

## Anharmonicity-Induced Solitons in One-Dimensional Periodic Lattices

Jacob Szeftel,<sup>1,2</sup> Pascal Laurent-Gengoux,<sup>3</sup> and Ernest Ilisca<sup>1</sup>

<sup>1</sup>Laboratoire de Physique Théorique de la Matière Condensée, case 7020, 2 Place Jussieu, 75251 Paris Cedex 05, France

<sup>2</sup>Laboratoire Léon Brillouin (CEA-CNRS), Centre d'Etudes de Saclay, 91191 Gif-sur-Yvette Cédex, France

<sup>3</sup>Ecole Centrale, Grande Voie des vignes, 92295 Chatenay-Malabry, France

(Received 2 April 1999)

All bell- and kink-shaped solitons sustained by an infinite periodic atomic chain of arbitrary anharmonicity are worked out by solving a second-order, nonlinear differential equation involving advanced and retarded terms. The asymptotic time decay behaves exponentially or as a power law according to whether the potential has a harmonic limit or not. Excellent agreement is achieved with Toda's model. Illustrative examples are also given for the Fermi-Pasta-Ulam and sine-Gordon potentials. Lattice and continuum solitons differ markedly from one another.

PACS numbers: 05.45.Yv, 05.50.+q, 63.20.Ry

The atomic motion in an anharmonic crystal is described [1] in terms of generic modes comprising localized vibrations such as breathers and standing waves, vibrational traveling waves, and solitons. The interest for solitons was kindled in the last century by the observation of nonoscillatory waves moving in a continuum at constant velocity while preserving a time-independent pattern [2] which is usually either bell or kink shaped. They show up as integrable solutions of a nonlinear partial differential equation [3]. Since then solitons have been investigated in a miscellany of frameworks pertaining to field theory [4] or solid state physics [2,5] such as hydrodynamics, optical fibers, or Josephson junctions. Recently solitons have been recognized to be of significance in atomic lattices too [6], as regards magnetic materials [7], spin-Peierls, or charge-density wave compounds [5]. The task of finding solitons in discrete matter is more difficult [8–10] than in a continuum because a nonlinear differential equation, including retarded and advanced terms, must be coped with, which is an unsolved problem so far. Thus all previous attempts [11] have consisted of moving breathers or static solitons over the Peierls-Nabarro barrier. As the resulting solutions either got deformed and damped by radiating phonons or displayed undamped oscillations called nanopterons [1,2,11], no conclusive statement could even be made upon the existence of solitons in anharmonic crystals, except for two particular models, the moving breather [12] and Toda's potential [13].

This work is concerned with working out for the first time all classical solitons of an anharmonic, infinite, and periodic atomic chain. Solitons are shown to exist in discrete lattices by taking advantage of the infinite chain being integrable for solitons, as already done for breathers [14]. The procedure will be exemplified for bell-shaped solitons as well as kink-shaped ones in the Toda, Fermi-Pasta-Ulam (FPU), and sine-Gordon models.

*Integrability.*—Let us consider an infinite chain of oscillators coupled by a pair potential  $V = \sum_i W(u_i, u_{i+1})$  where  $u_i$  designates the displacement coordinate of the

lattice site  $i$ .  $W(u_i, u_{i+1})$  is assumed to be an arbitrary anharmonic function. The equations of motion read at time  $t$

$$\ddot{u}_i(t) = -\partial V / \partial u_i = f(u_{i-1}, u_i, u_{i+1}). \quad (1)$$

$f(u_{i-1}, u_i, u_{i+1})$  is assumed to have one equilibrium position at  $u_i = 0$ ,  $\forall i$  for bell-shaped solitons, and two equilibrium positions at  $u_i = 0$  and  $u_i = a$ ,  $\forall i$  for kink-shaped solitons, so that  $f(0, 0, 0) = f(a, a, a) = 0$ . A soliton, propagating at constant velocity  $\tau^{-1} > 0$  while preserving its shape, is characterized by  $u_{i+1}(t) = u_i(t + \tau)$ ,  $\forall i, t$  (the lattice parameter is thus set equal to 1). Equation (1) is recast into

$$\ddot{u}(t) = f(u(t - \tau), u(t), u(t + \tau)). \quad (2)$$

Bell- and kink-shaped solitons are characterized, respectively, by  $u \rightarrow 0$  for  $|t| \rightarrow \infty$  and both  $u \rightarrow 0$  for  $t \rightarrow -\infty$ ,  $u \rightarrow a$  for  $t \rightarrow \infty$ . Besides it is required that  $\dot{u}(t)$  vanish a single time at  $t = 0$  for a bell-shaped soliton, whereas  $\dot{u}(t)$  keeps always the same sign and  $\ddot{u}(0) = 0$  for a kink-shaped soliton,  $a$  is realized to stand for the displacement amplitude of a kink-shaped soliton, whereas  $a = u(0)$  will refer hereafter to that of a bell-shaped soliton. Thus Eq. (2) turns out to be a nonlinear differential equation having the function  $u(t)$  as the single unknown and including advanced  $[u(t + \tau)]$  and retarded  $[u(t - \tau)]$  terms. For convenience the way to solve Eq. (2) will be presented for bell-shaped solitons.

As  $t$  does not come out explicitly in Eqs. (1) and (2), a solution  $u(t)$  such that  $u(-t) = u(t)$ ,  $\forall t$  is looked for. This requires  $W(u_i, u_{i+1})$  to be symmetric with respect to  $u_i, u_{i+1}$  and thence  $f(u_{i-1}, u_i, u_{i+1})$  to be symmetric with respect to  $u_{i-1}, u_{i+1}$ . As a matter of fact, after replacing  $t$  by  $-t$  in Eq. (2), it becomes  $\ddot{u}(t) = \ddot{u}(-t)$ , which is consistent with  $u(-t) = u(t)$ . Thus it suffices to consider the range  $t \leq 0$  only. Because of  $\dot{u}(t < 0) \neq 0$ ,  $u(t)$  is monotonous versus  $t$ . Hence  $u(t)$  can be inverted to give  $t(u)$ . This ensures the existence of the one to one mapping  $u(t) \rightarrow t \rightarrow u(t + \tau)$  for  $t \leq -\tau$ , which

defines the function  $g$ , referred to below as the time-shift operator, so that  $u(t + \tau) = g(u(t))$  and  $u(t - \tau) = g^{-1}(u(t))$ . Because of  $u \rightarrow 0$  for  $t \rightarrow -\infty$ , it entails that  $g(0) = g^{-1}(0) = 0$ . Equation (2) is then rewritten as

$$\ddot{u}(t) = h(u), \quad h(u) = f(g^{-1}(u), u, g(u)). \quad (3)$$

If  $g(u)$  is supposed to be known, Eq. (3) shows up an ordinary differential equation, similar to that encountered for the continuum soliton [2]. Accordingly, it is integrated thanks to the kinetic energy theorem, while taking into account  $\dot{u} = 0$  for  $u = 0$ , to yield

$$\dot{u}(t) = \sqrt{e(u(t))}, \quad e(u) = 2 \int_0^u h(y) dy. \quad (4)$$

As for continuum solitons, Eq. (4) requires  $uh(u) > 0$  for  $u \rightarrow 0$ ; that is, there is no restoring force in the neighborhood of  $u = 0$ . This unstable equilibrium position is the soliton signature. In case of a harmonic potential this would cause  $|u(t)| \rightarrow \infty$  for  $t \rightarrow \infty$ . Thus an anharmonic potential is a prerequisite for  $u(t)$  to remain finite. A similar statement has already been made regarding equilibrium with respect to breathers [14]; that is, anharmonicity can restore dynamical stability in a lattice unstable in the harmonic limit.

Equation (4) entails also that the infinite system of Eq. (1) is integrable in so far as the energy  $\epsilon = (\dot{u}_i)^2/2 - \int_0^{u_i} h(y) dy$  associated with each degree of freedom  $u_i$  is conserved (and equal to 0) for every site  $i$ . Notice that this prominent property could be borne out but by introducing the time-shift operator  $g(u)$ . It follows from Eq. (4) and  $\dot{u} = 0$  for  $u = a$  that  $e(u) = 2 \int_a^u h(y) dy$ . Further integration leads to

$$t = \int_a^u dx / \sqrt{e(x)}. \quad (5)$$

Because  $t(u)$  is obtained by two quadratures, as would be the case for a single oscillator, Eq. (2) is said to be integrable for solitons. Applying Eq. (5) to  $\tau$  gives

$$\tau = \int_{u(t)}^{u(t+\tau)} dx / \sqrt{e(x)}. \quad (6)$$

By differentiating Eq. (6) with respect to  $u(t)$ , it becomes

$$dg/du = \sqrt{[e(g(u))/e(u)]}, \quad (7)$$

where  $u(t + \tau) = g(u(t))$ .

*Asymptotic behavior.*—Taking the leading power of the Taylor expansion of  $h(u)$  in Eq. (3) at the equilibrium position  $u = 0$  to be proportional to  $u^l$  gives rise to  $dg/du = \sqrt{[g(u)/u]^{l+1}}$ . Replacing  $g(u)$  by  $ru^\alpha$  near  $u = 0$  leads to  $\alpha = 1$ ,  $r = r^{(l+1)/2}$ , whence  $l = 1$  or  $r = \frac{dg}{du}(u = 0) = 1$  are inferred to be the only possible assignments. If  $l = 1$  and  $r \neq 1$  are assumed [ $l = 1$  and  $r = 1$  give rise to  $u(t) = 0$ ,  $\forall t$ ],  $h(u)$  shows up a linear function of  $u$ , which entails that the potential  $W(u_i, u_{i+1})$  is quadratic with respect to  $u_i$ ,  $u_{i+1}$ , or equivalently has a harmonic limit. Therefore two kinds of bell- and kink-

shaped solutions have been found according to whether the potential  $W(u_i, u_{i+1})$  has a harmonic limit or not. They will be denoted  $A$  and  $B$  and correspond to  $r \neq 1$  or  $r = 1$ . They differ markedly by the respective asymptotic  $|t| \rightarrow \infty$  behaviors of  $u(t)$ .

In case of a potential having a harmonic limit ( $l = 1$ ,  $r \neq 1$ ), Eq. (2) reads near  $u = 0$  for a soliton  $A$ ,

$$\ddot{u} = \gamma u, \quad \gamma = r^{-1} \partial f / \partial u_{i-1} + \partial f / \partial u_i + r \partial f / \partial u_{i+1}, \quad (8)$$

where the partial derivatives of  $f$  are all calculated for  $u_{i-1} = u_i = u_{i+1} = 0$ . In order to get  $u(t) \rightarrow 0$  for  $t \rightarrow -\infty$ ,  $\gamma > 0$  is needed, whence it ensues that  $u \propto e^{t/T}$  and  $T^{-2} = \gamma$ . Furthermore, the asymptotic  $t \rightarrow -\infty$  exponential behavior entails that  $r = e^{\tau/T}$ . Replacing  $r$  by this expression in  $\gamma$  in Eq. (8) gives rise to what will be referred to below as the dispersion relation of solitons  $A$  by analogy with that of traveling phonons.

Contradistinctly in case of a potential having no harmonic limit, consistency of Eq. (7) with  $l > 1$  requires that  $r = 1$ . Therefore the associated soliton  $B$  displays an asymptotic behavior for  $u(t)$  which is no longer exponential but rather power-law-like, namely,  $u(|t|) \propto 1/|t|^{2/(l-1)}$  for  $|t| \rightarrow \infty$ .

All displacement patterns of bell- and kink-shaped solitons  $A, B$ , presented below, have been reckoned by solving Eq. (2) rather than Eq. (7). They depend on a single parameter, chosen here to be  $\tau$ . As the shooting method used for breathers [14] must be discarded because of the peculiarity of Eq. (2), a scheme combining the finite element and Newton's methods has been applied to the calculation of solitons  $A$  and  $B$  and will be detailed elsewhere. It is noteworthy that the time-shift operator  $g(u)$ , by affording explicitly the  $|t| \rightarrow \infty$  behavior of  $u(t)$ , has enabled us to deal with the case of the infinite crystal, which was beyond the scope of previous work.

*Bell-shaped solitons.*—The pair potential  $W_1(u_i, u_{i+1}) = \frac{(u_i - u_{i+1})^2}{2} - \frac{u_i^3 + u_{i+1}^3}{6} + \frac{u_i^4 + u_{i+1}^4}{8}$ , having a harmonic limit, has been studied for solitons  $A$ . The dispersion relation reads in this case

$$2T^2[\cosh(\tau/T) - 1] = 1, \quad (9)$$

which implies together with  $r = e^{\tau/T} > 1$  that the velocity  $\tau^{-1} > 1$ . The amplitude  $a = u(0)$  versus velocity  $\tau^{-1}$  is plotted in Fig. 1. No solution was found for  $\tau^{-1} < 1.06$ . It is interesting to compare with the continuum soliton. The equation of motion is worked out in this latter case by replacing [2] in Eq. (1)  $u_{i+1} - u_i$  by  $b \partial u / \partial x$ , where  $b$  stands for the lattice parameter and  $x$  is the abscissa, and taking the limit for  $b \rightarrow 0$ . It then becomes  $\partial^2 u / \partial t^2 - \partial^2 u / \partial x^2 = u^2 - u^3$ . The displacement  $u(x, t)$  depends on  $t$  and  $x$ . Not only does  $a$  increase with  $\tau^{-1}$  for the lattice soliton while  $a = 4/3$  shows up  $\tau$  independent for the continuum one, but the  $|t| \rightarrow \infty$  behavior as  $u(x, t) \propto (x - t/\tau)^{-2}$  differs qualitatively from

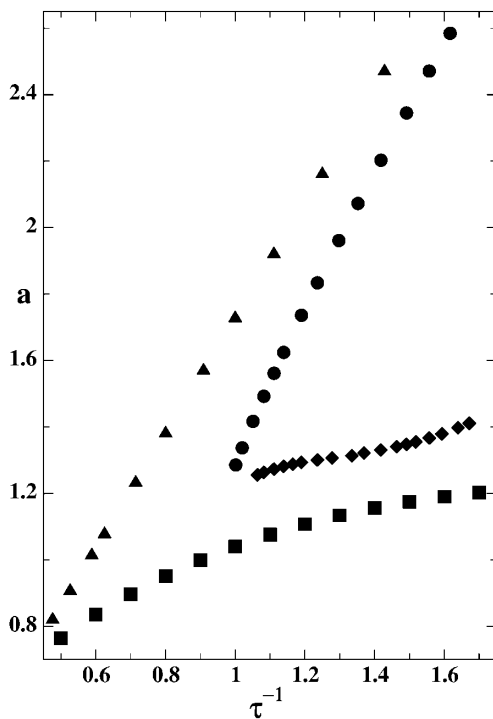


FIG. 1. Plots of  $a(\tau^{-1})$  for solitons sustained by the potentials  $W_1$  (filled diamonds),  $W_2$  (filled squares),  $W_4$  (filled circles), and  $W_5$  (filled triangles).

the exponential one typical of the lattice soliton  $A$ , as seen in Fig. 2.

The potential  $W_2(u_i, u_{i+1}) = -\frac{(u_i u_{i+1})^2}{2} + \frac{u_i^5 + u_{i+1}^5}{5}$ , having no harmonic limit, has been investigated for bell-shaped solitons  $B$  [see the displacement patterns  $u(t)$  in Fig. 2]. Accordingly,  $u(|t| \rightarrow \infty)$  decays like  $1/|t|$  and besides does not depend on  $\tau$ . The amplitude has been plotted versus velocity in Fig. 1. Notice that there are solutions for  $\tau^{-1} < 1$  by contrast with  $W_1$ .

*Toda's soliton.*—The pair potential [13] reads  $W_3(u_i, u_{i+1}) = e^{u_i - u_{i+1}}$  and sustains a kink-shaped soliton  $A$  having  $\dot{u}(t) < 0$ , the dispersion relation of which is given by Eq. (9). The equation of motion reads

$$\ddot{u}(t) = e^{u(t-\tau)-u(t)} - e^{u(t)-u(t+\tau)}. \quad (10)$$

As a consequence of  $W_3(u_i, u_{i+1})$  depending on  $u_i, u_{i+1}$  via their difference only, there are infinitely many equilibrium positions. Recalling that  $\ddot{u}(t = 0) = 0$ , the solution is sought to have the property that  $u(-t) + u(t) = 2u(0)$ , consistent with Eq. (10). However,  $W_3(u_i, u_{i+1})$  itself has no particular symmetry with respect to  $u_i, u_{i+1}$ . The sequence of iterations of Newton's method converges still faster than for the bell-shaped soliton and the agreement with Toda's results is gratifying; in particular, the relation  $|a| = \tau/T$ , valid for Toda's soliton, is checked accurately. No solitonlike solution having  $\dot{u}(t) > 0$  has been found for Eq. (10). This seems to confirm that the only soliton sustained by the potential  $W_3$  is that discovered by Toda.

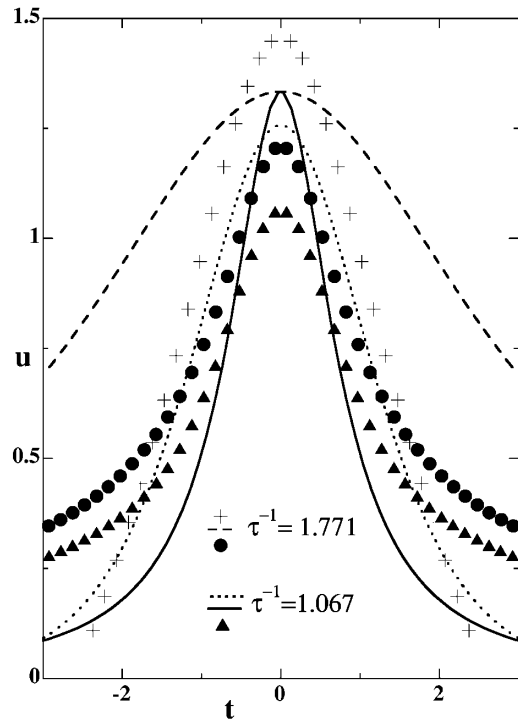


FIG. 2. Plots of  $u(t)$  for continuum (solid and dashed lines) and lattice bell-shaped solitons sustained by  $W_1$  (dotted line and +) and  $W_2$  (filled circles and triangles); respective velocities  $\tau^{-1}$  are indicated in the figure.

*FPU soliton.*—The FPU potential has been studied extensively [10]. The version of concern here reads  $W_4(u_i, u_{i+1}) = \frac{(u_i - u_{i+1})^2}{2} + \frac{(u_i - u_{i+1})^4}{4}$ . Our interest in the FPU potential stems from the property that its harmonic limit has a branch of acoustical phonons unlike most of the potentials used by other authors [1] which involve a local contribution ruling out any acoustical phonon. Thus  $W_4$  can describe the bulk atomic motion of a realistic, one-dimensional anharmonic solid. The dispersion relation is again given by Eq. (9). As  $W_4(u_i, u_{i+1})$  depends on  $u_i, u_{i+1}$  through their difference only like  $W_3$ , the kink-shaped soliton  $A$  sustained by  $W_4$  has the same properties as already discussed for Toda's soliton. However, it displays an additional property because  $W_4(u_i, u_{i+1})$  is even with respect to  $u_i, u_{i+1}$ ; namely, if there is a solution  $u(t)$  there is necessarily a solution  $2u(0) - u(t)$ . The amplitude  $a(\tau^{-1})$  is pictured in Fig. 1. It increases with the velocity but unlike Toda's soliton for which  $a(\tau^{-1} = 1) = 0$ , there comes out  $a(1) \neq 0$ . Displacement patterns  $u(t)$  are represented in Fig. 3.

The potential  $W_5(u_i, u_{i+1}) = \frac{(u_i - u_{i+1})^4}{4}$  has been studied for solitons  $B$ . It could mimic a solid driven out of equilibrium by a soft phonon. Although  $g(u)$  is generally not analytic at  $u = 0$  for every FPU potential having no harmonic limit, soliton existence has been established [15]. Besides, the asymptotic decay of  $u(|t| \rightarrow \infty)$  can be shown to be neither exponential nor power-law-like. The corresponding  $u(t)$ 's are pictured in Fig. 3, whereas the

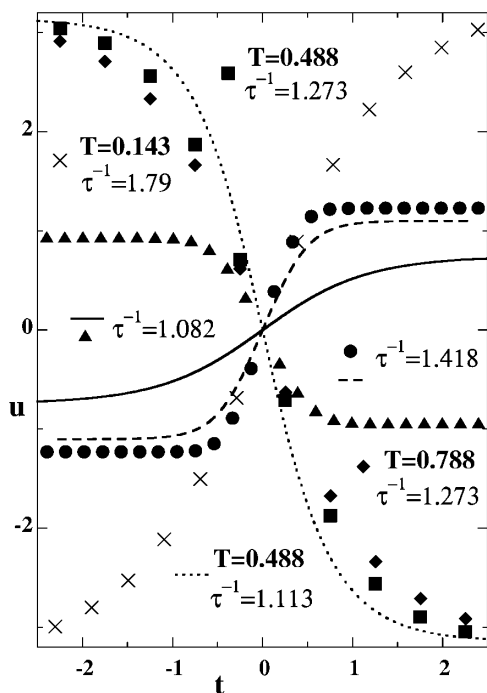


FIG. 3. Plots of  $u(t)$  for lattice solitons sustained by  $W_4$  (solid and dashed lines),  $W_5$  (filled triangles and circles) and the lattice (filled squares and  $\times$ ) and continuum (filled diamonds and dotted line) sine-Gordon potentials; respective  $\tau^{-1}$ ,  $T$ 's are indicated in the figure.

amplitude is plotted in Fig. 1. As is the case for a soliton  $B$ , there are solutions for  $\tau^{-1} < 1$ .

*sine-Gordon soliton.*—The pair potential has been taken as  $W_6(u_i, u_{i+1}) = \frac{(u_i - u_{i+1})^2 + \cos(u_i) + \cos(u_{i+1})}{2}$ , because no soliton has been found for the usual sine-Gordon potential [2,10,11] written with  $-\cos(u_i)$  instead of  $+\cos(u_i)$ . Although the configuration  $u_i = 0, \forall i$  of  $W_6$  is unstable, dynamical equilibrium could still be achieved owing to anharmonicity [14]. Since  $W_6(u_i, u_{i+1})$  like  $W_4, W_5$  is even with respect to  $u_i, u_{i+1}, u(t)$  and  $2u(0) - u(t)$  are simultaneously solutions. But the term  $\cos(u_i)$  imposes  $|a| = 2\pi$  so that the amplitude is independent of  $\tau$ . Note that  $W_4, W_5, W_6$  might as well sustain a bell-shaped soliton since they are symmetric with respect to  $u_i, u_{i+1}$ . Actually the restoring force proves too weak to allow for such a solution. The comparison with the soliton originating from the sine-Gordon equation [2]  $\partial^2 u / \partial t^2 - \partial^2 u / \partial x^2 = \sin(u)$  is all the more interesting since the continuum soliton displays also an asymptotic exponential behavior and has the same amplitude of  $2\pi$ . However, the respective dispersion relations  $T^2 [2 \cosh(\tau/T) - 1] = 1$  for the lattice soliton  $A$  and  $\tau^{-2} - T^2 = 1$  for the continuum one are quite different. Accordingly, the respective displacement patterns  $u(t)$  differ from one another as shown in Fig. 3.

In summary, even though the continuum soliton happens to present an exponential  $|t| \rightarrow \infty$  behavior, the respective properties as regards the dispersion relation or

the  $a(\tau^{-1})$  dependence are quite different. Therefore previous attempts to obtain the lattice soliton by continuous extrapolation from the continuum one might be misleading [2,9–11].

The existence of bell- and kink-shaped solitons moving at constant velocity while preserving a permanent shape has been demonstrated in one-dimensional, anharmonic crystals. This result could be achieved by showing first that the lattice equation of motion is integrable for solitons. Two classes of solutions,  $A$  and  $B$ , have been found depending on the potential having a harmonic limit. In case the potential has a harmonic limit (soliton  $A$ ), the asymptotic behavior is exponential and there is a dispersion relation between the decay time  $T$  and the propagation velocity  $\tau^{-1}$ . Potentials without any harmonic limit may sustain solitons  $B$  presenting a power-law-like or even nonanalytic asymptotic decay. An iteration procedure based on Newton's method has been devised to calculate the soliton displacement patterns  $u(t)$ . All features characterizing  $u(t)$  depend on a single parameter only, e.g.,  $\tau^{-1}$ . The amplitude  $a$  proved in all cases to increase with  $\tau^{-1}$ . Bell-shaped solitons require a bigger restoring force at  $t = 0$  than kink-shaped ones. The time-shift operator  $g(u)$  which proved to play a key role here, has been introduced owing to  $u(t)$  being invertible for solitons. Inversely this approach fails for moving breathers [12] because  $u(t)$  cannot be inverted. This comprehensive access to the lattice soliton properties opens a new field of investigation for nonlinear phenomena.

One of us (J.S.) thanks Michel Remoissenet for encouragement and criticism.

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