tag{2}$$

together with the sine-Gordon kink, are the simplest examples of topological solitons. More recently, interest has shifted towards the *discrete* ϕ^4 theories [3],

$$\ddot{\phi}_n=\frac{\phi_{n+1}-2\phi_n+\phi_{n-1}}{h^2}+f(\phi_{n-1},\phi_n,\phi_{n+1}), \tag{3}$$

and their solutions. Here h is the lattice spacing: $\phi_n(t)=\phi(x_n,t)$, with $x_n=hn$, and the function f is chosen to reproduce the nonlinearity (1) in the continuum limit:

$$f(\phi,\phi,\phi)=\tfrac{1}{2}\phi(1-\phi^2). \tag{4}$$

The discrete analogs of the ϕ^4 kinks have been used to describe charge-density waves in polymers and some metals [4], narrow domain walls in ferroelectrics [5], discommensurations in dielectric crystals [6], and topological excitations in hydrogen-bonded chains [7,8]. (For reviews and references, see [9].) The simplest, on-site, nonlinearity $f=\frac{1}{2}\phi_n(1-\phi_n^2)$ is employed most often; however, models with intersite nonlinear coupling are not unheard of in the physics literature either [10]. One of the sources of anharmonic coupling is the dipole-dipole interaction [8]; another is the geometric coupling of two degrees of freedom of the particle at the site [11].

Physically, one of the most significant properties of domain walls and topological defects is their mobility [12]. They transport the electron and proton charge in charge-density-wave condensates and hydrogen-bonded chains, respectively. The macroscopic mobile domain structures in ferroelectrics are of practical interest as the active components in optical switching and memory devices [5]. Mathematically, the discrete equations (3) are well known to admit stationary kink solutions [12,13]; however whether *traveling* discrete kinks exist remains to be an open question [3,14–18]. The continuous ϕ^4 equation (1) is Lorentz-invariant, and so the existence of the traveling kink (2) is an immediate consequence of the existence of the stationary soliton, Eq. (2) with $c=0$. The discretization breaks the Lorentz invariance and the existence of traveling discrete kinks becomes a nontrivial matter. Generically, the moving kink loses its energy through the resonant excitation of linear waves; as a result, it decelerates and eventually becomes pinned by the lattice.

In fact, the discretization even breaks the translation invariance of Eq. (1). Consequently, the stationary kink can be centered only at a countable number of points—usually on a site and midway between two adjacent sites [12,13]. This breaking of the translation invariance is connected with the presence of the Peierls-Nabarro barrier, an additional periodic potential induced by discreteness.

Miraculously, there are several *exceptional* discretizations which, while breaking the translation invariance of the equation, allow the existence of translationally invariant kinks; that is, kinks centered at an arbitrary point between the sites. One such discretization was discovered by Speight and Ward using a Bogomolny-type energy-minimality argument [15,16]:

$$f=\frac{2\phi_n+\phi_{n+1}}{12}\left(1-\frac{\phi_n^2+\phi_n\phi_{n+1}+\phi_{n+1}^2}{3}\right)+\frac{2\phi_n+\phi_{n-1}}{12}\times\left(1-\frac{\phi_n^2+\phi_n\phi_{n-1}+\phi_{n-1}^2}{3}\right). \tag{5}$$

Another exceptional discretization derives from the Ablowitz-Ladik integrable discretization of the nonlinear Schrödinger equation; it was reobtained by Bender and Tovbis [19] from the requirement of suppression of the kinks' resonant radiation:

$$f=\tfrac{1}{4}(\phi_{n+1}+\phi_{n-1})(1-\phi_n^2). \tag{6}$$

Finally, the nonlinearity

$$f=\frac{\phi_{n+1}+\phi_{n-1}}{4}-\frac{(\phi_{n+1}^2+\phi_{n-1}^2)(\phi_{n+1}+\phi_{n-1})}{8} \tag{7}$$

was identified by Kevrekidis [18], who demonstrated the existence of a two-point invariant associated with the stationary equation

$$\frac{\phi_{n+1}-2\phi_n+\phi_{n-1}}{h^2}+f(\phi_{n-1},\phi_n,\phi_{n+1})=0, \tag{8}$$

with f as in (6) and (7).

Although the translation invariance of a stationary kink does not automatically guarantee the existence of a traveling soliton, it is natural to expect it to be a prerequisite for kink mobility. For example, in the variational description of the slowly moving kink, the solution is sought as a stationary kink with a free continuous parameter defining its position on the line [15]. Also, the Stokes constants measuring the intensity of resonant radiation from the translationally invariant kinks were found to be at least an order of magnitude smaller than the corresponding constants in models with noninvariant kinks [20]. With an eye to a future attack on traveling kinks, it would be useful to identify all discretizations of the ϕ^4 theory supporting translationally invariant stationary kinks. The purpose of this note is to provide a general recipe for the generation of such exceptional discretizations $f(\phi_{n-1},\phi_n,\phi_{n+1})$.

We start with a simple observation which, however, holds the key to our construction. Assume we have a nonlinearity f which supports a continuous family of kinks of the form $\phi_n=g(n-x^{(0)},x^{(0)})$, where the continuous function $g(x,y)$, defined for all real x and y, is monotonically growing in x and periodic in y: $g(x,y+1)=g(x,y)$. (The function g will also depend on h parametrically but we omit this dependence for simplicity of notation.) It is important to emphasize that for generic discretizations, the function $g(x,y)$ can only be defined for $x=n$ and $x=n+\frac{1}{2}$. The *continuous* function with the above properties can exist only for a few *exceptional* discretizations.

The existence of the function $g(x,y)$ defined on the entire real line of x—the property we refer to as the translation invariance of the kink—implies that the stationary equation (8) derives from a two-point map. Indeed, since $g(x,y)$ is monotonic in x, we can write $n-x^{(0)}=g^{-1}(\phi_n,x^{(0)})$. Now since $\phi_{n+1}=g(n+1-x^{(0)},x^{(0)})$, we have $\phi_{n+1}=g[g^{-1}(\phi_n,x^{(0)})+1,x^{(0)}]$. Because $g(x,y)$ is defined for *any* x, this gives a well-defined one-dimensional map, $\phi_{n+1}=F(\phi_n,x^{(0)})$, with $x^{(0)}$ as a parameter. [If the function $g(x,y)$ is constant in y, the map does not depend on parameters other than h: $\phi_{n+1}=F(\phi_n)$.]

This observation suggests the following strategy for the construction of exceptional discretizations. Assume we have a one-dimensional (1D) map which we will write in the form

$$\phi_{n+1}-\phi_n=hH(\phi_{n+1},\phi_n). \tag{9}$$

Let H satisfy the following continuity condition:

$$H(\phi,\phi)=\tfrac{1}{2}(1-\phi^2). \tag{10}$$

This condition is necessary to make sure that the map (9) becomes

$$\phi_x=\tfrac{1}{2}(1-\phi^2) \tag{11}$$

in the continuum limit. The stationary ($c=0$) kink solution (2) of Eq. (1) is, simultaneously, a solution of the first-order equation (11). Imposing (10) we ensure that the discrete kink of (9) will have the correct continuum limit. Next, Eq. (10) implies that the map (9) has just one pair of fixed points, $\phi_*=\mp 1$. For small h, ϕ_{n+1} remains close to ϕ_n and hence, $H(\phi_{n+1},\phi_n)$ remains close to (10) which is positive for $|\phi|<1$. Consequently, no matter what $|\phi_0|<1$ we start with, the sequence ϕ_n is monotonically growing—at least until $|\phi_n|$ is not very close to 1. To ensure that it remains montonically growing near the fixed points, we assume that $\phi_*=-1$ is a source and $\phi_*=1$ a sink. (That is, small perturbations $\delta\phi_n=\phi_n-\phi_*$ satisfy $\delta\phi_{n+1}=\lambda\delta\phi_n$ with $\lambda>1$ near $\phi_*=-1$ and $0<\lambda<1$ near $\phi_*=1$.) Then, for any h smaller than some $\bar{h}$ and any ϕ_0 between -1 and 1, there is a number N such that $|\phi_N-\phi_*|$ is so small that all ϕ_n with $n>N$ are entrapped by the "linear neighborhood" of $\phi_*=1$ and those with $n<-N$ are all in a neighborhood of $\phi_*=-1$. This means that each ϕ_0 with $|\phi_0|<1$ defines a monotonic kink solution and so for any sufficiently small h we have a one-parameter family of stationary kinks. Speight [17] gives a less intuitively appealing but more rigorous proof of this fact; he also shows that our assumption on the character of the fixed points can be relaxed.

Next, squaring both sides of (9) and subtracting the square of its back-iterated copy,

$$\phi_n-\phi_{n-1}=hH(\phi_n,\phi_{n-1}), \tag{12}$$

produces an exceptional stationary Klein-Gordon equation

$$\frac{\phi_{n+1}-2\phi_n+\phi_{n-1}}{h^2}=\frac{H^2(\phi_{n+1},\phi_n)-H^2(\phi_n,\phi_{n-1})}{\phi_{n+1}-\phi_{n-1}}. \tag{13}$$

If H is symmetric: $H(\phi_n,\phi_{n-1})=H(\phi_{n-1},\phi_n)$, the numerator vanishes exactly where the denominator equals zero, so the discretization (13) is nonsingular.

If we want to have polynomial discretizations of the ϕ^4 theory, the function H^2 has to be a quartic polynomial. This leads to two possibilities, one where H is the square root of a polynomial, and the other where H is a polynomial itself. These can be written jointly as

$$(\phi_{n+1}-\phi_n)^m=h^mP_{2m}(\phi_{n+1},\phi_n), \tag{14}$$

where $m=1$ or 2, and $P_{2m}(u,v)$ is a polynomial of degree $2m$ that satisfies the symmetry and continuity conditions

$$P_{2m}(u,v)=P_{2m}(v,u), \tag{15}$$

$$P_{2m}(\phi,\phi)=2^{-m}(1-\phi^2)^m. \tag{16}$$

The condition (16) is a consequence of Eq. (10).

Before we proceed to the classification of the resulting models, it is pertinent to note that the linear part of the function f in (3) can always be fixed to $\frac{1}{2}\phi_n$ without loss of generality. Indeed, the most general function satisfying (4) is $f=a\phi_n+\frac{1}{2}(\frac{1}{2}-a)(\phi_{n+1}+\phi_{n-1})+$cubic terms. Since h^2 in (8) is a free parameter, we can always make a replacement $h\to\widetilde{h}$ such that $a-2/h^2=\widetilde{a}-2/\widetilde{h}^2$. In particular, we can set $\widetilde{a}=\frac{1}{2}$ which gives

$$f(\phi_{n-1},\phi_n,\phi_{n+1})=\tfrac{1}{2}\phi_n-Q(\phi_{n-1},\phi_n,\phi_{n+1}), \tag{17}$$

where Q is a homogeneous polynomial of degree 3.

Now let $m=2$ in Eq. (14). Provided P_4 satisfies conditions (15) and (16), the numerator $P_4(\phi_{n+1},\phi_n)-P_4(\phi_n,\phi_{n-1})$ of the fraction in the right-hand side of Eq. (13) divides $(\phi_{n+1}-\phi_{n-1})$ and so Eq. (13) will be of the form (8) with some cubic function f. The most general choice for such a polynomial is

$$P_4(u,v) = \tfrac{1}{4} - \mu(u-v)^2 - \tfrac{1}{2}uv + \tfrac{1}{20}[\alpha(u^4+v^4) + \beta uv(u^2+v^2) + \gamma u^2v^2], \tag{18}$$

where α, β, γ satisfy $2\alpha+2\beta+\gamma=5$ and μ is arbitrary. Picking the positive value of $\sqrt{P_4}$ and assuming that h is sufficiently small, one can check that the fixed points $\phi_*=\mp 1$ of the map (14) are a source and a sink, for any μ, α, and β. Consequently, the resulting cubic polynomial,

$$Q = \tfrac{1}{20}[\alpha(\phi_{n+1}+\phi_{n-1})(\phi_{n+1}^2+\phi_{n-1}^2) + \gamma\phi_n^2(\phi_{n+1}+\phi_{n-1}) + \beta\phi_n(\phi_{n+1}^2+\phi_n^2+\phi_{n-1}^2+\phi_{n+1}\phi_{n-1})] \tag{19}$$

with $\gamma=5-2(\alpha+\beta)$ defines a two-parameter family of models with translationally invariant kink solutions.

The discretization (19) includes, as particular cases, the Bender-Tovbis function (6) (which results from setting $\alpha=\beta=0$) and the Kevrekidis nonlinearity (7) (for which $\alpha=\frac{5}{2}$, $\beta=0$). Another simple function arises by letting $\alpha=\gamma=0$; this is a new model:

$$Q = \tfrac{1}{8}\phi_n(\phi_{n+1}^2+\phi_n^2+\phi_{n-1}^2+\phi_{n+1}\phi_{n-1}).$$

Now let $m=1$. The most general quadratic P_2 satisfying (15) and (16) is

$$P_2(u,v) = \tfrac{1}{2} - \alpha(u-v)^2 - \tfrac{1}{2}uv, \tag{20}$$

with an arbitrary α. Note that for $h<2$ and any α, $\phi_*=\mp 1$ are a source and a sink. Hence all resulting models will exhibit continuous families of kinks. Substituting Eq. (20) for H in (13), we obtain just a particular case of the nonlinearity (19), corresponding to the choice of the quartic (18) in the form of a complete square: $P_4=P_2^2$. To obtain *new* models, we need to note a conservation law $I_3(\phi_{n-1},\phi_n,\phi_{n+1})=0$ which follows from Eq. (14) with $m=1$. Here

$$I_3 \equiv P_2(\phi_{n+1},\phi_n)(\phi_n-\phi_{n-1}) + P_2(\phi_n,\phi_{n-1})(\phi_n-\phi_{n+1}).$$

Equation (13) remains valid if βI_3 is added to its right-hand side, with an arbitrary coefficient β. The resulting function Q has the form

$$\begin{aligned}Q = {}& \alpha^2(\phi_{n+1}^3+\phi_{n-1}^3) + 2\gamma(\alpha-\beta)\phi_{n+1}\phi_n\phi_{n-1} + \alpha(\alpha-\beta)\\ &\times\phi_{n+1}\phi_{n-1}(\phi_{n+1}+\phi_{n-1}) + [2\alpha^2+\gamma^2+\beta(\gamma-\alpha)]\\ &\times\phi_n^2(\phi_{n+1}+\phi_{n-1}) + \alpha(2\gamma+\beta)\phi_n(\phi_{n+1}^2+\phi_{n-1}^2)\\ &+ 2\alpha(\gamma+\beta)\phi_n^3,\end{aligned} \tag{21}$$

where $\gamma=\frac{1}{2}-2\alpha$. Equation (21) defines a two-parameter family of discretizations supporting translationally invariant kinks. These models cannot be obtained within the $m=2$ analysis above—unless $\beta=0$, of course.

Letting $\alpha=\beta=\frac{1}{6}$, we recover the model of Speight and Ward, Eq. (5). Another particularly simple, new, model is obtained by taking $\alpha=0$ and $\beta=-\frac{1}{2}$:

$$Q = \tfrac{1}{2}\phi_{n-1}\phi_n\phi_{n+1}.$$

It is instructive to compare discretizations furnished by our method with those arising from the requirement of the absence of resonant radiation from the kink [19]. The advance-delay equation associated with Eq. (8),

$$\phi(x+h) - 2\phi(x) + \phi(x-h) + h^2 f[\phi(x-h),\phi(x),\phi(x+h)] = 0, \tag{22}$$

can be solved to all orders as a perturbation expansion in h [20]; the resultant formal series depends continuously on the position parameter $x^{(0)}$. The series can only converge if all Stokes constants are zero [21]. The Stokes constants vanish if there exists a convergent solution in powers of z^{-1} to the equation

$$\varphi(z+1) - 2\varphi(z) + \varphi(z-1) - Q\,(\varphi(z-1),\varphi(z),\varphi(z+1))\big|_{h=0} = 0 \tag{23}$$

(see, e.g., [21]). This equation comes from a rescaling of Eq. (22) near the singularities of its leading-order solution (2) at $x_n=\pi i(1+2n)$, $n\in\mathbb{Z}$, in the limit $h\to 0$. The convergence of a power-series solution to Eq. (23) is necessary for the absence of oscillatory radiation tails in its "parent" equation (22).

In general, a numerical procedure is required to determine whether the series converges for a given Q, but we can easily generate a class of models for which it truncates after the first term. This was the method employed in Ref. [19] in deriving Eq. (6). It is a matter of direct substitution to check that the most general cubic polynomial for which $\varphi=2/z$ is a solution of Eq. (23), is

$$\begin{aligned}Q = {}& \sigma\phi_n(\phi_{n+1}+\phi_{n-1})^2 - 2\sigma\phi_{n+1}\phi_{n-1}(\phi_{n+1}+\phi_{n-1})\\ &+ \left(\frac{1}{4}-\frac{\beta}{2}\right)\phi_n^2(\phi_{n+1}+\phi_{n-1}) + \beta\phi_{n-1}\phi_n\phi_{n+1},\end{aligned} \tag{24}$$

with σ, β arbitrary constants.

The fact that the Stokes constants are zero is necessary but not sufficient for Eq. (22) to have continuous families of kinks for finite h. We have tested, numerically, a particular representative from the class (24):

$$Q = \phi_{n+1}\phi_{n-1}\frac{\phi_{n+1}+\phi_{n-1}}{2} - \phi_n\frac{\phi_{n+1}^2+\phi_{n-1}^2}{4}. \tag{25}$$

This model is obtained by letting $\sigma=-\frac{1}{4}$ and $\beta=\frac{1}{2}$. To check whether translationally invariant kinks exist or not, we have computed a stationary on-site kink for the model (25) and calculated eigenvalues of the associated linearized operator for an equidistant sequence of h values, ranging from $h=0$ to $h=1.179$ with an increment of 0.001. For h smaller than 0.556, the smallest-modulus eigenvalue was found to be smaller than 10^{-12} which is our numerical error of computation. However, as h increases from 0.556, the smallest eigenvalue grows to $\lambda=9\times10^{-7}$ at $h=0.955$, then decreases, crosses through zero at $h=0.993$, after which grows in modulus to $\lambda=-6\times10^{-4}$ at $h=1.179$ (Fig. 1). Thus, the zero eigenvalue, indicating the existence of a continuous family of solutions, is not present in the spectrum for $h>0.556$. For

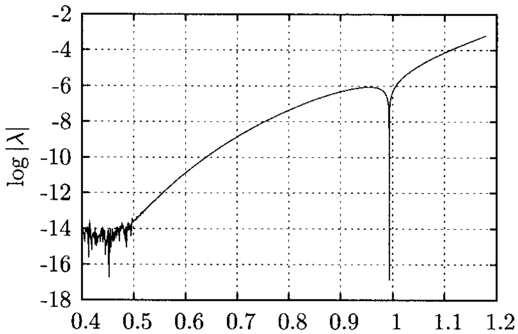

FIG. 1. The smallest-modulus eigenvalue as a function of h. The cusp occurs at the point $h=0.993$ where λ changes sign.

$h<0.556$, the smallest λ is apparently also nonzero (though very small). The only exception is the value $h=0.993$ for which the zero mode does exist. This means that the model (25) supports a continuous family of kinks for just one, isolated, value of h.

However, there exists a family of exceptional discretizations which reduces to (24) in the limit $h\to 0$. Indeed, when $\alpha=0$ in Eq. (20), the map (14) has one more conservation law: $I_2(\phi_{n-1},\phi_n,\phi_{n+1})=0$, where

$$I_2 \equiv \left(1+\frac{h^2}{4}\right)\phi_n(\phi_{n+1}+\phi_{n-1}) - 2\phi_{n-1}\phi_{n+1} - \frac{h^2}{2}.$$

We can add $\sigma(\phi_{n+1}+\phi_{n-1})I_2$ to the right-hand side of (13), along with βI_3 (with σ, β arbitrary constants.) This gives rise to the following family of discretizations:

$$\begin{aligned} Q = {} & \sigma\phi_n(\phi_{n+1}+\phi_{n-1})^2 - 2\sigma\phi_{n-1}\phi_{n+1}(\phi_{n+1}+\phi_{n-1}) \\ & + \left(\frac{1}{4}-\frac{\beta}{2}\right)\phi_n^2(\phi_{n+1}+\phi_{n-1}) + \beta\phi_{n-1}\phi_n\phi_{n+1} \\ & + \frac{1}{4}\sigma h^2\phi_n(\phi_{n+1}+\phi_{n-1})^2. \end{aligned} \tag{26}$$

Except for the last '$\mathcal{O}(h^2)$' term, this coincides with Eq. (24).

For the map (14), (20) with $\alpha=0$, the kink can be found explicitly. This implies that the discretizations (26) also share an explicit kink solution (for all β and σ): $\phi_n=\tanh(an-x^{(0)})$, with $\tanh a=h/2$.

Our final remark is on the conserved quantities of Eq. (3). The translation invariance of the stationary kink does not imply the invariance of Eq. (3) and hence the conservation of momentum. The discretization (13) [and hence (19)] conserves momentum [18] whereas the nonlinearities (21) and (26) (with $\beta,\sigma\neq 0$)—do not. Moreover, that the discretization f is exceptional does not guarantee that Eq. (3) has any integral of motion whatsoever. In particular, out of the three families (19), (21), and (26), only one model conserves energy, namely Speight and Ward's, Eq. (5).

In conclusion, we have identified three families of discretizations of the ϕ^4 equation which support translationally invariant stationary kinks: Eqs. (19), (21), and (26). In each case we have exhibited, explicitly, the underlying 1D map.

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