Multiple States of Intrinsic Localized Modes

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In the framework of the continuum approximation, localized modes in nonlinear lattices ('intrinsic localized modes' or 'discrete breathers') are described by the nonlinear Schrödinger (NLS) equation. We go beyond this approximation and analyze what kind of qualitatively new effects can be introduced by discreteness. Taking into account the higher-order linear and nonlinear dispersion terms in the NLS equation derived from a lattice model, we predict the existence of bound states of intrinsic localized excitations. These bound states of nonlinear localized modes are also found numerically for a discrete chain with linear and nonlinear cubic interparticle interaction.

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I. INTRODUCTION

Intrinsic localized modes (ILMs), highly localized vibrational excitations of anharmonic lattices, have been the subject of theoretical research for more than ten years [1] (see also the review papers [2]). In contrast to impurity modes in harmonic lattices with defects, ILMs in perfect lattices become possible due to anharmonicity in the interparticle interaction or on-site potential. Recent studies have revealed the existence of ILMs in realistic three-dimensional models of anharmonic crystals and suggested different methods for their excitation [3], so far such localized modes have not been yet observed experimentally. Nevertheless, the discovery of ILMs and their active theoretical study is an important step towards understanding the role of nonlinear spatially localized modes in realistic (usually nonintegrable and discrete) physical models, many years after the blossom of the theory of solitons in continuous models described by integrable nonlinear equations.

One of the important issues which has not been widely explored so far is the influence of the lattice discreteness on the stability and interaction of ILMs [4,5]. On the one hand, it is already well understood that ILMs can be linked to envelope solitons in the framework of the quasi-continuum approximation [6], in which case the mode profile is described by the nonlinear Schrödinger (NLS) equation. In that sense, ILMs are breather-like modes of nonlinear lattices, and they can be regarded as an extension of the soliton concept to nonintegrable nonlinear lattice models [7]. On the other hand, some of the properties of discrete nonlinear lattices, e.g. modulational instability of continuous wave solutions [8], have been found to display novel features introduced solely by discreteness.

The purpose of this paper is twofold. First, we analyze ILMs in the framework of the quasi-continuum approximation but go beyond the conventional approximation based on the NLS equation [6]. In particular, we derive a novel type of continuum model for ILMs described by a perturbed NLS equation with linear and nonlinear higher-order dispersion terms which appear due to discreteness. Second, analyzing the perturbed NLS equation and also the full lattice model, we reveal the existence of bound states of ILMs. Such localized states are somewhat similar to the multi-soliton modes obtained numerically by Rakhmanova and Mills [9] for an anisotropic Heisenberg spin chain, but in our case they appear in a lattice with nonlinear interparticle coupling. We believe that the existence of bound states is a common feature of the nonlinear dynamics of lattice models.

The paper is organized as follows. In Sec. II we first introduce our discrete model. Then, in Sec. II.B we consider the equations of motion in a quasi-continuum approximation and derive a perturbed NLS equation for the oscillation envelope which takes into account higher-order effects due to lattice discreteness. The analysis of homoclinic orbits of this novel nonlinear equation is presented in Sec. II.C, where we describe families of solutions including 'up-and-down' two-hump homoclinic orbits representing bound states of two localised modes with opposite phases. Section III is devoted to a search of similar bound states in the complete lattice model. We find several types of the bound states and verify that their stability is directly related to the stability of single ILMs of the same type. Finally, Sec. IV concludes the paper.

II. GENERALIZED NLS EQUATION

A. Lattice Model

We consider here the simplest model supporting ILMs [1], a monoatomic one-dimensional chain of particles ('atoms') coupled by interatomic anharmonic (symmetric) potential. More sophisticated models can be considered, but this simple model is good enough to present all basic properties of the multiple-state class of ILMs. The equation of motion describing the vibrational dynamics of the chain can be written in the following form (see, e.g., [1])

$$m\frac{d^2u_n}{dt^2} = k_2(u_{n+1} + u_{n-1} - 2u_n) + k_4[(u_{n+1} - u_n)^3 + (u_{n-1} - u_n)^3], \tag{1}$$

where u_n is the displacement of the particle at the site n, m is the mass of the particle, and the parameters k_2 and k_4 characterize the linear and nonlinear interparticle interactions within the chain. Only cubic nonlinearity is taken into account, assuming the potential to be symmetric.

Linear waves propagating in the chain (1) with frequency ω and wavenumber k are characterized by the dispersion relation, $\omega^2 = \omega_m^2 \sin^2(ka/2)$, where k is selected in the Brilloin zone, $|k| < \pi/2$, and $\omega_m = \sqrt{(4k_2/m)}$ is the maximum (cut-off) frequency of the linear spectrum band, $-\omega_m < \omega < \omega_m$.

As has been found earlier [1,2], the discrete model (1) can support the existence of highly localized nonlinear modes with vibrational frequency ω much larger than the cut-off frequency ω_m. These modes can be described analytically in two different limits. In the first limit, the mode is assumed to be localized only on a few particles which is valid for $\omega \gg \omega_m$. As a result, the mode structure is found by solving a finite system of just a few (in fact, only three) coupled nonlinear equations [1,2]. In the second limit, the deviation of the mode frequency from the cut-off, $(\omega^2 - \omega_m^2)^{1/2}$ can be taken as a parameter of asymptotic expansion in the oscillation amplitude to derive the NLS equation for the slowly varying wave envelope [6]. In spite of the fact that the rigorous analytical results for the existence and stability of ILMs are available [10], in general, the two limiting cases mentioned above are the only ones where the structure of ILMs can be presented in an analytical form.

B. Quasi-Continuum Approximation

To derive the effective nonlinear equation for the wave envelope, we follow the procedure of Refs. [6] and consider the localized lattice oscillation with the frequency $\omega > \omega_m$ in the form,

$$u_n(t) = (-1)^n A\phi_n \cos(\omega t), \tag{2}$$

where the factor $(-1)^n$ takes into account the structure of the chain oscillations with the opposite phases of the neighboring particles, A and ω are the mode amplitude and its frequency, respectively. The envelope ϕ_n of the lattice vibration can now be considered as a slowly varying function of the site n.

Substituting Eq. (2) into Eq. (1) and using the rotating wave approximation to evaluate the effect of higher order frequencies, we obtain the equation for the envelope function ϕ_n,

$$m\omega^2\phi_n = k_2(\phi_{n+1} + \phi_{n-1} + 2\phi_n) + \frac{3}{4}k_2A^2[(\phi_{n+1} + \phi_n)^3 + (\phi_{n-1} + \phi_n)^3]. \tag{3}$$

The discrete equation (3) can be further simplified by applying the continuum limit approximation, provided the mode localization length is much larger than the lattice spacing. Therefore, we can expand $\phi_{n\pm1}$ into Taylor series, treating the value $x = na$ as a continuous variable. In contrast to the conventional approach, here we keep not only the lowest-order term in nonlinearity and dispersion, as in Ref. [6], but also take into account the next-order terms that describe the higher-order linear and nonlinear dispersions originating from the lattice discreteness. The resulting equation for the continuous function $\phi(x)$ can be written in the form,

$$\frac{(m\omega^2 - 4k_2)}{k_2}\phi = \phi'' + \frac{1}{12}\phi'''' + \frac{12k_4}{k_2}A^2\left[\phi^3 + \frac{3}{4}\phi(\phi\,\phi')'\right]. \tag{4}$$

Equation (4) is a direct generalization of the NLS equation usually derived for the ILM envelope in the continuum approximation (see, e.g., Ref. [6]). The additional terms due to the next-order approximation of the discreteness are the fourth-order linear dispersion term and an additional nonlinear derivative-dependent dispersion.

Introducing the dimensionless parameter,

$$\lambda^2 = \frac{(m\omega^2 - 4k_2)}{k_2},$$

which characterizes the localization region of the mode, and the normalized mode envelope $v(x)$ through the relation,

$$\phi \to \left(\frac{k_2}{12k_4A^2}\right)^{1/2} v,$$

we obtain the normalized equation for the wave envelope in the following canonical form [11],

$$\frac{1}{12}v'''' + v'' - \lambda^2 v + v^3 + \frac{3}{4}v\,(v\,v'' + v'^2) = 0. \tag{5}$$

It can be easily shown that that Eq. (5) can be transformed into canonical form with Hamiltonian

$$H = \frac{\lambda^2}{2}v^2 + \frac{1}{2}v'^2 - \frac{1}{24}(v'')^2 - \frac{1}{4}v^4 + \frac{3}{4}v^2v'^2. \tag{6}$$

The nonlinear equation (5) resembles the two-parameter model arising in the theory of water waves with surface tension, for which the structure of solitary wave solutions has been recently investigated by Champneys and Groves [12]. However, in our case the nonlinearity is cubic, and therefore the properties of solitary waves are different.

C. Structure of Localized Solutions

To investigate the localized solutions of the Hamiltonian system (5), we note that for all values of λ^2, when viewed as a dynamical system in phase space variables (v, v', v'', v'''), it has odd symmetry and is reversible under

$$R : (v, v', v'', v''') \to (v, -v', v'', -v''')$$

and $-R$.

To obtain the localized solutions of the model (5), we should find solutions which are homoclinic to the equilibrium at $v = 0$. Note that the linearization there has two real and two pure imaginary eigenvalues $\pm[6(\sqrt{1 + (\lambda^2/3)} - 1)]^{1/2}$ and $\pm i[6(\sqrt{1 + (\lambda^2/3)} + 1)]^{1/2}$, and so the origin is a saddle-centre equilibrium for all $\lambda^2 > 0$. Hence, we should expect to find R or $-R$-symmetric homoclinic solutions only at isolated values of λ^2 [13] (see also Ref. [14] for a general overview of homoclinic orbits in autonomous Hamiltonian and reversible systems including numerical methods for their location).

Using numerical methods [14], for equation (5), R-symmetric one-pulse homoclinic solutions are found to exist at the discrete values of $\lambda^2 = 1.94618, 4.62637, 8.06146, 12.23219, 17.13291, \ldots$. The solutions at the first two of these values are depicted in Figs. 1(a) and 1(b). Note that they are monotonic increasing up to their point of symmetry. The solutions for larger λ are similar but with larger amplitude and are told apart by each one having one more small oscillation than its predecessor superimposed on the sech-like profile. This oscillation is almost undetectable unless the graph of the derivative v'' is plotted (actually, both the solutions in Fig. 1 have tiny oscillation superimposed when viewed in this way). Also, formally there is a zero-amplitude solution in the limit $\lambda \to 0$,

$$v(x) = \sqrt{2}\lambda\,\mathrm{sech}(x/\lambda) + \mathcal{O}(\lambda^2). \tag{7}$$

In addition, between each pair of λ^2-values at which the system (5) possesses one-pulse solutions, we find infinite sequences of -R-symmetric solutions which describe bound states of two primary solitary waves with opposite phases. The accumulation of these two-pulses on the one-pulses for $\lambda \neq 0$ is in full accordance with the theory [13] (see also Ref. [11]). Here we focus on the accumulation of bound states on the limit $\lambda \to 0$. Figure 2 shows such solutions as the dependence of the mode energy E versus the spectral parameter λ^2. As $\lambda^2 \to 0$, the separation between the localized modes increases $\propto 1/\lambda^2$, see Fig. 3. Note that this accumulation of bound states on a singular limit is qualitatively the same as occurs in the model of two-wave quadratic solitons due to second-harmonic generation [15].

III. MULTIPLE LOCALIZED MODES IN A LATTICE MODEL

The multi-pulse structure of the localized solutions of the generalized model (5) suggests to look for multiple-state solutions of the lattice equations (1). Using a path-following method [16], we have found numerically different types of localized solutions of the model (1), oscillating with the frequency ω_b. The following set of the parameters has been used: $k_2 = 1$, $m = 1$, and $k_4 = 5$, and $\omega_b = 20$. The system lengths used in search for numerically exact solutions were 100 or longer. The boundary conditions were either fixed (u_n clamped to zero) or periodic. They do not lead to any significant change in our numerical solutions.

The simplest solution for a localized mode has two distinct symmetries, already described in the literature. The localized mode centered at the lattice site is usually called *the Sievers-Takeno mode*, whereas the mode centered between the neighboring sites is known as *the Page mode* (see Refs. [1]). These two types of symmetries are easily recovered by our numerical technique, see Figs. 4(a) and 5(a), respectively.

Additionally to the simplest modes shown in Figs. 4(a) and 5(a), the lattice model (1) possesses multiple states which can be regarded as bound states of ILMs of lower symmetry, in analogy with the generalized NLS model. Some examples of such multiple modes are presented in Figs 4(b,c), for the modes generated by the Sievers-Takeno primary mode, and in Fig. 5(b,c), for the modes generated by the Page primary mode. All these numerical solutions are highly accurate, with a relative error of $\sum_n |\Delta u_n|$ converging to $10^{-11} \sim 10^{-12}$ in a Newton-Raphson iteration scheme.

Before discussing stability of the multiple localized modes, we would like to make two remarks. First of all, the stability of the primary localized modes is well known (see, e.g., the review papers [2] and references therein). The Sievers-Takeno mode is *structurally unstable*, the static mode configuration corresponds to the energy higher than that of the Page mode, this property can be attributed to the existence of an effective Peierls-Nabarro potential to the mode coordinate, qualitatively similar to that known for kinks. In the framework of this phenomenology, the Page mode corresponds to an effective minimum of the periodic potential.

Secondly, for a bound state we can expect the existence of a binding energy which prevents the individual modes to escape. This property may also affect the mode stability. In the continuum model (5), the binding energy was found to be zero, see a dotted line in Fig. 2. Therefore, the reason for the bound states to exist is the structure of the oscillating tails generated by the presence of the higher order linear and nonlinear dispersion terms.

From what is said above about the mode stability, it is not surprising that the bound states shown in Fig. 4(b,c) have been found to be *unstable*. In the full numerical simulation of system (1) using these numerical exact solutions as initial conditions, we found that these modes disintegrate into irregular lattice motion in both space and time. In contrast, the localized mode centered between the neighboring sites, i.e. the Page mode, is known to be stable. As a result, all the modes shown in Figs. 5(a,b,c) are found to be dynamically stable, they persist for thousands of oscillation without any appreciable changes.

It is interesting to note that, within the accuracy of the numerical method, we do not identify any effect of the binding energy. For example, the energy of the mode shown in Fig. 5(a) is $E_0 = 1.680381 \times 10^4$, whereas the bound state shown in Fig. 5(b) has the energy $E_b = 3.360924 \times 10^4$ which is a bit larger than $2E_0$. The bound state in Fig. 5(c) has an energy almost equal to $2E_0$ within our numerical accuracy. Therefore, the mode stability comes from the stability of individual modes. Such a feature is probably due to the fact that we have found all mode structures at a fixed value of the mode frequency, $\omega_b = 20$, whereas the existence of a binding energy should correspond to the energy lower than $2E_0$, and probably to a different value of the mode frequency. Such an argument is hard to verify because a localized mode is characterized by several parameters which do not allow for a simple picture based on an effective particle, as we have in the case of kinks.

We believe that the existence of bound states of two and more localized modes can be viewed as a result of the lattice discreteness. On a qualitative level, the stable mode with the Page configuration corresponds to an effective minimum of the Peierls-Nabarro periodic potential. Two such modes can be situated in any two minima giving birth to a discrete set of stable bound states. Weak overlapping of the modes corresponds to the energy slightly higher than the sum of the energies of two individual modes, the difference is lower than the potential barrier produced by the discreteness so that the bound state remains stable. All these features are in a qualitative agreement with the properties of the modes found numerically.

Finally, it is interesting to note the agreement in the form of localised modes found for this discrete model and its continuous counterpart, (5). Using the notation of Sec. II.C, the Sievers-Takeno mode (Fig. 4(a)) represents an R-reversible solution, whereas the Page mode (Fig. 5(a)) is $-R$-reversible. We therefore might identify the Sievers-Takeno mode with the one-pulse solution in Fig. 1(a) and Page mode with simplest two-pulse solution (e.g. the panel in Fig. 2(b) representing the solution at $\lambda^2 \approx 1.2$). Note further, from the discrete model, that the bound states of the Sievers-Takeno mode (Figs. 4(b),(c)) are $-R$ reversible in this analogy, as they are for the continuous model. Moreover, bound states of the $-R$-reversible Page mode (Figs. 5(b),(c)) correspond to R-reversible solutions (these would be 4-pulse solutions of (5)). The property that R-reversible pulses have $-R$-reversible bound states, and vice-versa, is in full accordance with the sign condition [13] that may be calculated from the Hamiltonian 6.

IV. CONCLUDING REMARKS

We would like to emphasize that the intrinsic localized modes have been extensively investigated for different types of physical models as a natural extension of the soliton concept, well developed for continuous integrable models, to the case of realistic lattice models of solids. Such a study, however, did not allow to display clearly the specific properties of the lattice discreteness which may bring novel features of the localized modes, not found in integrable and continuous models. Our analysis revealed that some of these features can be modeled by a perturbed NLS equation, allowing to make the next step in describing the properties of intrinsic localized modes in terms of continuous models. This equation includes the effect of discreteness through both linear and nonlinear dispersion terms. One of the main features found for this novel continuous model for localized modes is the possibility to form bound states of two and more localized modes. The existence of bound states of different types of localized modes has been verified for the lattice model, and their stability has been investigated by means of direct numerical simulations. We expect similar features to be found for other types of nonlinear lattices and localized modes, e.g. those recently found in ferromagnetic chains.

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[1] A.S. Dolgov, Fiz. Tverd. Tela **28**, 1641 (1986) [Sov. Phys. Solid State **28**, 907 (1986)]; A.J. Sievers and S. Takeno, Phys. Rev. Lett. **61**, 970 (1988); J.B. Page, Phys. Rev. B **41**, 7835 (1990).

[2] A.J. Sievers and J.B. Page, In: *Dynamical Properties of Solids*, Vol. 7, Ed. G.K. Horton and A.A. Maradudin (North-Holland, Amsterdam, 1995), p. 137; S.A. Kiselev, S.R. Bickham, and A.J. Sievers, Comments Cond. Mat. Phys. **17**, 135 (1995); S. Flach and C.R. Willis, Phys. Rep. **295**, 181 (1998).

[3] See, e.g., D. Bonart, A.P. Mayer, and U. Schröder, Phys. Rev. Lett. **75**, 870 (1995); T. Rössler and J.B. Page, Phys. Rev. Lett. **78**, 1287 (1997).

[4] D. Cai, A.R. Bishop, and N. Grønbech-Jensen, Phys. Rev. E **56**, 7246 (1997).

[5] K.Ø. Rasmussen, D. Cai, A.R. Bishop, and N. Grønbech-Jensen, Phys. Rev. **E** 6151 (1997).

[6] K. Yoshimura and S. Watanabe, J. Phys. Soc. Jpn. **60**, 82 (1991); Yu.S. Kivshar, Phys. Lett. A **161**, 80 (1991).

[7] D. Cai, A.R. Bishop, and N. Grønbech-Jensen, Phys. Rev. Lett. **72**, 591 (1994).

[8] Yu.S. Kivshar and M. Peyrard, Phys. Rev. A **46**, 3198 (1992).

[9] S. Rakhmanova and D.L. Mills, Phys. Rev. B **54**, 9225 (1996).

[10] R.S. MacKay and S. Aubry, Nonlinearity **7**, 1623 (1994); D. Bambusi, Nonlinearity **9**, 433 (1996).

[11] A more general model has been recently introduced by A.R. Champneys and J. Härterich (submitted to Nonlinearity), who analyzed cascades of homoclinic orbits to a saddle-center for different reversible and perturbed Hamiltonian systems. However, that general model may not correspond to a relevant physical system.

[12] A.R. Champneys and M.D. Groves, J. Fluid Mech. **342**, 199 (1997).

[13] A. Mielke, P. Holmes, and O. O'Reilly, J. Dynam. Differ. Equations **4**, 95 (1992).

[14] A.R. Champneys, Physica D **112**, 158-186 (1998).

[15] A.V. Buryak and Yu.S. Kivshar, Phys. Lett. A **197**, 407 (1995).

[16] J.C. Eilbeck, "Numerical studies of solitons on lattices", pp143 - 150 and references therein in *Lecture Notes in Physics — Nonlinear Coherent Structures in Physics and Biology*, Edited by M. Remoissenet and M. Peyard (Spring Verlag, New York, 1991).

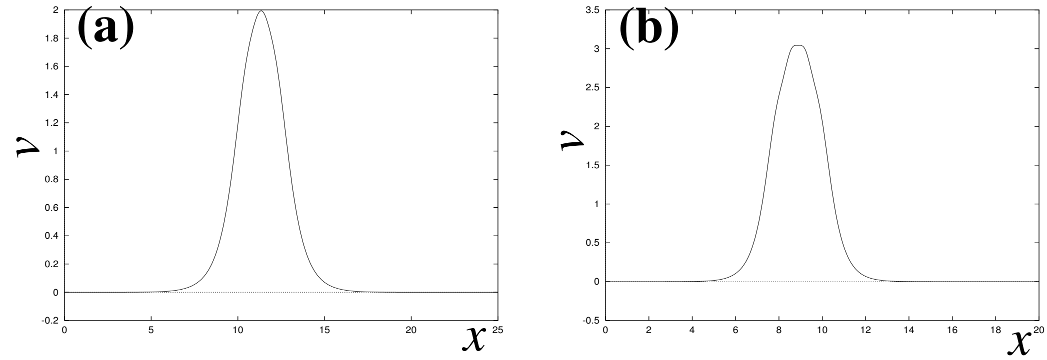

FIG. 1. Examples of the one-pulse localized solutions of Eq. (5) with the lowest values of λ^2: (a) $\lambda^2 = 1.94618$, (b) $\lambda^2 = 4.62637$.

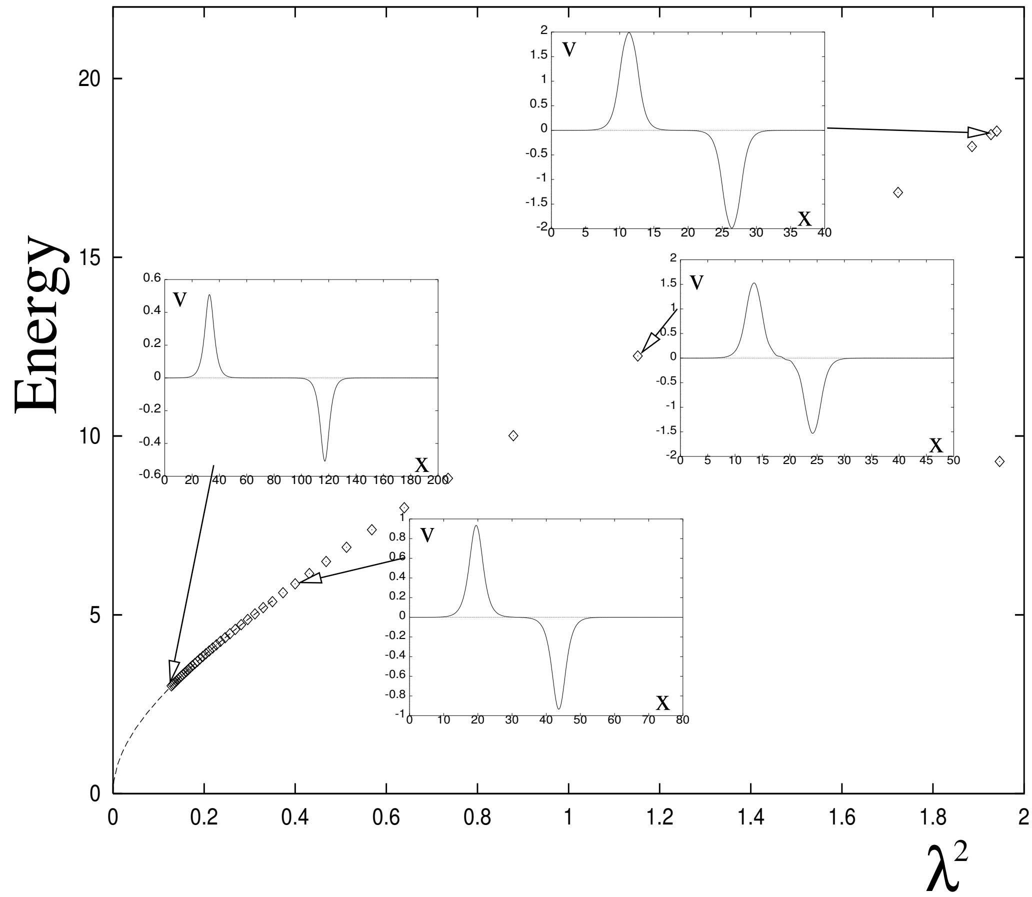

FIG. 2. Sequence of two-pulse localized solutions of Eq. (5) accumulating on $\lambda = 0$. The 'energy' is defined as $\int v^2(x)dx$, the value directly proportional to the physical energy calculated in the rotating wave approximation for large ω^2. The dotted line plots twice the energy of the approximate primary solution (7). The two-pulses continue down to $\lambda = 0$ but due to their slow-accumulation on this limit, we have plotted then only to $\lambda^2 \approx 0.15$.

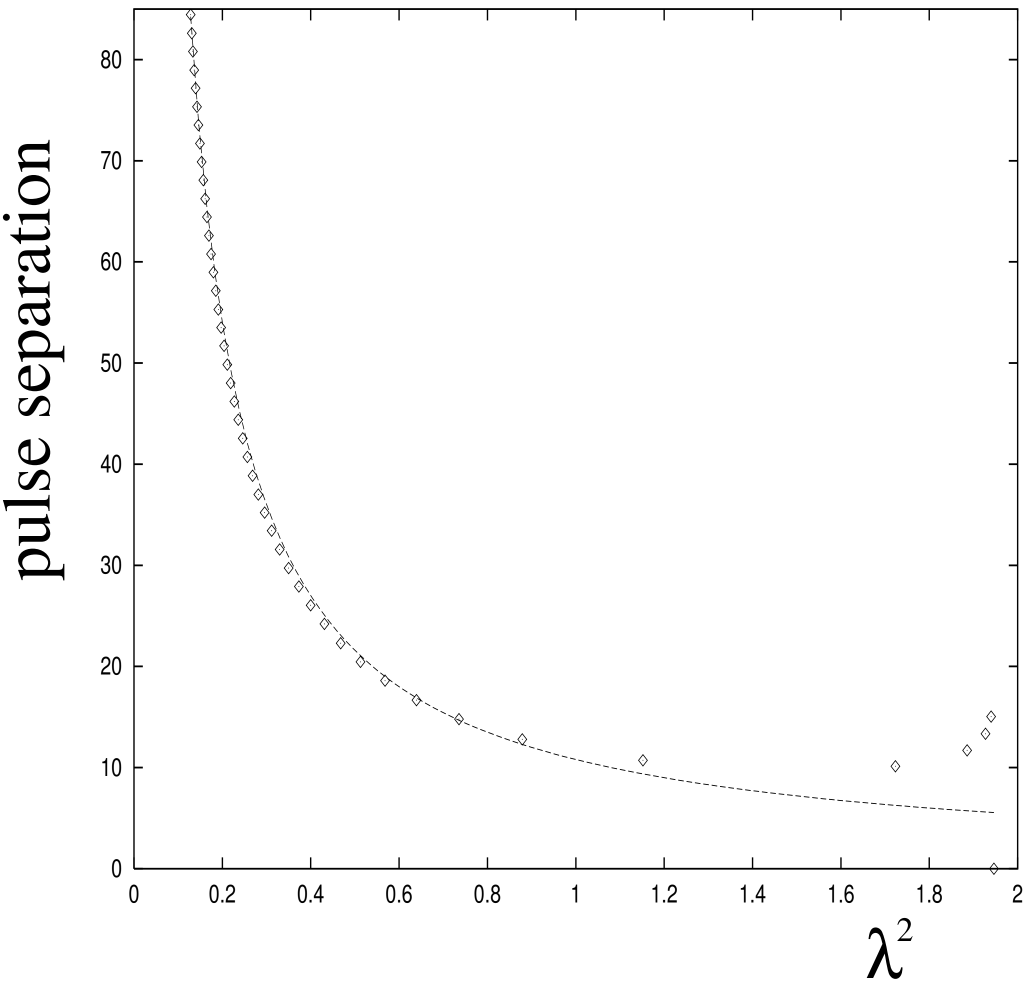

FIG. 3. The same solutions as in Fig. 2 plotted as the separation between the primary solitons in the bound states versus λ^2. The dashed curve is a data fit to $10.8/\lambda^2$. The solutions to the right are bound states accumulating on the one-pulse solution at $\lambda^2 = 1.94618$.

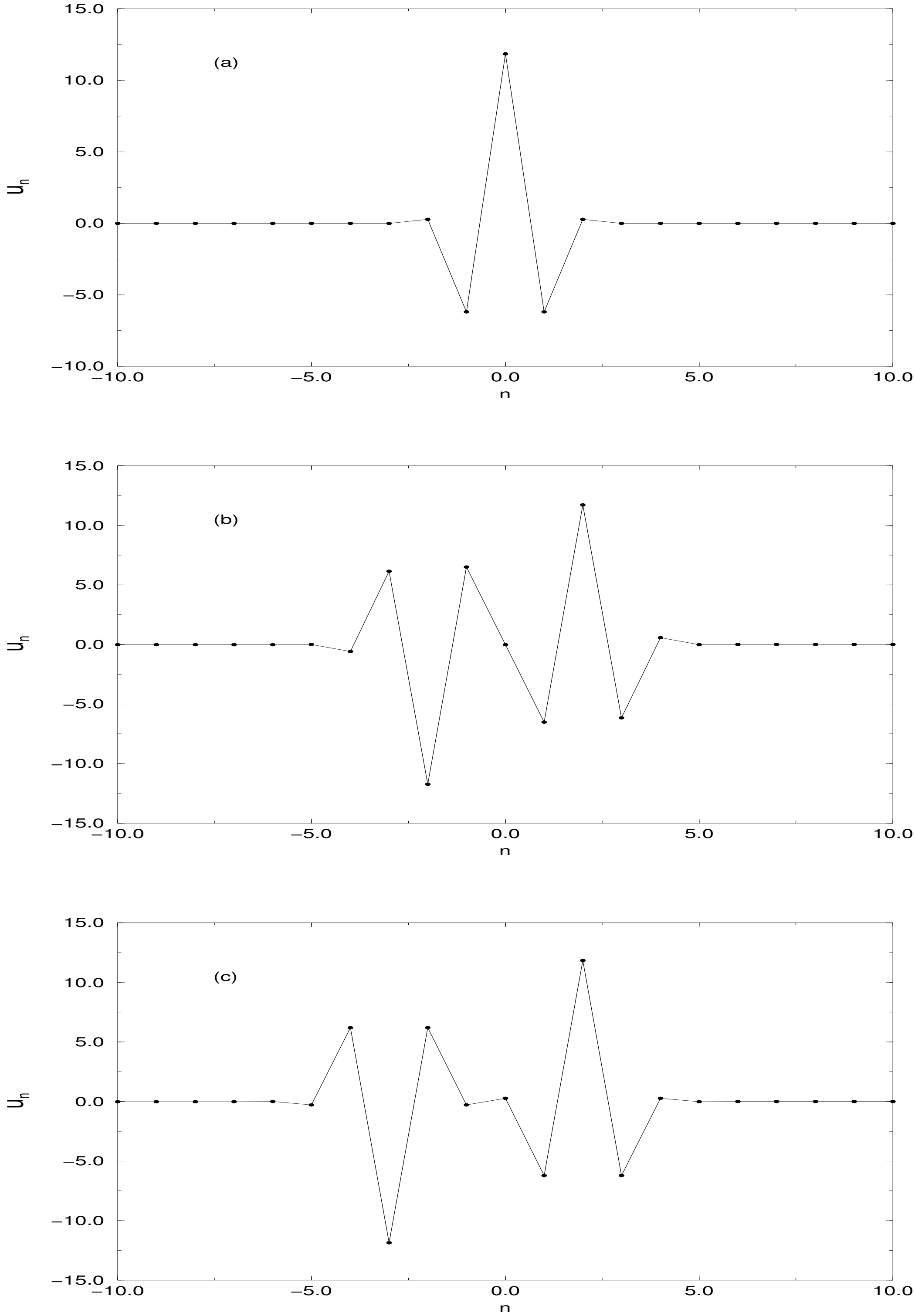

FIG. 4. Examples of ILMs for the lattice model (1): (a) Sievers-Takeno localized mode centered on a lattice site; (b),(c) two examples of a bound state of two Sievers-Takeno modes.

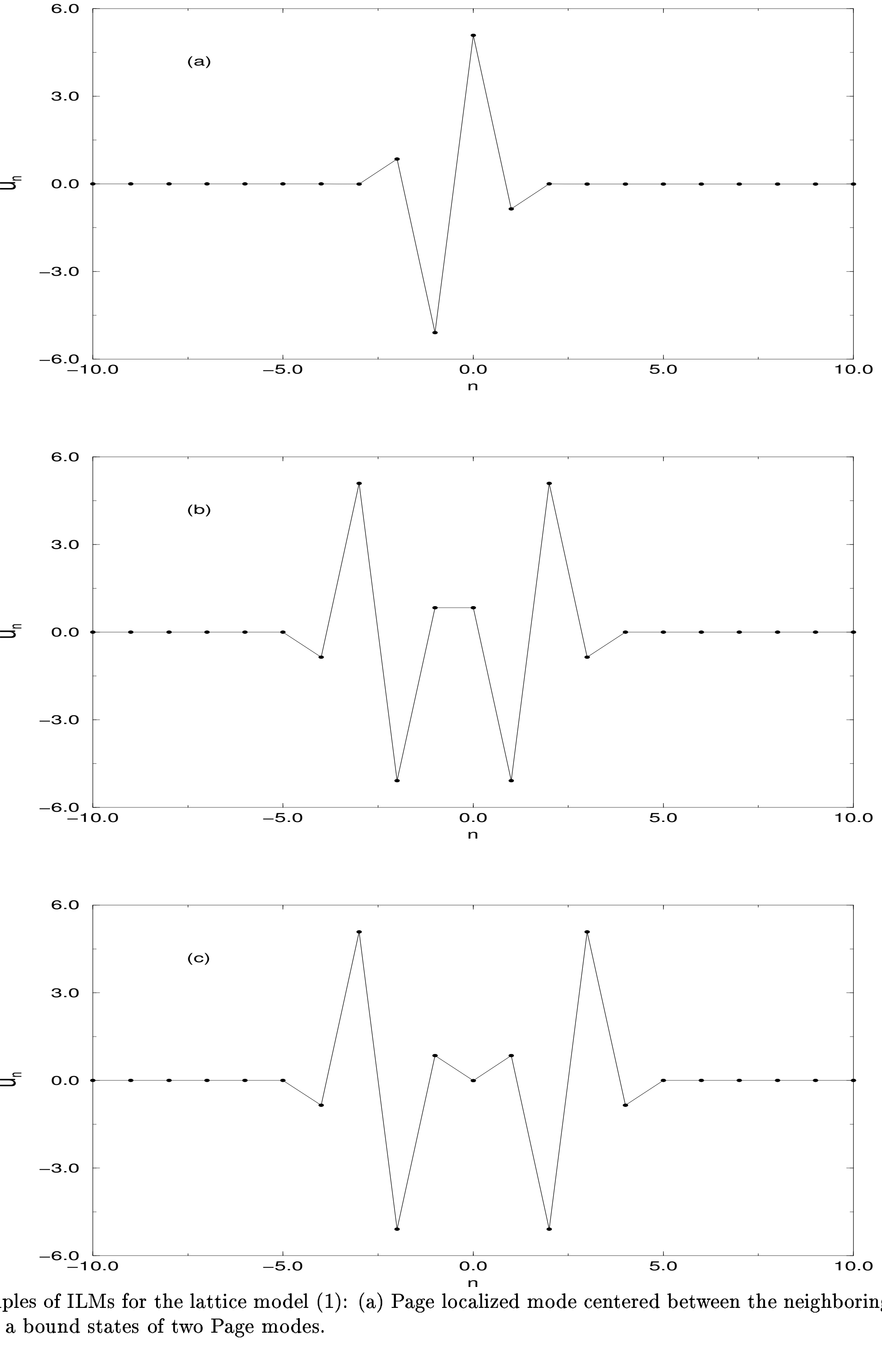

FIG. 5. Examples of ILMs for the lattice model (1): (a) Page localized mode centered between the neighboring sites; (b),(c) two examples of a bound states of two Page modes.