Intrinsic localized modes as solitons with a compact support

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It is shown that nonlinear localized modes in purely anharmonic lattices may be treated as compactons, i.e., solitons with finite wavelength [see Ph. Rosenau and J. M. Hyman, Phys. Rev. Lett. 70, 564 (1993)]. An explicit analytical solution for a compacton with an internal frequency is found for the chain of particles interacting via the quartic interatomic potential. It is demonstrated that in two particular cases, when the compacton is centered at a particle site or between neighboring particle sites, this solution gives exact expressions for two intrinsic localized modes found earlier in the framework of the rotating-wave approximation.

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As is well known, dynamical solitons appear in a result of a balance between weak nonlinearity and dispersion. However, when the wave dispersion is purely nonlinear, some novel features in the nonlinear dynamics may be observed and the most remarkable one is the existence of the so-called compactons, i.e., solitons with a compact support, which have been recently discovered by Rosenau and Hyman [1] for a special class of the Korteweg–de Vries (KdV) -type equations with nonlinear dispersion. These traveling-wave solutions have a remarkable property: Unlike the standard KdV soliton, which narrows as the amplitude increases, the compacton’s width is independent of the amplitude. Having a constant width, such solutions cannot be obtained, however, in a result of a proper continuum limit to discrete models (see, however, a special case mentioned in Ref. [1]). Indeed, primary physical models of solids are inherently discrete, with the lattice spacing being a fundamental physical parameter. Soliton-bearing equations may be derived from such discrete models in a result of expansions in the wave amplitude and inverse pulse width that normally need a scaling procedure. In other words, the continuum limit approach yields the condition of the slowly varying wave envelope, which is consistent with the effect of weak nonlinearity balanced by a weak dispersion. As soon as we deal with compactons instead of standard solitons, the continuum limit approximation cannot be properly justified because higher-order derivatives will be only numerically small.

The purpose of the present paper is to introduce a discrete compacton-bearing model that supports solutions with a finite wavelength. Moreover, I show that intrinsic localized modes, which have been recently extensively discussed for the case of one-dimensional lattices (see, e.g., the pioneer works by Sievers and Takeno [2] and Page [3]), may be treated as discrete compactons, showing excellent agreement with approximate solutions found earlier [2, 3].

I consider a one-dimensional lattice in which each atom interacts only with its nearest neighbors by purely anharmonic forces. If \( u_n(t) \) is the dimensionless displacement of the \( nth \) atom from its equilibrium position, and the atoms interact via quartic anharmonic potentials, the equation of motion for the \( nth \) atom is given by

\[
\frac{d^2 u_n}{dt^2} = [(u_{n+1} - u_n)^2 + (u_{n-1} - u_n)^2],
\]

where dimensionless units have been used.

In the continuum limit, when the particle number is treated as a continuous variable, long-wavelength excitations of the nonlinear model (1) are described by

\[
u_{tt} = (\nu^3)_{xx} + \cdots,
\]

where the indices stand for partial derivatives in \( t \) and \( x = an \), a being the lattice spacing assumed below to be equal to 1, and the function \( u_n \equiv u_{n+1} - u_n \) is treated as slowly varying. For short-wavelength excitations the continuum limit approximation may be applied to the wave envelope \( \phi_n \) defined through the relation \( u_n = (-1)^n \phi_n \), so that the partial differential equation for \( \phi_n \) takes the form

\[
\phi_{tt} + 16\phi^3 + 6\phi(\phi^2)_{xx} + \cdots = 0.
\]

Equations (2) and (3) have compacton properties similar to those of the generalized KdV equation with the nonlinear dispersion introduced in [1]. However, these equations have higher-order dispersion terms omitted that are in fact only numerically small for constant-width solutions, so that they cannot be neglected (e.g., as was done in Ref. [4]). Therefore, discrete nonlinear chains are rather natural models to look for compacton solutions (i.e., those with finite wavelength), provided in the continuum limit such models are approximately described by partial differential equations with purely nonlinear dispersion.

I look for standing oscillating solutions of Eq. (1) in the form

\[
u_n(t) = (-1)^n \phi_n \phi(t),
\]

where the function \( \phi_n \) is assumed to be independent of time. Substituting Eq. (4) into Eq. (1), I reduce it to the following equation:
\[
- \frac{1}{G^3} \frac{d^2G}{dt^2} = \frac{(\phi_{n+1} + \phi_n)^3 + (\phi_{n-1} + \phi_n)^3}{\phi_n}. \tag{5}
\]

It is clear that the left-hand side of Eq. (5) depends only on time, whereas its right-hand side depends only on the particle number \(n\). This simply means that both the parts are equal to the same constant value, giving rise to the system of two decoupled equations:

\[
\frac{d^2G}{dt^2} + CG^3 = 0, \tag{6}
\]

\[
(\phi_{n+1} + \phi_n)^3 + (\phi_{n-1} + \phi_n)^3 = C\phi_n, \tag{7}
\]

\(C\) being a constant value. Equation (6) is easily integrated and its periodic solution with amplitude \(A\) is described by the result

\[
G(t) = A \cn(\omega t; k), \tag{8}
\]

where

\[
\omega = A\sqrt{C} \quad \text{and} \quad k = \frac{1}{\sqrt{2}}, \tag{9}
\]

and \(\cn(x; k)\) is the Jacobi elliptic function with the modulus \(k\).

To find a localized solution of Eq. (7), I use the fundamental idea proposed by Rosenau and Hyman [1], assuming that such a localized solution may be taken as a part (a half of the period) of a quasilinear periodic solution with finite wavelength. In fact, the primary form of the solution may be found with the help of Eq. (3) (which has in fact properties similar to those in the equation analyzed in [1]). Thus, I seek the solution of Eq. (7) in the form

\[
\phi_n = \cos[q(n - n_0)], \quad \text{when} \quad |q(n - n_0)| < \frac{\pi}{2}, \tag{10}
\]

and \(\phi_n = 0\), otherwise. Substituting Eq. (10) into Eq. (7), I find two relations,

\[
\tan^2 \left( \frac{q}{2} \right) = \frac{1}{3}, \quad \text{i.e.,} \quad q = \frac{\pi}{3}, \tag{11}
\]

and

\[
C = \frac{27}{4}. \tag{12}
\]

Therefore, the compacton solution of the lattice equation (1) may be written as

\[
u_n(t) = (-1)^n A \cos \left[ \frac{\pi}{3} (n - n_0) \right] \cn \left( \omega t; \frac{1}{\sqrt{2}} \right), \tag{13}
\]

where \(\omega = \sqrt{27/4} A^2\),

\[
\text{when} \quad |n - n_0| < \frac{3}{2},
\]

and \(u_n(t) = 0\), otherwise. If one takes the compacton's amplitude as an independent parameter, then the compacton's frequency \(\omega\) is defined through the relation [see Eqs. (9) and (12)]

\[
\omega^2 = \frac{27}{4} A^2, \tag{14}
\]

which may be treated as the nonlinear dispersion relation.

The compacton (13) may be centered in the lattice at any position, because it is characterized by an arbitrary parameter \(n_0\) that defines a continuous shift of the compacton's center. If \(n_0 = 0\), the compacton is centered at the particle site \(n = 0\), and the corresponding pattern structure is shown in Fig. 1(a). As a result, being extended only for three lattice spacings, the compacton mode involves only three neighboring particles oscillating with the opposite phases. At \(n_0 = 0\) the solution (13) may be rewritten in the form

\[
\nu_n(t) = A(\ldots, 0, -\frac{1}{2}, 1, -\frac{1}{2}, 0, \ldots) \cn \left( \omega t; \frac{1}{\sqrt{2}} \right), \tag{15}
\]

which clearly shows the mode pattern through the amplitudes of the oscillating particles. The other limit case of the solution (13) is realized when the compacton is centered just between the neighboring particle sites, i.e., at \(n_0 = \frac{1}{2}\). In this latter case only two neighboring particles oscillate, the other being at rest [see Fig. 1(b)]. The mode pattern is given by the expression

\[
u_n(t) = \frac{\sqrt{3}}{2} A(\ldots, 0, 1, -1, 0, \ldots) \cn \left( \omega t; \frac{1}{\sqrt{2}} \right), \tag{16}
\]

and to keep the total energy unchanged, mode (16) has a renormalized amplitude \((\sqrt{3}/2)A\). In fact, the solution (13) describes an infinite family of different localized modes, which are characterized by a certain value of \(n_0\) \((0 < n_0 < \frac{1}{2})\).

As a matter of fact, the spatial structures similar to those of the localized modes (15) and (16) have been extensively discussed in connection with the so-called intrinsic localized modes first predicted by Sievers and Takeno [2] for the one-dimensional chain of particles interacting via harmonic and quartic anharmonic interatomic potentials. The model is described by [cf. Eq. (1)]

*FIG. 1.* The compacton pattern in two particular cases: (a) the compacton centered at the particle site, and (b) the compacton centered between the neighboring particle sites. Shown is the function \((-1)^n \phi_n\), where \(\phi_n\) is defined by Eqs. (10) and (11).
\[
\begin{align*}
\frac{d^2 w_n}{dt^2} &= k_2(w_{n+1} + w_{n-1} - 2w_n) \\
&\quad + k_4[(w_{n+1} - w_n)^3 + (w_{n-1} - w_n)^3].
\end{align*}
\]

(17)

Looking for a solution to Eq. (17) in the so-called "rotating-wave approximation" when only a contribution of the first harmonic is taken into account, Sievers and Takeno [2] found the so-called \(s\)-like localized mode,

\[
w_n(t) = A(..., 0, -\frac{1}{2}, 1, -\frac{1}{2}, 0, ...) \cos(\Omega t),
\]

(18)

which is in fact an approximate solution of Eq. (17) in the limit \((k_4 A^2/k_2) \gg 1\), \(\Omega\) being the mode frequency lying above the cutoff frequency \(\Omega_m^2 = 4k_2/m\) of the linear spectrum band. The other type of the intrinsic localized mode was introduced by Page [3]:

\[
w_n(t) = A(..., 0, -1, 1, 0, ...) \cos(\Omega t).
\]

(19)

I would like to note that in the case \(k_4 A^2 \gg k_2\) the contribution of the nonlinear interaction between particles in the chain (17) becomes much more important than that of a linear coupling term, so that the model (17) may be treated as the model (1) for the function \(w_n = w_n \sqrt{k_4/m}\), which is perturbed by small linear coupling. That is why the approximate solutions (18) and (19) are somehow close to the exact solutions (15) and (16), respectively. At the same time, it should be pointed out that the rotating-wave approximation cannot be properly justified because the oscillation described by the elliptic function \(cn(\nu t; k)\) at \(k = \frac{1}{\sqrt{2}}\) is far from any harmonic oscillation. In spite of this fact, one meets here the situation when the exact solutions (15) and (16), having even a more complicated temporal evolution, do reproduce qualitatively well the spatial structure of the localized modes found with the help of the rotating-wave approximation.

It is relevant to mention briefly one more peculiarity of the localized modes in the model (17) in comparison with the compacton solution (13) for the purely anharmonic lattice (1). As has been recently demonstrated by Sandusky, Page, and Schmidt [5], the mode (18) may show a dynamical instability in the framework of the model (17), whereas the mode (19) seems to be absolutely stable. A recent explanation [6] of this instability effect is based on the phenomenon of the so-called Peierls-Nabarro potential to the localized mode [7], an effective periodic potential to the coordinate of the localized mode, which appears to be due to the model discreteness. The existence of the exact compacton solution (13) with an arbitrary \(n_0\) clearly indicates that this Peierls-Nabarro potential is absent for the compactons, and they may, therefore, move freely in the lattice, provided the interatomic coupling is purely anharmonic. It seems that this is the first example where the Peierls-Nabarro barrier may appear to be due to a linear interparticle coupling, which itself does not destroy the integrability of discrete linear models.

In conclusion, it has been demonstrated that a chain of particles interacting via purely anharmonic forces is a natural model to support discrete compactons, i.e., solitons with finite wavelength. Such a compacton solution has been found for the chain of particles with quartic interatomic potentials, and it has been pointed out that this solution may be naturally used to explain the phenomenon of the intrinsic localized modes [2, 3]. In particular, I have shown that the general compacton solution reproduces excellently two localized mode patterns found earlier in the framework of the rotating-wave approximation. Namely, when the compacton (13) is centered at the particle site, it gives the so-called \(s\)-mode pattern found by Sievers and Takeno [2]. In the other case, when the compacton (13) is centered between the nearest particle sites, it gives the pattern of the \(p\) mode introduced by Page [3].

In conclusion, I would like to point out that the ideas of the discrete compactons formulated in the present paper are rather general to be applied to other strongly nonlinear models of solids. However, the model (1) itself may support also other types of compacton solutions, such as pulse compactons, kinklike compactons, and moving breather compactons, and the properties of such compactons as well as their stability and collisions are still to be analyzed in detail.

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