Origin of Multikinks in Nonlinear Dispersive Systems

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We develop the first analytical theory of multikinks in strongly dispersive nonlinear systems, considering the examples of the weakly discrete sine-Gordon model and the generalized Frenkel-Kontorova model with a piecewise parabolic potential. We reveal the existence of *discrete sets* of the $2\pi N$-kinks, and also show their bifurcation structure in driven damped systems, in agreement with earlier reported numerical simulations.

Nonequilibrium dynamics of many physical systems can be characterized by the creation and motion of topological excitations or defects. In particular, when a nonlinear system possesses a degeneracy of its ground state, such excitations are *kinks*, the simplest and probably most studied nonlinear modes. The concept of a kink is vital for many physical problems such as dislocation and mass transport in solids, charge-density waves, commensurable-incommensurable phase transitions, conductivity, tribology, Josephson transmission lines, etc (see, e.g., the recent review [1] and references therein).

In application to problems in solid state physics, the kink's motion is strongly affected by the inherent lattice discreteness. Earlier numerical simulations [2] of the kink's motion in a lattice described by the discrete sine-Gordon (SG) equation, also known as the Frenkel-Kontorova (FK) model [1], demonstrated a number of interesting features not observed in the dynamics of solitons of integrable (either continuous or discrete) models. In particular, Peyrard and Kruskal [2] found that a single kink becomes unstable when it moves in a discrete lattice at sufficiently large velocity, whereas two (or more) kinks are stable and propagate as *multikinks*. The former effect is associated with the mechanism of resonant interaction between a kink and radiation [3], and resonances are even observed experimentally [4]. In contrast, the latter phenomenon, i.e. the formation of multikinks, *"... has no clear analytical explanation yet"* (see [1], p. 25).

Recently, different physical systems have been studied numerically where multikinks are found to play an important role since they appear in the region where single kinks are unstable. For example, multikinks are responsible for *a mobility hysteresis* in a damped driven commensurable chain of atoms at zero [5] and nonzero [6] temperatures. In arrays of Josephson junctions, instabilities of fast kinks lead to the generation of *bunched fluxon states* also described by multikink modes [7].

The main purpose of this Letter is to provide the first step towards *an analytical theory of multikinks* in strongly dispersive nonlinear nonintegrable systems, including the analysis of the existence and codimension of $N-$kink states. In particular, we consider a weakly discrete SG model and demonstrate the existence of *a finite number of multikinks* due to a higher-order dispersion. We also find analytical solutions for multikinks and describe the effect of an external field and damping on their existence and qualitative features.

As the starting physical model for our analysis, we consider the dynamics of a commensurable chain of atoms in a periodic substrate potential (see, e.g., [1]). In a normalized form, the equations of motion for the atomic displacements u_n can be written as

$$\ddot{u}_n - V'_{\rm int}(u_n - u_{n-1}) + V'_{\rm int}(u_{n+1} - u_n) + W'_{\rm sub}(u_n) = 0,$$

where $V_{\rm int}(u)$ is the effective potential describing the interaction between neighboring atoms, and $W_{\rm sub}(u)$ is a substrate potential with period a. For small anharmonicity, the potential $V_{\rm int}(u)$ can be expanded into a Taylor series to yield:

$$\ddot{u}_n - g(u_{n+1} + u_{n-1} - 2u_n) + W'_{\rm sub}(u_n) = 0,$$

where $g \equiv V''_{\rm int}(a)$. We consider the quasi-continuum limit of this lattice model and, taking into account a higher-order dispersion, obtain the normalized equation

$$u_{tt} - u_{xx} - \beta u_{xxxx} + W'_{\rm sub}(u) = 0, \qquad (1)$$

where, for harmonic interaction, $\beta = a^2/12$.

Equation (1) takes into account the effect of lattice discreteness through a fourth-order dispersion term, and for $\beta = 0$ and $W'_{\rm sub}(u) = \sin u$, it transforms into the well-known exactly integrable SG equation that has an analytical solution for *a single 2π-kink* moving with the velocity v, $u_k = 4\tan^{-1}\{\exp[(x - vt)/\sqrt{1-v^2}]\}$. Similar kinks exist for a rather general topology of the substrate potential $W_{\rm sub}(u)$ [1]. However, our aim in this Letter is to study *a new class of localised solutions* of Eq. (1) for $\beta \neq 0$ in the form of $2\pi N$-multikinks.

First, following the original study of Peyrard and Kruskal [2], we consider the harmonic substrate potential

$$W_{\rm sub}(u) = 1 - \cos u\,. \qquad (2)$$

We look for kink-type localised solutions of Eq. (1) that move with velocity v ($v^2 < 1$), i.e. we assume

$u_k(z) = u_k(x - vt)$. Linearizing Eq. (1) and taking $u(z) \sim e^{\lambda z}$, we find eigenvalues λ of the form,

$$\lambda^2 = \frac{1}{2\beta}[(v^2 - 1) \pm \sqrt{(1 - v^2)^2 - 4\beta}],$$

so that for $\beta > 0$ there always exist two real and two purely imaginary eigenvalues. Thus, the origin $u = 0$ is a saddle-centre point and hence kinks, which are homoclinic solutions to $u = 0 \pmod{2\pi}$, should occur for *isolated values* of v for fixed β (see Refs. [8,9]). That is they are of codimension one. Moreover, this codimension is only true if the solutions are themselves reversible, that is invariant under one of the transformations:

$$R_1: \quad u(\mathrm{mod}\, 2\pi) \to -u(\mathrm{mod}\, 2\pi), \; u'' \to -u'', \quad t \to -t,$$

$$R_2: \quad u' \to -u', \quad u''' \to -u''', \quad t \to -t,$$

where prime stands for differentiation with respect to z.

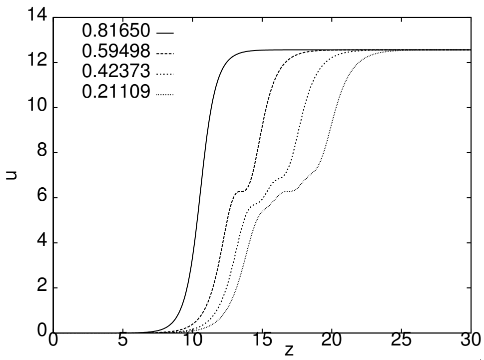

FIG. 1. The four 4π-kink solutions of Eq. (1) with $W'_{\mathrm{sub}}(u) = \sin u$ propagating at the given velocities.

To find all solutions of this type, first we fix $\beta = 1/12$, which corresponds to $a = 1$. Then, we perform numerical shooting for a range of values of v and find a discrete family of 4π-kinks at different values of v. We reveal that there exist *only four such solutions* at four different values of v. The first solution has an analytical form [10]

$$u_k(z) = 8\tan^{-1}\exp\left\{(3\beta)^{1/4} z\right\}, \tag{3}$$

where $v^2 = 1 - 2\sqrt{\beta/3}$, i.e. for our choice of β, $v_{4\pi}^{(1)} = \sqrt{2/3}$. Other values are: $v_{4\pi}^{(2)} = 0.59498\ldots$, $v_{4\pi}^{(3)} = 0.42373\ldots$, and $v_{4\pi}^{(4)} = 0.21109\ldots$. All these solutions are presented in Fig. 1. We may regard this discrete family as part of an infinite sequence of bound-states of two 2π-kinks that converges to the limit of infinite separation at a value of $v^2 < 0$. Actually the key parameter is $\mu = 1 - v^2$, and further numerical evidence reveals that the bound states converge to $\mu = -\infty$ at which value a 2π-kink exists only formally.

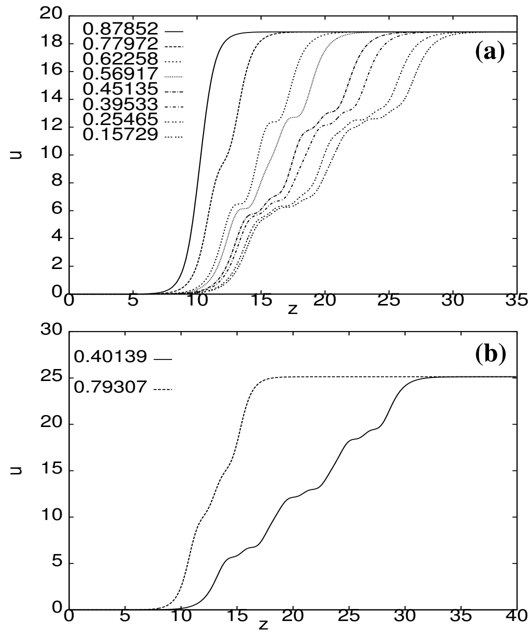

FIG. 2. Examples of (a) 6π- and (b) 8π-kinks of Eq. (1) with the potential (2) at given velocities.

Furthermore, the numerics reveals that there are no values of v at which 2π-kinks occur. However, there are v-values at which $2\pi N$-kinks occur for all $N > 2$. Figure 2 shows several examples of 6π- and 8π-kinks. According to the theory of the dynamical systems [8], on the existence of bound states of homoclinic solutions to saddle-centre equilibria in reversible Hamiltonian systems, again thinking of the 4π-kinks as bound states of 2π-kinks, one should expect to see *precisely two 6π-kinks for each 4π-kink.* These would occur at $v_{6\pi}^{(i),\pm}$ satisfying $v_{6\pi}^{(i)-} < v_{4\pi}^{(i)} < v_{6\pi}^{(i)+}$; all eight of which are depicted in Fig. 2(a). Moreover, there would be two *infinite sequences of 8π-kinks* at $v_{8\pi}^{(i,j)\pm}$ such that $v_{8\pi}^{(i,j)-} \to v_{4\pi}^{(i)}$ from below as $j \to \infty$ and $v_{8\pi}^{(i,j)+} \to v_{4\pi}^{(i)}$ from above. *Our numerical simulations have revealed precisely this structure of all multikink families.*

Finally, it appears that the above structure is *largely independent* of β. Figure 3 shows the results of continuation (using the method for homo/heteroclinic orbits [11] in the software AUTO) of the four 4π-kinks in the $(v, 1/\sqrt{\beta})$ plane. The curves are similar to the curve obtained numerically in Ref. [2] for the discrete SG equation. Note that no curve passes through $v = 1$, they only reach there asymptotically as $\beta \to 0$. In the process the slope of each kink at its midpoint steepens, so that the solution becomes singular in the limit.

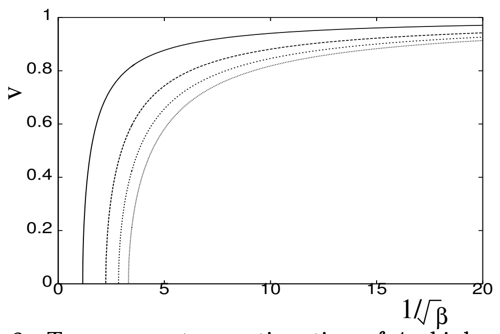

FIG. 3. Two-parameter continuation of 4π-kink solutions for the model (1) with the harmonic nonlinearity (2).

The above numerical results may be verified by the construction of *exact solutions in closed form* when the substrate potential is approximated by a piecewise parabolic potential that generates in Eq. (1) the effective force, $W'_{\rm sub}(u) =$

$$\begin{cases} u - 2n\pi \ : (2n-1)\pi + \pi/2 < u < 2n\pi + \pi/2, \\ (2n+1)\pi - u \ : 2n\pi + \pi/2 < u < (2n+1)\pi + \pi/2. \end{cases}$$

Looking for kinks moving with velocity v, we solve the linear equation (1) that defines a four-dimensional dynamical system in the phase space $(u, u', u'', u''') \in (-\pi/2, 3\pi/2] \times \mathbf{R}^3$. The phase space is separated into two distinct domains:

$$\underline{\text{Region 1}} : |u| < \pi/2, \quad \underline{\text{Region 2}} : \pi/2 < u < 3\pi/2.$$

Thus, 4π-kinks can be constructed by first noticing that, in order for these solutions to be of codimension-one (i.e. occur at isolated v-values), they should be reversible under the transformation R_1 above. Hence, we look for solutions which satisfy, for some unknown z_2, the conditions: $u(-\infty) \to 0$, $u(z_2) = 2\pi$, and $u''(z_2) = 0$, so that $u(z)$ is in Region 1 for all $z < 0$, in Region 2 for $0 < z < z_1$, for some unknown $z_1 < z_2$, and is in Region 1 again for all $z_1 < z < z_2$.

The boundary condition can be satisfied by noticing that such solutions at $z = 0$ (the first point of transition between Regions 1 and 2) satisfy $u(0) = \pi/2$, $u'(0) = \lambda\pi/2$, $u''(0) = \lambda^2\pi/2$, and $u'''(0) = \lambda^3\pi/2$, where $\lambda^2 = 6(\sqrt{\mu^2 + 2/3\pi} - \mu)$ is the unique real positive eigenvalue of the linear system in Region 1. Hence the asymptotic boundary condition at $z = -\infty$ in Region 1 becomes an initial condition at $z = 0$ for u in Region 2. The general solutions in Regions 1 and 2 are:

$$u_1(z) = A_1 e^{\lambda z} + B_1 e^{\lambda z} + C_1 \cos(\omega z) + D_1 \sin(\omega z)$$

and, providing $\mu > \mu_{\rm min} := \sqrt{2/3\pi}$,

$$u_2(z) = A_2 \cos(\omega_1 z + B_2) + C_2 \cos(\omega_2 z + D_2)$$

where $\omega^2 = 6(\sqrt{\mu^2 + 2/3\pi} + \mu)$ and $\omega_{1,2}^2 = 6(\mu \pm \sqrt{\mu^2 - 2/3\pi})$, A_j, B_j, C_j, and D_j are unknown coefficients. Therefore, we can explicitly solve for the coefficients to find $u_2(z)$ in closed form. This expression defines an implicit equation for z_1; $u_2(z_1) = 3\pi/2$. The value of $u_2(z_1)$ and its derivatives then defines initial conditions at $z = z_1$, hence determining the constants A_1, B_1, C_1, and D_1. This in turn defines z_2 implicitly as $u_1(z_2) = 2\pi$. To have a 4π-kink we additionally require $u_1''(z_2) = 0$, and so should only expect to find zeros of this final quantity by varying v. Hence we can define a 'test function' for 4π-kinks $K(v; z_1, z_2) := u_2''(z_2)$. Using the above construction, this K can be written in closed form in terms of v, z_1, and z_2. The unknown transition points $z_{1,2}$ are the solution to given transcendental equations, in each case only the first solution of which has meaning.

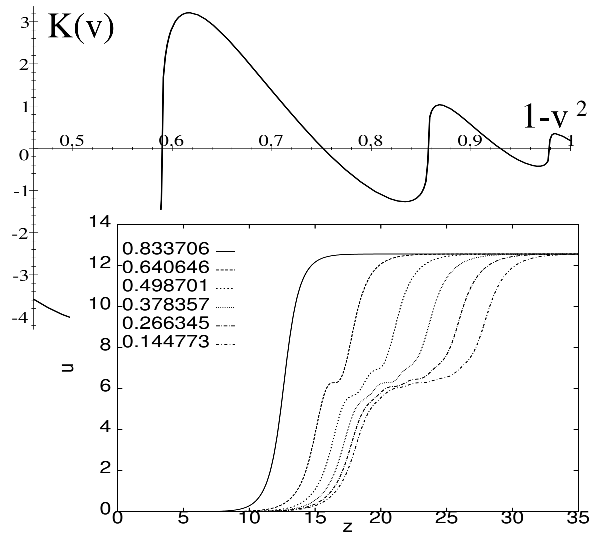

FIG. 4. The function $K(v)$ for multikinks of Eq. (1) with piecewise parabolic potential. Inset: the corresponding 4π-kinks and their associated v-values.

Figure 4 shows a graph of K as a function of $\mu = 1 - v^2 \in (\mu_{\rm min}, 1)$, which has been computed using MAPLE with the implicit equations solved for their smallest positive solutions. The five zeros of K correspond to 4π-kinks, graphs of which are shown in the insert to the figure. These zeros occur for $v = 0.64064609$, 0.49870155, 0.37835717, 0.26634472, 0.14477294. It is also possible to construct solutions for $\mu < \mu_{\rm min}$ in a analogous manner, but with the solution in Region 2 replaced by one corresponding to complex eigenvalues. This gives the additional solution given in the insert to Fig. 4 for $v = 0.833706$.

In this way, we find *analytically* a finite set of v-values giving 4π-kinks for the piecewise parabolic potential model, having *qualitatively the same structure* as the solutions found numerically for the sinusoidal nonlinearity (2). One could go on to construct $2\pi N$-kinks for $N > 2$, but the calculations presented already serve to corroborate the earlier numerical results.

To analyse the robustness of multikinks in realistic physical systems, we add to the right-hand side of Eq.

(1) the driven damped term $F - \delta u_x$, where F is an external DC force and δ is a damping coefficient (see, e.g., [5,6]). Importantly, for each of the kinks so far found, it is possible to use numerical continuation to trace curves that lie on sheets in the parameter space (v, δ, F) corresponding to the existence of multikinks. For example, taking the explicit 4π-kink solution given by Eq. (3), a curve was computed at $\beta = 1/12$ in the (F, δ)-plane with fixed $v = \sqrt{2/3}$, reaching a maximum with respect to δ at $\delta = 0.069326$. Taking the fixed value $\delta = 0.05$ from this curve the locus of kinks in the (v, F)-plane can then be traced out, as depicted in Fig. 5.

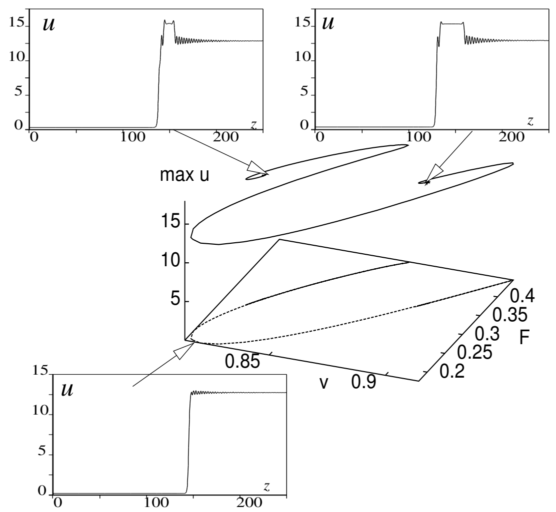

FIG. 5. The kink's velocity v and maximum amplitude against external force F for the simplest 4π kink with $\delta = 0.05$. Note that each limb of the curve spirals back on itself. The insets illustrate example solutions on the locus.

Two interesting features can be noted from this curve. First, all kinks have developed oscillations around the equilibrium close to $u = 4\pi$. This is because, for $\delta > 0$, the corresponding equation for travelling waves is no longer Hamiltonian or reversible, and the linearization around the asymptotic value $u_\star = \sin^{-1} F$ now has *three stable eigenvalues*, two of which have non-zero imaginary part. These oscillations may be regarded as *radiation that travels at the kink's velocity*, as was earlier observed in direct numerical simulations [7]. The second interesting feature of the computed curve is that it ends at a point where a transition takes place involving a heteroclinic connection with $u \approx 5\pi$. This suggests that π-kinks are possible for sufficiently large values of F.

Finally, we mention that the case $\beta < 0$ in Eq. (1) can also occur in generalised nonlinear lattices provided we take into account the next-neighbor interactions, e.g. due to the so-called *helicoidal terms* in nonlinear models of DNA dynamics [12]. In this case, the analysis is much simpler and, similar to the nonlocal SG equations [13], leads to existence and stability of continuous families of multikinks parameterized by v. ¿From the mathematical point of view, for $\beta < 0$ the origin changes from a saddle-center to a saddle-focus, and rigorous variational principles [14] give families of stable $2\pi N$-kinks for all $N > 1$.

In conclusion, we have developed the first analytical theory of multikinks in strongly dispersive nonlinear systems, considering the important examples of the weakly discrete SG model and the generalized FK model with a piecewise parabolic potential. We have revealed the existence of a discrete set of $2\pi N$-kinks, and also found exact analytical solutions for the multikinks. The analysis of a driven damped system has shown that multikinks exist in a wide region of the physical parameters above a certain threshold in the applied force amplitude. We believe that general features of multikinks and the physical mechanism for their formation are similar in many other strongly dispersive nonlinear models.

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