Strongly localized gap solitons in diatomic lattices

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It is shown that strongly localized discrete gap solitons may exist in a diatomic chain of particles interacting via a harmonic and a quartic anharmonic potential. In the framework of the rotating-wave approximation, several types of such nonlinear modes are found in the limit of large nonlinearity.

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The existence of gaps in the spectrum of linear waves propagating in crystal lattices with a complex unit cell is a rather fundamental physical phenomenon in solids. One of the typical and well-known examples is a frequency gap between the acoustic and optical branches of the linear spectrum of a diatomic chain. The interest to the study of the spectrum gaps has been stimulated also by the recent discovery of three-dimensionally periodic dielectric structures that can exhibit what is called a "photonic band gap" [1] by analogy with electronic band gap in semiconductor crystals.

In the linear case, a spectrum gap means that wave propagation of certain wavelengths is forbidden. Going to the nonlinear case, one may allow such waves to propagate in the form of so-called *gap solitons* [2]. Gap solitons, being spatially localized nonlinear modes which exist with the frequencies lying just within the gap frequency band, are a result of balance between weak nonlinearity and dispersion, the latter is essential near the gap edges. Various properties of gap solitons have been investigated in respect to their potential applications in nonlinear optics (see, e.g., Refs. [3–7]), whereas the instability-induced generation of a pulse train consisting of gap solitons has recently been shown experimentally [8] as a novel way to generate a periodic stream of short optical pulses from a cw signal.

A wider class of gap solitons has been found recently for one-dimensional *diatomic* lattices with nonlinearity introduced either through on-site (substrate) potential [9] or through nonlinear interparticle interaction in the chain [10]. These gap modes may be described by a system of two coupled nonlinear equations, and one class of these modes is also possible in a monoatomic chain as a result of the nonlinearity-induced gap in the spectrum band [11].

Up to now, all the studies of gap solitons assumed *weak* nonlinearity effects so that the gap solitons were described by slowly varying envelope functions being solutions of partial differential equations (see, e.g., Refs. [5, 6, 9, 10]). However, recently, interest in *strongly localized modes* in anharmonic lattices has been heightened by the identification of a new kind of localized mode in a homogeneous nonlinear monatomic lattice, the so-called "intrinsic localized modes" (see Refs. [12–14] and references therein). Being spatially localized, the intrinsic localized mode has the frequency lying above the upper cutoff frequency of the linear spectrum band and for large values of the parameter $(k_4/k_2)A^2$ (where A is the mode amplitude, k_4 and k_2 are strengths of harmonic and anharmonic forces), such a mode is localized only on a few particles.

The purpose of the present paper is to describe *strongly localized gap modes* which are similar to intrinsic localized modes but they exist with the frequency lying *within* the linear (wide) frequency gap, so that they may be considered as *a discrete version of the gap solitons.* We also describe the standard intrinsic localized modes in the diatomic chain of particles interacting via harmonic and quartic anharmonic potential.

We consider vibrations of a one-dimensional diatomic lattice composed of particles (atoms) with masses m and M $(M > m)$ in which each particle interacts only with its neighbors. Let $u_n(t)$ be the displacement of the nth particle from its equilibrium position and let k_2 and k_4 be nearest-neighbor harmonic and quartic anharmonic potential constants, respectively. The equations of motion are given by

$$m_n\ddot{u}_n = k_2(u_{n+1} + u_{n-1} - 2u_n) + k_4[(u_{n+1} - u_n)^3 + (u_{n-1} - u_n)^3], \quad (1)$$

where $m_n = m$ for $n = 2j + 1$ and $m_n = M$ for $n = 2j$. The linear spectrum of this diatomic chain has two branches describing acoustic and optical modes, respectively. These modes are separated by the gap $\Delta\omega^2 = \omega_{01}^2 - \omega_{02}^2$, where the frequencies $\omega_{01}^2 = 2k_2/m$ and $\omega_{02}^2 = 2k_2/M$ are the gap edge frequencies. The maximum (cutoff) frequency of the linear spectrum band is $\omega_{0m}^2 = 2k_2(m + M)/mM$.

The most interesting part of the spectrum is the vicinity of the maximum value of k $(k = \pi/2)$ where two branches with the opposite signs of dispersion are neigh-

boring. The lower branch corresponds to the mode for which heavy particles oscillate with the higher amplitudes than the light ones, and at $k = \pi/2$ light particles are at rest and the heavy ones oscillate with the opposite phases. For the upper branch, the heavy particles practically do not move while the light atoms vibrate with the opposite phases. In the limit $M = m$ the gap in the linear spectrum disappears.

Substituting the trial solution $u_n(t) = A\Phi_n \cos(\omega t)$ into Eq. (1) and using the so-called "rotating-wave" approximation, i.e., keeping just the terms which are proportional to $\cos\omega t$ on the right-hand side of Eq. (1), we may obtain the set of algebraic equations to real coefficients Φ_n. Let us introduce two functions for the odd and even atomic displacements $\Phi_{2j} = v_n$, $\Phi_{2j+1} = w_n$. Then the system of equations for v_n and w_n may be written in the following form:

$$-\omega^2 M v_n = k_2(w_n + w_{n-1} - 2v_n) + \frac{3}{4}k_4 A^2\left[(w_n - v_n)^3 + (w_{n-1} - v_n)^3\right], \quad (2)$$

$$-\omega^2 m w_n = k_2(v_{n+1} + v_n - 2w_n) + \frac{3}{4}k_4 A^2\left[(v_{n+1} - w_n)^3 + (v_n - w_n)^3\right], \quad (3)$$

or

$$\left(1 - \frac{\omega^2}{\omega_{02}^2}\right) v_n = \frac{1}{2}(w_n + w_{n-1}) + \alpha\left[(w_n - v_n)^3 + (w_{n-1} - v_n)^3\right], \quad (4)$$

$$\left(1 - \frac{\omega^2}{\omega_{01}^2}\right) w_n = \frac{1}{2}(v_n + v_{n+1}) + \alpha\left[(v_{n+1} - w_n)^3 + (v_n - w_n)^3\right], \quad (5)$$

where $\alpha \equiv 3k_4A^2/8k_2$.

Near the edge of the Brillouin zone, the neighboring atoms of the same kind are vibrating with the opposite phases. Therefore, substituting into Eqs. (4) and (5) the solutions $v_n = 0$, $w_n = (-1)^n w_0$ or $w_n = 0$, $v_n = (-1)^n v_0$ we can find *how the gap frequencies are modified by the nonlinearity*

$$\omega_1^2 = \frac{1}{m}\left(2k_2 + \frac{3}{2}k_4 A^2 w_0^2\right) \equiv \omega_{01}^2\left(1 + \frac{1}{2}\alpha w_0^2\right) \quad (6)$$

and

$$\omega_2^2 = \frac{1}{M}\left(2k_2 + \frac{3}{2}k_4 A^2 v_0^2\right) \equiv \omega_{02}^2\left(1 + \frac{1}{2}\alpha v_0^2\right). \quad (7)$$

At the cutoff frequency the atoms in the diatomic chain oscillate with the minimum wave length. This means that to find the nonlinear cutoff frequency, one has to look for solutions in the form $w_n = w_0$, $v_n = v_0$ and Eqs. (4) and (5) are reduced to the following ones:

$$-\omega^2 M v_0 = 2k_2(w_0 - v_0) + \frac{3}{2}k_4 A^2(w_0 - v_0)^3,$$
$$-\omega^2 m w_0 = 2k_2(v_0 - w_0) + \frac{3}{2}k_4 A^2(v_0 - w_0)^3. \quad (8)$$

From Eq. (8) we get the exact result $v_0 = -(m/M)w_0$ and

$$\omega_m^2 = \omega_{0m}^2\left[1 + \frac{3k_4}{4k_2}A^2 w_0^2 \frac{(m+M)^2}{M^2}\right]. \quad (9)$$

The frequencies, which are defined by Eqs. (6) and (7), are the characteristic frequencies of the nonlinear spectrum band found in the rotating-wave approximation.

It is important to note that the gap frequencies (6) and (7) depend on the mode amplitudes, so that it may happen that they have a cross provided $v_0^2 > w_0^2$. Thus our first conclusion to the nonlinear spectrum band is that the linear gap may be *completely suppressed by nonlinearity.* We would like to mention that this effect seems opposite to the phenomenon of the nonlinearity-induced spectrum gap recently described in Ref. [11].

Since the frequency of the nonlinear waves is determined by the wave amplitude, we introduce as an independent variable its deviation from the lower edge of the linear spectrum band,

$$\epsilon^2 = \frac{\omega^2}{\omega_{02}^2} - 1. \quad (10)$$

In this case the system (4) and (5) can be rewritten in the following form:

$$-\epsilon^2\phi_n = \frac{1}{2}(\psi_n - \psi_{n-1}) + (\psi_n - \phi_n)^3 - (\psi_{n-1} + \phi_n)^3, \quad (11)$$

$$\beta\psi_n = \frac{1}{2}(\phi_n - \phi_{n+1}) + (\phi_n - \psi_n)^3 - (\phi_{n+1} + \psi_n)^3, \quad (12)$$

where $\beta \equiv 1 - \mu - \mu\epsilon^2$, $\mu \equiv m/M$, and we have introduced the new functions ϕ_n and ψ_n through the relations $v_n = (-1)^n\phi_n/\sqrt{\alpha}$ and $w_n = (-1)^n\psi_n/\sqrt{\alpha}$. Now strongly localized modes may be determined as those for which the inequality $\epsilon \gg 1$ is satisfied provided the linear gap $\Delta\omega^2$ is wide enough. Then, for this case, on the right-hand side of Eq. (11) we can neglect the first linear term. In a general case, this cannot be done in the second equation since for $\mu \ll 1$ we have $\beta \sim 1$, and two linear terms of Eq. (12) become of the same order. This case is of the most interest since we are looking for localized modes with the frequencies lying within the linear spectrum gap, i.e., gap solitons.

To calculate the spatial shapes of the localized modes, we use Eqs. (11) and (12). The parameter ϵ determines the width of such solutions, so that we can expect that the modes will be strongly localized provided the condition $\epsilon \gg 1$ is fulfilled. From the continuous approximation [9,10] the shapes of the gap modes are known, i.e., in a gap soliton the envelope of the heavy-atom vibrations is of a constant sign whereas light particles oscillate with a sign-changing envelope. The structure of the gap-soliton solutions found in Refs. [9,10] does help us to obtain the corresponding solutions in the limit of strongly localized modes when the continuous limit approximation is not valid.

In the case of strongly localized solutions the mode

may be centered either at heavy or at light particles. Designating the solution center by the number $n = 0$, we will have equations symmetric with respect to $n \to -n$, defining two different cases.

(i) The mode center is at a heavy particle (symmetric mode). In this case the first equation of the system (11) and (12) has the form

$$-\epsilon^2\phi_0 = \psi_1 + 2(\psi_1 - \phi_0)^3. \tag{13}$$

(ii) The mode center is at a light particle (asymmetric mode). In this case we have the following two first equations:

$$\psi_0 = 0, \quad -\epsilon^2\phi_1 = \frac{1}{2}\psi_1 + (\psi_1 - \phi_1)^3 - \phi_1^3. \tag{14}$$

The following equations of this system for both cases have the following form:

$$\phi_{n+1} = \phi_n - 2\beta\psi_n - 2(\phi_{n+1} + \psi_n)^3 + 2(\phi_n - \psi_n)^3, \tag{15}$$

$$\psi_{n+1} = \psi_n - 2\epsilon^2\phi_{n+1} - 2(\psi_{n+1} - \phi_{n+1})^3 + 2(\psi_n + \phi_{n+1})^3, \tag{16}$$

Therefore, our system of equations has one unknown variable ϕ_0 in the first case or ϕ_1 in the second one. Applying for the function ϕ_n the conditions $\phi_{n+1} < \phi_n$ (because we are looking for localized solutions of these equations) and $\phi_n \geq 0$, we can use a simple iteration method to find a unique value of ϕ_0 (or ϕ_1) giving the localized mode pattern.

The results are summing up in the Table I and the structures of two such solutions are presented in Figs. 1(a) and 1(b). Note that the solution is stronger localized for smaller μ and larger ϵ. The solid and dashed curves in Figs. 1(a) and 1(b) indicate the envelopes of the particles' vibration amplitudes which have been analyzed in the continuum approximation in Ref. [10], and in this limit the gap solitons may be described by explicit analytical solutions.

The diatomic lattice we have analyzed in the present paper may support also the intrinsic localized modes of a standard type [12–15] with the frequencies lying above the upper cutoff frequency ω_m. To analyze such modes

TABLE I. Structure of the discrete gap solitons.

μ	ϵ^2	ϕ_0	ϕ_1	ϕ_2	ϕ_3	ϕ_4
		ψ_0	ψ_1	ψ_2	ψ_3	ψ_4
0.01	10.0	3.3545	1.8083	0.1346	0.0036	0.0001
			0.7752	0.8509	0.0733	0.0020
			2.9001	0.5770	0.0178	0.0005
		0.0	1.1682	0.3012	0.0097	0.0003
0.08	10.0	3.3480	1.8399	0.1735	0.0167	0.0024
			0.7704	0.9509	0.3175	0.0572
			2.9071	0.6397	0.0446	0.0059
		0.0	1.1862	0.5678	0.1332	0.0208

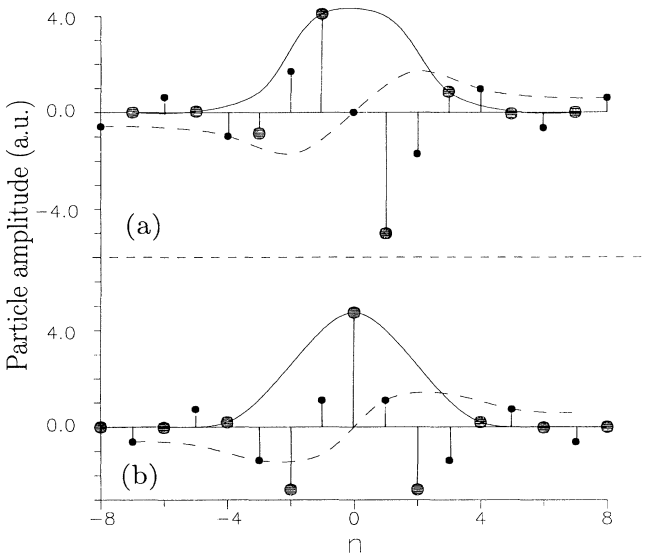

FIG. 1. Localized patterns corresponding to discrete gap solitons at $\mu = 0.08$ and $\epsilon^2 = 10.0$: (a) the mode centered at a light particle, and (b) the mode centered at a heavy particle. Solid and dashed lines are used to show envelopes of heavy and light particles, respectively. These curves are close to the analytical solutions of Ref. [10] found in the continuous approximation.

analytically we first note that for the modes with the large frequencies, $\omega^2 \gg \omega_{01}^2$, ω_{02}^2, we may simplify Eqs. (2) and (3) to the form

$$\gamma^2 f_n = g_n + g_{n-1} + 2f_n + (g_n + f_n)^3 + (g_{n-1} + f_n)^3, \tag{17}$$

$$\gamma^2\mu g_n = f_n + f_{n+1} + 2g_n + (f_{n+1} + g_n)^3 + (f_n + g_n)^3, \tag{18}$$

where

$$f_n = v_n\sqrt{\frac{3}{4}k_4A^2}, \quad g_n = -w_n\sqrt{\frac{3}{4}k_4A^2}\,, \tag{19}$$

and $\gamma^2 = \omega^2 M/k_2$. To find the structure of a localized mode let us suppose that the center of the mode is centered at a heavy particle. Then the first equation for the central particle will be $\gamma^2 f_0 = 2(g_1 + f_0) + 2(g_1 + f_0)^3$. Equations for the next-atom displacements can be rewritten as $\gamma^2\mu g_n = f_{n+1} + f_n + 2g_n + (f_{n+1} + g_n)^3 + (f_n + g_n)^3$; from there we find v_{n+1} knowing v_n and w_n with the help of the relation

$$\gamma^2 f_{n+1} = g_{n+1} + g_n + 2f_{n+1} + (f_{n+1} + g_{n+1})^3 + (g_n + f_{n+1})^3, \tag{20}$$

and g_{n+1} through g_n and f_{n+1}. Thus the only unknown variable is f_0 and we can find it using iteration method as in the previous case. The results are summed up in Table II and one of the modes is shown in Fig. 2. The

TABLE II. Structure of the intrinsic localized modes in the diatomic chain.

μ	γ^2	f_0	f_1	f_2	f_3
			g_1	g_2	g_3
0.5	10.0	0.3814	0.1450	0.0050	0.0002
			0.5949	0.0412	0.0017
0.1	30.0	0.0604	0.0289	0.0011	0.0000
			0.5816	0.0302	0.0011
0.8	10.0	0.7377	0.1126	0.0023	0.0000
			0.5932	0.0195	0.0004

mode pattern shown in Fig. 2 looks very much like the intrinsic localized mode of Sievers and Takeno [12], but it exists in *a diatomic chain* composed of the atoms of two different kinds. Such kinds of modes have been recently observed in direct numerical simulations by Aoki [16].

At last, we would like to note that in the diatomic chain one more type of nonlinear mode may exist. Indeed, when the effects of nonlinearity become large in a diatomic lattice with a relatively small ratio of particle masses, the linear spectrum gap may be suppressed by nonlinearity. This means that instead of spatially localized modes we may obtain modes on a nonvanishing background, i.e., in fact *dark gap solitons*. These dark solitons (or kink-profile modes) are somehow similar to the modes recently found in a monoatomic chain [17].

In conclusion, we have shown analytically that strongly localized nonlinear modes with the frequencies lying within the gap of the linear spectrum band are possible in a diatomic chain of particles interacting via harmonic and quartic anharmonic interatomic potential. We have found such solutions in the rotating-wave approximation, and we have shown that they may be treated as a discrete version of gap solitons.

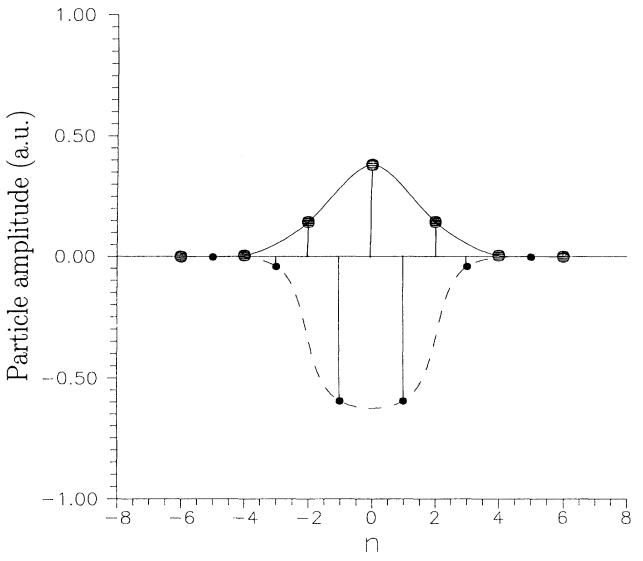

FIG. 2. Localized pattern corresponding to intrinsic localized modes in the diatomic chain at $\mu = 0.5$ and $\gamma^2 = 10.0$ (the upper mode in Table II).

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[1] E. Yablonovitch, Phys. Rev. Lett. **58**, 2059 (1987).
[2] W. Chen and D.L. Mills, Phys. Rev. Lett. **58**, 169 (1987).
[3] D.L. Mills and S.E. Trullinger, Phys. Rev. B **36**, 947 (1987).
[4] C.M. de Sterke and J.E. Sipe, Phys. Rev. A **38**, 5149 (1988); **42**, 2858 (1990).
[5] D.N. Christodoulides and R.I. Joseph, Phys. Rev. Lett. **62**, 1746 (1989).
[6] A.B. Aceves and S. Wabnitz, Phys. Lett. A **141**, 37 (1989).
[7] C.M. de Sterke, Phys. Rev. A **45**, 2012 (1992).
[8] H.G. Winful, R. Zamir, and S. Feldman, Appl. Phys. Lett. **58**, 1001 (1991).
[9] Yu. S. Kivshar and N. Flytzanis, Phys. Rev. A **46**, 7972 (1992).
[10] O.A. Chubykalo, A.S. Kovalev, and O.V. Usatenko, Phys. Rev. B **47**, 3153 (1993).
[11] Yu.S. Kivshar, Phys. Rev. B **46**, 8652 (1992).
[12] A.J. Sievers and S. Takeno, Phys. Rev. Lett. **61**, 970 (1988).
[13] J.B. Page, Phys. Rev. B **41**, 7835 (1990).
[14] K.W. Sandusky, J.B. Page, and K.E. Schmidt, Phys. Rev. B **46**, 6161 (1992).
[15] Ch. Claude, Yu.S. Kivshar, O. Kluth, and K.H. Spatschek, Phys. Rev. B **47**, 14 228 (1993).
[16] M. Aoki, J. Phys. Soc. Jpn. **61**, 3024 (1992).
[17] O.A. Chubykalo and Yu. S. Kivshar, Phys. Lett. A **178**, 123 (1993).