Exceptional discretizations of the sine-Gordon equation

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The method of one-dimensional maps was recently introduced as a means of generating exceptional discretizations of the ϕ^4 theory, i.e., discrete ϕ^4 models which support kinks centered at a continuous range of positions relative to the lattice. In this paper, we employ this method to obtain exceptional discretizations of the sine-Gordon equation (i.e., exceptional Frenkel-Kontorova chains). We also use one-dimensional maps to construct a discrete sine-Gordon equation supporting kinks which move with arbitrary velocities without emitting radiation.

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I. INTRODUCTION

Discrete analogs of nonlinear evolution equations have been the subject of intense investigation over the last 15 years. A great deal of insight has been gained into the properties of the discretized nonlinear Schrödinger, Landau-Lifschitz, Korteweg-de Vries, ϕ^4, and other equations which were originally introduced in the context of continuous nonlinear media. As for the discrete sine-Gordon equation that we study in this paper, it preceded the appearance of its continuum counterpart in the physics literature. The equation dates back to 1938 when it was proposed by Yakov Frenkel and Tatyana Kontorova to model stationary and moving crystal dislocations [1].

The original Frenkel-Kontorova model consisted of a chain of harmonically coupled atoms in a spatially periodic potential:

$$\ddot{\theta}_n = \frac{1}{h^2}(\theta_{n+1} - 2\theta_n + \theta_{n-1}) - \sin\theta_n. \qquad (1)$$

Here θ_n is the position of the nth atom in the chain, $1/h^2$ is a coupling constant, and the overdots indicate differentiation with respect to time: $\ddot{\theta}=d^2\theta/dt^2$. An alternative interpretation of Eq. (1) is that of a chain of torsionally coupled pendula, with θ_n being the angle the nth pendulum makes with the vertical. Finally, Eq. (1) can be seen simply as a discretization of the sine-Gordon equation

$$\ddot{\theta} = \theta_{xx} - \sin\theta, \qquad (2)$$

which was conceived for the numerical simulation of this partial differential equation.

Since its original inception as the Frenkel-Kontorova model, the discrete sine-Gordon equation (1) has reappeared in a great number of physical contexts, including domain walls in ferro- and antiferromagnetic crystals, charge-density waves in solids, crowdions in metals, vortices in arrays of Josephson junctions, incommensurate structures in metals and insulators, and nonlinear excitations in hydrogen-bonded molecules. (See [2,3,33] for review and references.) The equation has also been generalized in a variety of ways. In the present paper we study, systematically, two classes of such generalizations. In the models of the first class the main part of the intersite coupling is still harmonic, as in the original Frenkel-Kontorova model, but in addition there is an anharmonic part of the interaction arising from the modified periodic potential. These types of models are of interest primarily in the stationary case where they define nontrivial systems of statistical mechanics (systems with convex interactions) [3,4,33]. The stationary discretizations in this class have the form

$$\frac{1}{h^2}(\theta_{n+1} - 2\theta_n + \theta_{n-1}) = f(\theta_{n-1}, \theta_n, \theta_{n+1}), \qquad (3)$$

where the function f (not necessarily a periodic function) reduces to $\sin\theta$ in the continuum limit:

$$f(\theta_{n-1}, \theta_n, \theta_{n+1}) \to \sin\theta_n \quad \text{as} \quad \theta_{n-1}, \theta_{n+1} \to \theta_n.$$

The other class consists of all-periodic discretizations:

$$\frac{1}{h^2}\sin(\theta_{n+1} - 2\theta_n + \theta_{n-1}) = f(\theta_{n-1}, \theta_n, \theta_{n+1}). \qquad (4)$$

Here f is a periodic function of each of its three arguments, such that $f(\theta_n, \theta_n, \theta_n)=\sin\theta_n$. Equations of this type govern arrays of electric dipoles or magnetic spins in which the interactions between the neighboring elements are characterized by the trigonometric functions of the corresponding angles. These models are commonly referred to as the "sine lattices" [5]. In the stationary case, examples of the sine lattices include the usual and the chiral one-dimensional *XY* model in the magnetic field [3,6]. In the time-dependent setting, the sine lattices were used to model the rotational dynamics of methyl groups in 4-methyl-pyridine [7], CH_2 units in crystalline polyethylene [8], and bases in a DNA macromolecule [8,9]; to study conformational defects in polymer crystals [10] and nonlinear waves in chains of electric dipoles [11].

In addition to Eqs. (3) and (4), we also consider some other discretizations which have the special property of exhibiting exact solutions.

In most physical applications of the sine-Gordon theory, both continuum and discrete, the central role is played by its solitary-wave solution, called a kink. The kink represents a

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dislocation in the crystal, a 2π-twist wave in the chain of pendula, and a quantum of magnetic flux in a long Josephson junction. In the continuum model (2), the kink solution is available explicitly; in particular, the stationary kink has the expression

$$\theta(x) = 4 \arctan[\exp(x - x^{(0)})]. \tag{5}$$

The stationary kink (5) depends on a single parameter, the position of its center $x^{(0)}$, which can be varied continuously: $-\infty < x^{(0)} < \infty$. In generic discretizations of the sine-Gordon theory, however, the kink can only be centered on a lattice site or strictly midway between two neighboring sites [12–15]. Mathematically, this is a consequence of the breaking of the translation symmetry of the continuum model. The physical interpretation is that the discrete kink can only remain stationary when placed at a minimum or a maximum of the so-called Peierls-Nabarro barrier, a periodic potential induced by the discretization of Eq. (2) [12–16].

Speight and Ward [17] were the first to realize that the breaking of the translation symmetry does not necessarily preclude the existence of a one-parameter family of stationary discrete kinks with an arbitrary centering relative to the lattice. In other words, despite not being translation invariant, the lattice equation may support a kink solution which depends on a continuous translation parameter. This "spontaneous symmetry restoration" is a nongeneric phenomenon which may only occur in isolated, or *exceptional*, discretizations of the sine-Gordon model. Physically, it implies that the discretization does not induce the Peierls-Nabarro barrier, or that the barrier is transparent to kinks. Flach, Zolotaryuk, and Kladko have discovered a similar phenomenon in a class of discrete Klein-Gordon systems with nonlinearities of a special form [18].

The classification of the exceptional discrete sine-Gordon equations, i.e., equations supporting families of stationary kinks with a continuously variable position relative to the lattice, is of fundamental interest. First, the discrete kinks tend to be more mobile in exceptional discrete models. There are some isolated velocities at which kinks in the exceptional models may *slide*, i.e., travel without losing energy to radiation [19]. For other velocities, the moving kinks do radiate but the amplitude of radiation is much smaller than in generic systems [17,19–21]. In addition, the collisions of kinks were reported to be more elastic in the exceptional models [22]. We also show in this paper that some exceptional systems admit time-dependent versions which support sliding kinks with *arbitrary* velocities. Furthermore, there are indications [23] that all exceptional discretizations possess a conservation law: they conserve either energy or momentum. Therefore exceptional discrete models appear to be "better" approximations of the partial-differential Eq. (2)—at least as far as the kink solutions are concerned—as they preserve important properties of the continuum model.

The objective of the present paper is to identify exceptional Frenkel-Kontorova models within the families (3) and (4). We are not going to attempt a complete classification here; instead, we focus on identifying simple particular cases which may be of practical use in the future. We also construct two discrete models with *exact* (stationary and moving) kink solutions.

An outline of the rest of the paper is as follows. In the next section (Sec. II), we present the method of one-dimensional maps as applied to discrete sine-Gordon equations. In Sec. III, the method is used to identify simple exceptional discretizations of the form (3) involving ratios of trigonometric and linear functions. The symmetric maps found in this section have one further use; in Sec. IV we utilize them to construct purely trigonometric discretizations [of the form (4)]. In the subsequent sections we present discrete sine-Gordon equations with *exact* stationary (Sec. V) and moving (Sec. VI) kink solutions. Finally, several concluding remarks are made in Sec. VII which summarizes the results of this study.

II. METHOD OF ONE-DIMENSIONAL MAPS

To derive an exceptional discrete sine-Gordon model, Speight and Ward used the Bogomolny energy-minimality argument [17]. The energy minimality requirement has naturally led them to consider a one-dimensional map rather than the original, second-order, difference equation. In the follow-up work [24], Speight utilized the energy-minimizing map (the Bogomolny map) to prove the existence of a one-parameter family of kinks for their discretization of the ϕ^4 theory, i.e., the exceptionality of their ϕ^4 model.

A further insight was due to Kevrekidis [25]. Inspired by Herbst and Ablowitz' results on the discrete nonlinear Schrödinger equation [26], Kevrekidis reformulated the exceptionality of a stationary discrete Klein-Gordon equation as the existence of a two-point invariant. He also provided two phenomenological recipes of construction of stationary discretizations with such invariants. Thus the existence of a two-point invariant replaced the energy minimality requirement as the crucial property of exceptional discretizations.

The universality of one-dimensional maps as generators of translationally invariant families of solutions has been fully realized in Ref. [27]. Instead of trying to identify discretizations exhibiting a two-point invariant, the authors of [27] proposed to generate exceptional discretizations departing from a postulated map. (That is, the two-point invariant has now become a starting point rather than the final objective of the analysis.) In this way, the classification of exceptional discretizations has been reduced to the classification of one-dimensional maps. This will be our approach in this paper as well.

We start by considering a discrete sine-Gordon equation of the form (3) and assume that the corresponding stationary equation,

$$\frac{1}{h^2}(\theta_{n+1} - 2\theta_n + \theta_{n-1}) = f(\theta_{n-1}, \theta_n, \theta_{n+1}), \tag{6}$$

has a solution of the form $\theta_n = g(nh)$, where the continuous function $g(x)$ is defined for $-\infty < x < \infty$ and is monotonically growing, with $g(-\infty) = 0$ and $g(\infty) = 2\pi$. Since n does not appear in Eq. (6) explicitly, from the existence of the above solution it follows that Eq. (6) also has a whole family of solutions $\theta_n=g(nh-x^{(0)})$, with any real $x^{(0)}$, and therefore that the model (6) is exceptional. For each $x^{(0)}$, the solution $\theta_n=g(nh-x^{(0)})$ represents a discrete kink; if we interpret values $x_n=nh$ as positions of the lattice sites on the x axis, the kink θ_n appears centered on the point $x=x^{(0)}$. It is important to emphasize that we do not need to know an explicit form of g; all we need to know is that a function with these properties exists (for example, as an implicit function).

As $g(x)$ is a monotonically growing function, we can invert it to obtain $\theta_{n+1}=g(g^{-1}(\theta_n)+h)\equiv F(\theta_n)$. Since $g(x)$ is defined for all real x, the function $F(\theta_n)$ is defined for any θ_n. Thus the fact that the discretization is exceptional implies that the kink solution θ_n satisfies a one-dimensional map [27]. The opposite is also true. Namely, assume Eq. (6) results from the iteration of a one-dimensional map $\theta_{n+1}=F(\theta_n)$ (in a similar way as a second-order differential equation can be derived by differentiating a first-order one). In addition, let the function F be such that $F(\theta)>\theta$ for any θ between 0 and 2π, whereas $F(0)=0$ and $F(2\pi)=2\pi$. A simple cobwebbing argument shows then that for any θ_0 within the range $0<\theta_0<2\pi$, the map generates a discrete kink solution $\dots,\theta_{-1},\theta_0,\theta_1,\dots$. Therefore, we have a one-parameter family of kinks and so Eq. (6) represents an exceptional discretization.

This observation implies that we can find exceptional discretizations of the sine-Gordon equation by considering a one-dimensional map

$$\theta_{n+1}-\theta_n = hH(\theta_{n+1},\theta_n), \tag{7}$$

where the function H satisfies several requirements. First of all, it should satisfy the condition

$$H(\theta,\theta)=2\sin\frac{\theta}{2}, \tag{8}$$

which ensures that the map (7) reduces to equation

$$\theta_x = 2\sin\frac{\theta}{2} \tag{9}$$

in the continuum limit (where $\theta_{n+1}-\theta_n\to h\theta_x$). Equation (9) is the Bogomolny equation for the stationary continuum sine-Gordon theory: the sine-Gordon equation $\theta_{xx}=\sin\theta$ follows from Eq. (9) by differentiation, while its kink solution (5) is simultaneously a solution of Eq. (9). Therefore the condition (8) selects maps which generate discretizations of the sine-Gordon rather than some other equation. Our second requirement is that $H(\theta_n,\theta_{n+1})$ should be bounded and positive for all pairs of θ_n and θ_{n+1} with a sufficiently small value of the difference $|\theta_{n+1}-\theta_n|$ (where $0<\theta_n,\theta_{n+1}<2\pi$). Using this property of H, assuming that h is sufficiently small, and invoking the implicit function theorem, we can show that Eq. (7) defines, for any $0<\theta_n<2\pi$, a function $\theta_{n+1}=F(\theta_n)$, with $\theta_{n+1}>\theta_n$. Thus Eq. (7) will give rise to an *exceptional* discretization of the sine-Gordon equation.

This discretization results from squaring both sides of Eq. (7) and subtracting the square of its back-iterated copy,

$$\theta_n-\theta_{n-1}=hH(\theta_n,\theta_{n-1}).$$

This yields [27]

$$\frac{\theta_{n+1}-2\theta_n+\theta_{n-1}}{h^2}=\frac{H^2(\theta_{n+1},\theta_n)-H^2(\theta_n,\theta_{n-1})}{\theta_{n+1}-\theta_{n-1}}. \tag{10}$$

If H is symmetric [i.e., invariant under the permutation of its arguments: $H(x,y)=H(y,x)$], the numerator in Eq. (10) vanishes whenever the denominator equals zero and hence the right-hand side of Eq. (10) is nonsingular. Thus the classification of exceptional discretizations reduces to the classification of all symmetric functions $H(x,y)$ with the above properties. The next section summarizes the results of this analysis.

III. RATIONAL-TRIGONOMETRIC DISCRETIZATIONS

A. $H^2(x,y)=\mathcal{F}(x)+\mathcal{F}(y)$

The simplest possibility is to let $H^2(x,y)=\mathcal{F}(x)+\mathcal{F}(y)$. From $H(x,x)=2\sin(x/2)$ it follows that $\mathcal{F}(x)=2\sin^2(x/2)$ and so

$$H^2(x,y)=2\sin^2\frac{x}{2}+2\sin^2\frac{y}{2}. \tag{11}$$

This function gives rise to one of Kevrekidis' discretizations [25]:

$$\frac{\theta_{n+1}-2\theta_n+\theta_{n-1}}{h^2}=-\frac{\cos\theta_{n+1}-\cos\theta_{n-1}}{\theta_{n+1}-\theta_{n-1}}, \tag{12a}$$

or, equivalently,

$$\frac{\theta_{n+1}-2\theta_n+\theta_{n-1}}{h^2}=2\frac{\sin[(\theta_{n+1}-\theta_{n-1})/2]}{\theta_{n+1}-\theta_{n-1}}\sin\left(\frac{\theta_{n+1}+\theta_{n-1}}{2}\right). \tag{12b}$$

B. $H^2(x,y)=\mathcal{F}(x+y)$

Letting $H^2(x,y)=\mathcal{F}(x+y)$ and substituting into the continuum limit condition, yields

$$H^2(x,y)=4\sin^2\frac{x+y}{4}. \tag{13}$$

This symmetric function generates the discretization of the form

$$\frac{\theta_{n+1}-2\theta_n+\theta_{n-1}}{h^2}=4\frac{\sin[(\theta_{n+1}-\theta_{n-1})/4]}{\theta_{n+1}-\theta_{n-1}}\times\sin\left(\frac{\theta_{n+1}+2\theta_n+\theta_{n-1}}{4}\right). \tag{14}$$

C. $H^2(x,y)=\mathcal{F}(x)\mathcal{F}(y)$

Another simple possibility is to assume that $H^2(x,y)=\mathcal{F}(x)\mathcal{F}(y)$. From the continuum limit we obtain $\mathcal{F}(x)=2\sin(x/2)$ and so

$$H^2(x,y)=4\sin\frac{x}{2}\sin\frac{y}{2}. \tag{15}$$

By substituting into Eq. (10) we find the following discretization:

$$\frac{\theta_{n+1}-2\theta_n+\theta_{n-1}}{h^2}=8\frac{\sin[(\theta_{n+1}-\theta_{n-1})/4]}{\theta_{n+1}-\theta_{n-1}}\times\sin\left(\frac{\theta_n}{2}\right)\cos\left(\frac{\theta_{n+1}+\theta_{n-1}}{4}\right). \quad (16)$$

D. $H^2(x,y)=[\mathcal{F}(x)+\mathcal{F}(y)]^2$

Considering the symmetric function of the form $H^2(x,y)=[\mathcal{F}(x)+\mathcal{F}(y)]^2$, we obtain from the continuum limit

$$H^2(x,y)=\left(\sin\frac{x}{2}+\sin\frac{y}{2}\right)^2. \quad (17)$$

This gives rise to the following discretization:

$$\frac{\theta_{n+1}-2\theta_n+\theta_{n-1}}{h^2}=2\frac{\sin[(\theta_{n+1}-\theta_{n-1})/4]}{\theta_{n+1}-\theta_{n-1}}\cos\left(\frac{\theta_{n+1}+\theta_{n-1}}{4}\right)\times\left(\sin\frac{\theta_{n+1}}{2}+2\sin\frac{\theta_n}{2}+\sin\frac{\theta_{n-1}}{2}\right). \quad (18)$$

E. $H^2(x,y)=\mathcal{F}(x)\mathcal{F}(y)+\mathcal{G}(x)\mathcal{G}(y)$

A simple symmetric generalization involving two functions of a single argument, say $\mathcal{F}(x)$ and $\mathcal{G}(x)$, is $H^2(x,y)=\mathcal{F}(x)\mathcal{F}(y)+\mathcal{G}(x)\mathcal{G}(y)$. Setting $x=y$ yields

$$\mathcal{F}^2(x)+\mathcal{G}^2(x)=4\sin^2\frac{x}{2}.$$

One possibility here is to assume that the functions $\mathcal{F}$ and $\mathcal{G}$ have the form

$$\mathcal{F}(x)=2\eta(x)\sin\frac{x}{2}, \quad \mathcal{G}(x)=2\xi(x)\sin\frac{x}{2},$$

where η and ξ satisfy $\eta^2(x)+\xi^2(x)=1$. The simplest trigonometric choice for η and ξ is

$$\eta(x)=\sin(ax), \quad \xi(x)=\cos(ax),$$

where a is a parameter. Taking, for instance, $a=\frac{1}{2}$, gives us the following expression for $H^2(x,y)$:

$$H^2(\theta_{n+1},\theta_n)=4\sin\frac{\theta_{n+1}}{2}\sin\frac{\theta_n}{2}\cos\frac{\theta_{n+1}-\theta_n}{2}. \quad (19)$$

The function (19) is obviously positive for $|\theta_{n+1}-\theta_n|<\pi$ and therefore the resulting discretization

$$\frac{\theta_{n+1}-2\theta_n+\theta_{n-1}}{h^2}=4\frac{\sin[(\theta_{n+1}-\theta_{n-1})/2]}{\theta_{n+1}-\theta_{n-1}}\times\sin\left(\frac{\theta_n}{2}\right)\cos\left(\frac{\theta_{n+1}-\theta_n+\theta_{n-1}}{2}\right) \quad (20)$$

is exceptional for sufficiently small h.

Another simple symmetric combination of two functions of a single argument is $H^2(x,y)=\mathcal{F}(x)\mathcal{G}(y)+\mathcal{F}(y)\mathcal{G}(x)$; however, this H^2 gives rise to the discretization that we have already identified, Eqs. (12a) and (12b).

F. More complex symmetric functions

It is not difficult to construct more examples of symmetric functions $H(x,y)$ with increasing complexity. One possibility is to take

$$H^2(x,y)=\sum_{n=1}^{N}\mathcal{F}_n(x)\mathcal{F}_n(y),$$

where $\mathcal{F}_n(x)$ $(n=1,2,\ldots,N)$ are appropriate trigonometric functions. Another symmetric combination is

$$H^2(x_1,x_2)=\prod_{n=1}^{N}\mathcal{F}_n(x_{|n|})+\prod_{n=1}^{N}\mathcal{F}_n(x_{|n+1|}),$$

where $|n|\equiv n \bmod 2$.

IV. PURELY TRIGONOMETRIC DISCRETIZATIONS

Our original one-dimensional map (7) can be modified to produce periodic discretizations. Instead of Eq. (7), we consider the map

$$\ell\sin\frac{\theta_{n+1}-\theta_n}{\ell}=hH(\theta_{n+1},\theta_n), \quad (21)$$

where $H(\theta_{n+1},\theta_n)$ is a trigonometric function of its arguments and ℓ is a positive integer. Subtracting from the square of Eq. (21) the square of its back-iterated copy yields the discrete model

$$\frac{\ell^2}{h^2}\sin\frac{\theta_{n+1}-2\theta_n+\theta_{n-1}}{\ell}=\frac{H^2(\theta_{n+1},\theta_n)-H^2(\theta_n,\theta_{n-1})}{\sin[(\theta_{n+1}-\theta_{n-1})/\ell]}. \quad (22)$$

As in Eq. (7), we assume that $H(\theta_{n+1},\theta_n)$ is positive, symmetric, and has the continuum limit $H(\theta,\theta)=2\sin(\theta/2)$. For sufficiently small h and $|\theta_{n+1}-\theta_n|$, Eq. (21) defines an implicit function $\theta_{n+1}=F(\theta_n)$, with $\theta_{n+1}>\theta_n$. Consequently, the discretization (22) is exceptional.

The discretizations (22) are different from those in Eq. (10) in that every term in Eq. (22) is periodic in each of its three arguments, θ_{n-1}, θ_n, and θ_{n+1}. The models of the form (22) find their applications in the description of coupled chains of elements where each element is characterized by a periodic variable (an angle) and the coupling of elements does not violate this periodicity. One example is given by the Speight-Ward discretization [17]

$$\frac{4}{h^2}\sin\left(\frac{\theta_{n+1}-2\theta_n+\theta_{n-1}}{4}\right)=\sin\left(\frac{\theta_{n+1}+2\theta_n+\theta_{n-1}}{4}\right), \quad (23)$$

which has recently been shown to describe chains of electric dipoles constrained to rotate in the plane containing the chain [11]. Another example is the one-dimensional chiral *XY* model

$$\sin(\chi_{n+1}-\chi_n-\gamma)-\sin(\chi_n-\chi_{n-1}-\gamma) = K\sin(p\chi_n) \quad (p=1,2,\ldots), \tag{24a}$$

or, equivalently,

$$\frac{\ell}{h^2}\sin\left(\frac{\theta_{n+1}-2\theta_n+\theta_{n-1}}{\ell}\right)\cos\left(\frac{\theta_{n+1}-\theta_{n-1}}{\ell}-\gamma\right)=\sin\theta_n, \tag{24b}$$

where $\theta_n = p\chi_n$, $\ell=2p$, and $h^2=pK$. The chiral XY model (24a) and (24b) describes arrays of spins with the nearest-neighbor interactions in an external magnetic field [3,6]. It is used to model helimagnetic materials, discotic and ferroelectric smectic liquid crystals, crystalline polymers, thin magnetic films, and Josephson junction arrays.

The classification of discretizations of the form (22) reduces to the classification of all possible symmetric functions $H(x,y)$—the task completed in Sec. III above. Each function $H^2(x,y)$ identified in Sec. III gives rise to a number of purely periodic discretizations of the form (22), with various ℓ; that is, each rational-trigonometric exceptional model (10) has a set of purely trigonometric counterparts (22). We will restrict ourselves to the simplest representative(s) of these sets by choosing appropriate value(s) of ℓ. The resulting models can be summarized as follows.

Picking the symmetric function (11) of Sec. III A and letting $\ell=2$ gives rise to a very simple exceptional discretization

$$\frac{2}{h^2}\sin\left(\frac{\theta_{n+1}-2\theta_n+\theta_{n-1}}{2}\right)=\sin\left(\frac{\theta_{n+1}+\theta_{n-1}}{2}\right). \tag{25}$$

If, instead, we took $\ell=4$, we would obtain a slightly more complicated model:

$$\frac{4}{h^2}\sin\left(\frac{\theta_{n+1}-2\theta_n+\theta_{n-1}}{4}\right) = \sin\left(\frac{\theta_{n+1}+\theta_{n-1}}{2}\right)\cos\left(\frac{\theta_{n+1}-\theta_{n-1}}{4}\right). \tag{26}$$

Finally, if we "extend" the symmetric function (11) by adding a term that vanishes in the continuum limit,

$$H^2(x,y)=2\sin^2\frac{x}{2}+2\sin^2\frac{y}{2}+2\sin^2\frac{x-y}{2},$$

then, keeping $\ell=4$, we will arrive at a (still reasonably simple) exceptional model

$$\frac{2}{h^2}\sin\left(\frac{\theta_{n+1}-2\theta_n+\theta_{n-1}}{4}\right) = \sin\left(\frac{\theta_{n+1}-\theta_n+\theta_{n-1}}{2}\right)\cos\left(\frac{\theta_{n+1}-\theta_{n-1}}{4}\right)\cos\frac{\theta_n}{2}. \tag{27}$$

Next, choosing the symmetric function (13) of Sec. III B and letting $\ell=4$ yields Speight and Ward's model, Eq. (23). On the other hand, taking the symmetric function (15) of Sec. III C and letting $\ell=4$, gives the discretization

$$\frac{4}{h^2}\sin\left(\frac{\theta_{n+1}-2\theta_n+\theta_{n-1}}{4}\right)=2\sin\left(\frac{\theta_n}{2}\right)\cos\left(\frac{\theta_{n+1}+\theta_{n-1}}{4}\right). \tag{28}$$

Equation (28) reduces to Eq. (23) with the lattice spacing constant $\tilde{h}=h(1+h^2/4)^{-1/2}$, if we use an identity

$$2\sin\left(\frac{\theta_n}{2}\right)\cos\left(\frac{\theta_{n+1}+\theta_{n-1}}{4}\right) = \sin\left(\frac{\theta_{n+1}+2\theta_n+\theta_{n-1}}{4}\right)-\sin\left(\frac{\theta_{n+1}-2\theta_n+\theta_{n-1}}{4}\right). \tag{29}$$

Picking the symmetric function of the form (17) from Sec. III D, and letting $\ell=4$, gives an exceptional discretization

$$\frac{4}{h^2}\sin\left(\frac{\theta_{n+1}-2\theta_n+\theta_{n-1}}{4}\right) = \frac{1}{2}\cos\left(\frac{\theta_{n+1}+\theta_{n-1}}{4}\right)\left(\sin\frac{\theta_{n+1}}{2}+2\sin\frac{\theta_n}{2}+\sin\frac{\theta_{n-1}}{2}\right). \tag{30}$$

Finally, choosing the symmetric function in the form (19) from Sec. III E and letting $\ell=2$ produces an exceptional model

$$\frac{2}{h^2}\sin\left(\frac{\theta_{n+1}-2\theta_n+\theta_{n-1}}{2}\right)=2\sin\left(\frac{\theta_n}{2}\right)\cos\left(\frac{\theta_{n+1}-\theta_n+\theta_{n-1}}{2}\right). \tag{31}$$

Writing the right-hand side as a sum of sines, we reproduce Eq. (25) with h replaced with $\tilde{h}=h(1+h^2/2)^{-1/2}$.

The models (25)–(27) and (30) constitute our list of exceptional periodic discretizations of the sine-Gordon equation. This list can be generalized and extended in a variety of ways. For example, we can replace the sine function in Eq. (21) with $\tan[(\theta_{n+1}-\theta_n)/\ell]$ or, more generally, with $\sin[(\theta_{n+1}-\theta_n)/\ell]\cos^p[m(\theta_{n+1}-\theta_n)]$ with arbitrary m and p. Also, we can add a sum $\Sigma A_n \sin^2[B_n(x-y)]$ with arbitrary A_n and B_n to any of the symmetric functions $H^2(x,y)$. Since we are mainly interested in simple discretizations, we are not pursuing these possibilities in our present work.

V. DISCRETE SINE-GORDON EQUATION WITH EXACT KINK SOLUTIONS

In this section we consider one more exceptional discretization of the sine-Gordon equation. In addition to admitting an arbitrary centering relative to the lattice, the kinks in this model are available in exact explicit form.

We start with what may seem to be an unrelated map,

$$\phi_{n+1}-\phi_n = h(1-\phi_n\phi_{n+1}).$$

Writing the square of this map as

$$\frac{(\phi_{n+1}-\phi_n)^2}{1-\phi_{n+1}\phi_n}=h^2(1-\phi_n\phi_{n+1})$$

and subtracting its back-iterated copy gives

$$\phi_{n+1} - 2\phi_n + \phi_{n-1} + \phi_n(\phi_n^2 - \phi_{n+1}\phi_{n-1}) = -h^2\phi_n(1 - \phi_{n+1}\phi_n)(1 - \phi_n\phi_{n-1}). \tag{32a}$$

Equation (32a) with

$$\phi_n = \cos\frac{\theta_n}{2}, \tag{32b}$$

that is, equation

$$\cos\frac{\theta_{n+1}}{2} - 2\cos\frac{\theta_n}{2} + \cos\frac{\theta_{n-1}}{2} + \cos\frac{\theta_n}{2}\left(\cos^2\frac{\theta_n}{2} - \cos\frac{\theta_{n+1}}{2}\cos\frac{\theta_{n-1}}{2}\right) = -h^2\cos\frac{\theta_n}{2}\left(1 - \cos\frac{\theta_n}{2}\cos\frac{\theta_{n+1}}{2}\right) \times\left(1 - \cos\frac{\theta_n}{2}\cos\frac{\theta_{n-1}}{2}\right), \tag{33}$$

provides an exceptional discretization of the sine-Gordon equation. Indeed, the continuum limit of Eq. (32a) is

$$\phi_{xx}(1-\phi^2) + \phi\phi_x^2 = -\phi(1-\phi^2)^2, \tag{34}$$

which is nothing but the stationary sine-Gordon equation $\theta_{xx}=\sin\theta$ written in terms of $\phi=\cos(\theta/2)$.

Equation (32a) has an exact kink solution

$$\phi_n = \tanh(kn - x^{(0)}), \quad \tanh k = h,$$

where $x^{(0)}$ is a translation parameter which can be chosen arbitrarily. Applying the transformation (32b) to ϕ_n produces an explicit kink solution of the discrete sine-Gordon equation (33):

$$\theta_n = 4\arctan[\exp(kn - x^{(0)})], \quad \tanh k = h. \tag{35}$$

We are not aware of any physical systems represented by Eq. (33). This discrete model may find its uses, however, in numerical simulations of the continuum sine-Gordon equation. Like other exceptional discretizations of the sine-Gordon equation, this model preserves an "effective translation invariance" of the continuum equation. The fact that the stationary discrete kinks of the model (33) are available in exact explicit form is an additional computational advantage.

VI. TRAVELING KINKS

In this section we show how the method of one-dimensional maps can be used to construct moving kinks.

The discretization breaks the Lorentz invariance of the continuum model (2) in the same way as it breaks its translation symmetry; hence the mobility of the kink becomes a nontrivial property in the discrete case. As the kink moves in the Peierls-Nabarro potential, it excites resonant radiation and decelerates as a result of that [12,14,20,28,29]. Surprisingly, some discrete models exhibit isolated values of the kink velocity for which the kink can *slide*, i.e., travel without experiencing radiative friction [18,19,30,31].

A pertinent question here is whether there are exceptional discretizations where the kink can slide with an *arbitrary* velocity. A discrete nonlinear Schrödinger equation with this property is well-known; it is the Ablowitz-Ladik model whose solitons are radiationless irrespective of their velocities. On the other hand, no discrete Klein-Gordon equations whose kink velocities would *all* be sliding velocities have been found so far—neither in the Frenkel-Kontorova class of models nor among the discrete ϕ^4 theories.

In this section we construct such a discrete sine-Gordon equation. Its kink solutions are given by explicit expressions, and, as will become obvious from these explicit formulas, all its kinks travel without emitting radiation.

We start with a nonstationary equation

$$\phi_{xx} - \phi_{tt} - 2\phi\frac{\phi_x^2 - \phi_t^2}{1+\phi^2} = \phi\frac{1-\phi^2}{1+\phi^2}, \tag{36}$$

which transforms into the sine-Gordon equation $\theta_{xx}-\theta_{tt}=\sin\theta$ by the substitution $\phi=\tan(\theta/4)$. Our first observation is that if $\phi(x,t)$ is a simultaneous solution of two first-order equations

$$\phi_x = \frac{1}{\sqrt{1-v^2}}\phi \tag{37}$$

and

$$\phi_t = -\frac{v}{\sqrt{1-v^2}}\phi, \tag{38}$$

then it also satisfies Eq. (36). In Eqs. (37) and (38), v is a parameter; $-1<v<1$. Note that Eq. (36) does not contain v explicitly; hence finding a solution of Eqs. (37) and (38) for *all* v amounts to finding a one-parameter family of solutions to Eq. (36).

Next, we discretize Eq. (37) according to

$$\frac{1}{h^2}(\phi_{n+1}-\phi_n)^2 = \frac{1}{1-v^2}\phi_n\phi_{n+1} \tag{39}$$

and divide both sides by the same expression to get

$$\frac{1}{h^2}\frac{(\phi_{n+1}-\phi_n)^2}{(1+\phi_{n+1}^2)(1+\phi_n^2)} = \frac{1}{1-v^2}\frac{\phi_n\phi_{n+1}}{(1+\phi_{n+1}^2)(1+\phi_n^2)}. \tag{40}$$

We also consider a discrete version of Eq. (38):

$$\dot{\phi}_n = -\frac{v}{\sqrt{1-v^2}}\phi_n. \tag{41}$$

Subtracting Eq. (40) from its back-iterated copy and replacing ϕ_n with $\tan(\theta_n/4)$, gives

$$\frac{1}{h^2}\sin\left(\frac{\theta_{n+1}-2\theta_n+\theta_{n-1}}{4}\right) = \frac{1}{2}\frac{1}{1-v^2}\sin\left(\frac{\theta_n}{2}\right)\cos\left(\frac{\theta_{n+1}+\theta_{n-1}}{4}\right). \tag{42}$$

On the other hand, Eq. (41) yields

$$\ddot{\phi}_n - 2\phi_n \frac{\dot{\phi}_n^2}{1+\phi_n^2} = \frac{v^2}{1-v^2}\phi_n \frac{1-\phi_{n-1}\phi_{n+1}}{1+\phi_{n-1}\phi_{n+1}}, \tag{43}$$

where we have used the relation $\phi_{n+1}\phi_{n-1}=\phi_n^2$ which is straightforward from Eq. (39). Letting $\phi_n=\tan(\theta_n/4)$ in Eq. (43), we get

$$\frac{\ddot{\theta}_n}{4}\cos\left(\frac{\theta_{n+1}-\theta_{n-1}}{4}\right) = \frac{1}{2}\frac{v^2}{1-v^2}\sin\left(\frac{\theta_n}{2}\right)\cos\left(\frac{\theta_{n+1}+\theta_{n-1}}{4}\right). \tag{44}$$

Finally, subtracting Eq. (42) from Eq. (44) yields a discrete sine-Gordon equation

$$\cos\left(\frac{\theta_{n+1}-\theta_{n-1}}{4}\right)\frac{\ddot{\theta}_n}{4} = \frac{1}{h^2}\sin\left(\frac{\theta_{n+1}-2\theta_n+\theta_{n-1}}{4}\right) - \frac{1}{2}\sin\left(\frac{\theta_n}{2}\right)\cos\left(\frac{\theta_{n+1}+\theta_{n-1}}{4}\right). \tag{45}$$

For any h, this equation has an explicit moving kink solution which is a compatible solution of the first-order difference Eq. (39) and the first-order differential Eq. (41):

$$\theta_n = 4\arctan\left[\exp\left(kn - \frac{vt}{\sqrt{1-v^2}}\right)\right], \tag{46}$$

where k is defined by

$$2\sinh\left(\frac{k}{2}\right) = \frac{h}{\sqrt{1-v^2}} \tag{47}$$

and v can take any value between -1 and 1. As $h\to 0$, the solution (46), (47) tends to the traveling kink solution of the continuum sine-Gordon equation,

$$\theta_n \to 4\arctan\left[\exp\left(\frac{x_n-vt}{\sqrt{1-v^2}}\right)\right], \quad x_n = hn.$$

Using identity (29), Eq. (45) can be cast in the form

$$\cos\left(\frac{\theta_{n+1}-\theta_{n-1}}{4}\right)\ddot{\theta}_n = \frac{4}{\tilde{h}^2}\sin\left(\frac{\theta_{n+1}-2\theta_n+\theta_{n-1}}{4}\right) - \sin\left(\frac{\theta_{n+1}+2\theta_n+\theta_{n-1}}{4}\right), \tag{48}$$

where $\tilde{h}=h(1+h^2/4)^{-1/2}$. The solution to Eq. (48) is given by the same Eq. (46) where k should now be defined by

$$\sinh\left(\frac{k}{2}\right) = \frac{1}{\sqrt{1-v^2}}\frac{\tilde{h}}{\sqrt{4-\tilde{h}^2}}. \tag{49}$$

Solution (46), (49) exists for any $|v|<1$ and $0<\tilde{h}<2$.

We close this section by noting that the stationary limit of Eq. (48) coincides with the stationary part of the Speight-Ward model [17],

$$\cos^{-1}\left(\frac{\theta_{n+1}-\theta_{n-1}}{4}\right)\ddot{\theta}_n = \frac{4}{\tilde{h}^2}\sin\left(\frac{\theta_{n+1}-2\theta_n+\theta_{n-1}}{4}\right) - \sin\left(\frac{\theta_{n+1}+2\theta_n+\theta_{n-1}}{4}\right). \tag{50}$$

(Here $\cos^{-1}\alpha$ should be understood as $1/\cos\alpha$ and not as $\arccos\alpha$.) The simulations of Speight and Ward [17] have demonstrated that the motion of the kink in their Eq. (50) is accompanied by a much weaker radiation than the kink propagation in a typical nonexceptional model. Now that we have another time-dependent version of the same stationary model, in which the radiation is completely suppressed for all velocities, the low level of radiation from the moving Speight-Ward kink can be explained simply by the proximity of their Eq. (50) to our model (48).

VII. CONCLUDING REMARKS

The results of this work can be summarized as follows.

(1) Using the method of one-dimensional maps, we have derived several exceptional discretizations of the sine-Gordon equation involving ratios of trigonometric to linear functions: Eqs. (14), (16), (18), and (20). We have also recovered the exceptional system of Kevrekidis, Eqs. (12a) and (12b), which was originally obtained within a different approach [25].

(2) We have identified several purely trigonometric exceptional discretizations, in particular Eqs. (25), (26), and (30):

$$\ddot{\theta}_n = \frac{2}{h^2}\sin\left(\frac{\theta_{n+1}-2\theta_n+\theta_{n-1}}{2}\right) - \sin\left(\frac{\theta_{n+1}+\theta_{n-1}}{2}\right);$$

$$\ddot{\theta}_n = \frac{4}{h^2}\sin\left(\frac{\theta_{n+1}-2\theta_n+\theta_{n-1}}{4}\right) - \sin\left(\frac{\theta_{n+1}+\theta_{n-1}}{2}\right)\cos\left(\frac{\theta_{n+1}-\theta_{n-1}}{4}\right);$$

$$\ddot{\theta}_n = \frac{4}{h^2}\sin\left(\frac{\theta_{n+1}-2\theta_n+\theta_{n-1}}{4}\right) - \frac{1}{2}\cos\left(\frac{\theta_{n+1}+\theta_{n-1}}{4}\right)\left(\sin\frac{\theta_{n+1}}{2} + 2\sin\frac{\theta_n}{2} + \sin\frac{\theta_{n-1}}{2}\right).$$

(3) We have derived a discretization with exact explicit kink solutions, Eq. (33).

(4) We have constructed a discrete sine-Gordon model which supports kinks traveling with arbitrary velocities:

$$\ddot{\theta}_n\cos\left(\frac{\theta_{n+1}-\theta_{n-1}}{4}\right) = \frac{4}{h^2}\sin\left(\frac{\theta_{n+1}-2\theta_n+\theta_{n-1}}{4}\right) - \sin\left(\frac{\theta_{n+1}+2\theta_n+\theta_{n-1}}{4}\right). \tag{51}$$

The latter result deserves an additional comment. By analogy with the derivation of the model (51), it is not difficult to construct discrete ϕ^4 theories supporting sliding kinks with arbitrary velocities. One such model has the form

$$\ddot{\phi}_n \frac{1-\phi_{n+1}\phi_{n-1}}{1-\phi_n^2} = \frac{\phi_{n+1}-2\phi_n+\phi_{n-1}}{h^2} + \frac{\phi_n}{2}(1-\phi_{n+1}\phi_{n-1}). \tag{52}$$

(This is a time-dependent generalization of the exceptional stationary ϕ^4 model derived in [27].) The moving kink solution to Eq. (52) has the form

$$\phi_n = \tanh\left(kn - \frac{vt}{2\sqrt{1-v^2}}\right), \quad \frac{4\tanh^2 k}{1+\tanh^2 k} = \frac{h^2}{1-v^2}.$$

Another time-dependent discretization of the ϕ^4 theory with sliding kinks is

$$\ddot{\phi}_n \frac{1-\phi_{n+1}\phi_{n-1}}{1-\phi_n^2} = \frac{\phi_{n+1}-2\phi_n+\phi_{n-1}}{h^2} + \frac{\phi_n}{2}\left[1-\frac{\phi_n}{2}(\phi_{n+1}+\phi_{n-1})\right]. \tag{53}$$

(This is a time-dependent generalization of the exceptional ϕ^4 model identified by Bender and Tovbis [32] and Kevrekidis [25].) The sliding kink solution has the form

$$\phi_n = \tanh\left(kn - \frac{1}{2\sqrt{1+\tanh^2 k}}\frac{vt}{\sqrt{1-v^2}}\right), \quad 4\tanh^2 k = \frac{h^2}{1-v^2}.$$

The analogy between Eq. (51) and the Ablowitz-Ladik model is also worth commenting upon. The Ablowitz-Ladik model is the only discrete nonlinear Schrödinger equation whose solitons can slide with any chosen velocity. The absence of the accompanying radiation is usually explained by the integrability of this equation. The similar behavior of the kinks of Eq. (51) makes one wonder whether the latter equation could also be integrable. We have tested the integrability of Eq. (51) numerically, by simulating a collision of a kink and an antikink. The scattering was found to be inelastic: the velocities of the kink and antikink changed as a result of the collision, and a significant amount of radiation was detected. Consequently, we conclude that Eq. (51) is not integrable. This example demonstrates that, contrary to common belief, integrability is not a prerequisite for the existence of a discrete soliton sliding at an arbitrarily chosen velocity.

Finally, it is interesting to compare traveling kink solutions of our model (51) with traveling kinks of another modification of the Speight-Ward model proposed by Zakrzewski [31]. Zakrzewski's model is different from the Speight-Ward Eq. (50) in the presence of a factor $(1+\alpha\dot{\theta}_n^2)^{-1}$ in front of the left-hand side of Eq. (50), with α=const. The model has an exact solution in the form of a sliding kink; however, similarly to radiationless moving kinks in other systems [18,19,30], this kink can only slide with one particular velocity which is determined by the parameters h and α. Unlike this codimension-1 solution, our sliding kinks (46), (49) have codimension 0 in the sense that they can move with an arbitrary velocity independent of h.

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