Creation of nonlinear localized modes in discrete lattices

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Creation of intrinsic localized modes in homogeneous nonlinear lattices is discussed, taking as a special example a chain of particles interacting via harmonic and even-power anharmonic potentials. The analysis is based on an effective equation for the wave envelope that, in particular, seems to be an alternative discrete version of the well-known nonlinear Schrödinger equation. It is pointed out that modulational instability and nonlinearity-induced blowup may be considered as two main physical mechanisms for generation of highly localized modes in homogeneous nonlinear chains.

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As is well known, spatially localized oscillations called "intrinsic localized modes" can exist in *strongly anharmonic* homogeneous lattices when nonlinearity is introduced through interatomic interactions [1, 2] or an external on-site potential [3]. Highly localized modes involve only a few particles and in the case when interatomic coupling is purely nonlinear, they may be treated as *compactons*, i.e., discrete solitons with a compact support [4]. As has been mentioned recently in [5, 6], two stationary localized modes proposed by Sievers and Takeno [1] and Page [2] may be attributed to extrema points of an effective periodic potential, the so-called Peierls-Nabarro relief, generated by the lattice discreteness.

One of the principal problems in the theory of intrinsic localized modes is to predict and discuss possible mechanisms of energy localization leading to the formation of large-amplitude nonlinear excitations in discrete lattices. When a lattice is *with* impurities, inhomogeneities may effectively localize energy at [7] or between [8] impurity sites leading to an effective process by which energy, being initially distributed in a nonlinear lattice, can localize itself into large-amplitude excitations. However, this mechanism of the energy localization is certainly not possible for *homogeneous* lattices. However, to make a conclusion about importance of the intrinsic localized modes in transport properties of strongly nonlinear discrete lattices, one should propose simple mechanisms (other than those involving impurities) of the energy localization in lattices which might be responsible for formation of highly localized large-amplitude modes.

The purpose of the present paper is to discuss possible mechanisms leading to the formation of intrinsic localized modes in chains with strong nonlinear interatomic interaction. The analysis presented is based on an effective *discrete* nonlinear equation for the wave envelope of relative particle displacements. It is pointed out that nonlinearity-induced *modulational instability* and, for the case of supercritical power nonlinearity, *collapse dynamics* seem to be important effects responsible for formation of highly localized nonlinear modes in discrete systems.

I consider the dynamics of a one-dimensional chain made of particles (atoms) with mass m coupled with their neighbors by harmonic and even-power anharmonic potentials (see, e.g., Ref. [2]). Denoting by $u_n(t)$ the displacement of atom n, its equation of motion is

$$m\ddot{u} = k_2(u_{n+1} + u_{n-1} - 2u_n) + k_r[(u_{n+1} - u_n)^{2r+1} + (u_{n-1} - u_n)^{2r+1}], \quad r \geq 1, \tag{1}$$

where k_2 and k_r are the corresponding coupling constants which are assumed to be positive. The model (1) is an important generalization of the models considered in [1, 2] because dealing with *large-amplitude* oscillating modes one should naturally expect an importance of higher-order nonlinearities rather than low-order ones. At the same time, the model (1) takes into account a linear interparticle interaction ($\sim k_2$) for, at least, two reasons: (i) this allows one to save many features of linear lattices, e.g., the spectrum of linear excitations, to understand how nonlinearities do modify the lattice properties, and (ii) the model covers the well-known case $r = 1$ treated previously when the effective nonlinear Scrödinger equation has stable solutions.

Introducing the relative displacements, $v_n = u_{n+1} - u_n$, Eq. (1) may be reduced to the following:

$$m\ddot{v}_n = k_2(v_{n+1} + v_{n-1} - 2v_n) + k_r(v_{n+1}^{2r+1} + v_{n-1}^{2r+1} - 2v_n^{2r+1}), \tag{2}$$

where the dot stands for the time derivative. Linear oscillations in the chain of the frequency ω and wave number q are described by the dispersion relation

$$\omega^2 = 4\left(\frac{k_2}{m}\right)\sin^2\left(\frac{qa}{2}\right), \tag{3}$$

a being the lattice spacing. As shown by Eq. (3), the linear spectrum is limited by the cutoff frequency $\omega_m = (4k_2/m)^{1/2}$ due to discreteness.

Analyzing oscillating localized modes with frequencies lying much above the cutoff frequency ω_m, I look for a solution of Eq. (2) in the form

$$v_n(t) = (-1)^n \psi_n(t) e^{i\omega_m t} + \text{c.c.}, \tag{4}$$

where c.c. stands for complex conjugate, and the envelope ψ_n of the relative particle displacements is assumed to be *slowly varying in time* (but not in space), i.e., satisfying the inequality $\dot{\psi}_n \ll \omega_m \psi_n$. Substituting Eq. (3) into Eq. (2) and keeping only the lowest order in the rapidly oscillating multiplier $\exp(i\omega_m t)$, I obtain the discrete equation for the envelope ψ_n,

$$i\dot{\psi}_n + D(\psi_{n+1} + \psi_{n-1} - 2\psi_n) + \lambda_r(|\psi_{n+1}|^{2r}\psi_{n+1} + |\psi_{n-1}|^{2r}\psi_{n-1} + 2|\psi_n|^{2r}\psi_n) = 0, \quad (5)$$

where

$$D = \frac{k_2}{2m\omega_m}, \quad \lambda_r = \frac{k_r}{2m\omega_m}\frac{(2r+1)!}{(r+1)!r!}, \quad r \geq 1. \quad (6)$$

Equation (5) is used below to analyze localized modes in the chain (1) and mechanisms of their formation. However, I would like to point out that the assumption of slow variation of the envelope in time as well as the neglecting of higher-order harmonics to derive (5), assume that the frequency ω_m is large with respect to other frequencies in the system, i.e., nonlinearity-induced effects are not large in comparison with effects produced by discreteness. This condition simply means that structure of localized modes to Eq. (5) found below is an *approximate* one and the corresponding accuracy of such an approximation is similar to that of the so-called "rotating-wave approximation" used in [1, 2]. Nevertheless, Eq. (5) is very convenient for studying nonlinearity-induced *instabilities* in the lattice (1).

As is well known, nonlinear physical systems may exhibit an instability that leads to a self-induced modulation of the steady state as a result of an interplay between nonlinear and dispersive effects. This phenomenon, referred to as *modulational instability*, seems to be one of the main physical mechanisms responsible for energy localization and formation of large-amplitude excitations in homogeneous discrete systems (see, e.g., [9, 10]). Here I will show a feature of this mechanism which may lead to creation of *finite-width* localized modes which seem to be a discrete analog of the so-called compactons [11, 4].

For the discrete model (5),(6) derived in the single-frequency approximation, modulational instability can be easily analyzed by the method previously used in Ref. [10]. Equation (5) has an exact continuous wave (cw) solution with the wave number k,

$$\psi_n(t) = \psi_0 e^{i\theta_n} \quad \text{with} \quad \theta_n = kan - \omega t, \quad (7)$$

where the frequency ω obeys the *nonlinear dispersion relation*,

$$\omega = 4D\sin^2\left(\frac{ka}{2}\right) - 4\lambda_r\psi_0^2\cos^2\left(\frac{ka}{2}\right). \quad (8)$$

The linear stability of the cw solution (7),(8) can be investigated by looking for a perturbed solution of the form

$$\psi_n(t) = (\psi_0 + b_n)\exp(i\theta_n + i\chi_n), \quad (9)$$

where the modulation of the amplitude $b_n = b_n(t)$ and the phase difference $\chi_{n+1} - \chi_n = \chi_{n+1}(t) - \chi_n(t)$ are assumed to be small in comparison with the corresponding parameters of the carrier wave. In the linear approximation two coupled equations for these functions are

$$\dot{b}_n + D\sin(ka)(b_{n+1} - b_n) + \psi_0(D + \lambda_r\psi_0^{2r})\cos(ka)(\chi_{n+1} + \chi_{n-1} - 2\chi_n) + \lambda_r\psi_0^{2r}(2r+1)\sin(ka)(b_{n+1} - b_{n-1}) = 0, \quad (10)$$

$$-\psi_0\dot{\chi}_n + D\cos(ka)(b_{n+1} + b_{n-1} - 2b_n) - \psi_0(D + \lambda_r\psi_0^{2r})\sin(ka)(\chi_{n+1} - \chi_{n-1}) \lambda_r\psi_0^{2r}\cos(ka)[(2r+1)(b_{n+1} + b_{n-1}) - 2b_n] + 4r\lambda_r\psi_0^{2r}b_n = 0. \quad (11)$$

Looking for a solution of Eqs. (10) and (11) in the form $b_n, \chi_n \sim b_0, \chi_0 \exp(iQna - i\Omega t)$, I find the dispersion relation for small modulations of the cw solution. In the case of standing waves, i.e., at $k = 0$, the dispersion relation takes the form

$$\Omega^2 = 4(D + \lambda_r\psi_0^{2r})\sin^2(Qa) \times \left[(D + \lambda_r\psi_0^{2r})\tan^2\left(\frac{Qa}{2}\right) - 2r\lambda_r\psi_0^{2r}\right]. \quad (12)$$

In the long-wavelength limit, when $Qa \ll 1$, and for a strong linear coupling, when $D \gg \lambda_r\psi_0^{2r}$, Eq. (12) reduces to the standard expression for the continuous nonlinear Schrödinger (NLS) equation with an even-power nonlinearity.

Equation (12) determines the instability region,

$$\tan^2\left(\frac{Qa}{2}\right) < \frac{2r}{1+\Delta}, \quad \text{where } \Delta = \frac{D}{\lambda_r\psi_0^{2r}}, \quad (13)$$

of a nonlinear (standing) plane wave in the lattice. The maximum grow rate of such an instability, i.e., the minimum of the function $\Omega^2(Q)$, is realized at $Q = Q_*$, where Q_* is a solution of the equation

$$\tan^2\left(\frac{Q_* a}{2}\right) = \frac{r}{(r+1)+\Delta}, \quad (14)$$

and Δ is defined above.

The important issue of the present analysis of modulational instability is the characteristic value Q_* which in fact defines the width of pulses generated in result of development of such an instability. As follows from Eq. (14), in the limit $\Delta \ll 1$, i.e., for large-amplitude nonlinearities, the grow rate *does not depend on the wave amplitude and it tends to a fixed value.* The latter result means that the characteristic width d of the pulses created due to this instability is also fixed, e.g., at $r = 1$ a simple estimate yields $d \sim 2.55a$. This estimate is rather close to the width $d = 3a$ of an *exact compacton solution* recently proposed in [4] for a lattice with purely anharmonic interaction, i.e., Eq. (1) at $k_2 = 0$.

The growth rate of modulational instability for the discrete equation (5) differs drastically from the corresponding result for the standard discrete NLS equation (see, e.g., Ref. [12]) where the instability analysis predicts [10] the existence of arbitrary narrow pulses when the oscillation energy is mostly localized at a single particle site. In the case of the model (5), the spatial extension of localized modes will be not less than three particles. The spatial structure of the localized modes can be directly obtained from (5) following the method of Ref. [2]. I seek highly localized standing solutions to the NLS equation (5) in the form $\psi_n(t) = Ae^{i\Omega t}f_n$, where I take $f_0 = 1$, $f_{-n} = f_n$ assuming $|f_n| \ll f_1$ for $|n| > 1$. Equations at $n = 0$, $n = 1$, etc. then yield an infinite system of coupled nonlinear equations to calculate oscillation amplitudes at each site. It is easy to check that in the case

$$\xi \equiv \frac{D}{\lambda_r A^{2r}} \ll 1, \tag{15}$$

the structure of a highly localized mode centered at the site $n = 0$ is given by

$$\psi_n(t) = Ae^{i\Omega t}(\ldots 0, \tfrac{1}{2}, 1, \tfrac{1}{2}, 0, \ldots), \tag{16}$$

where the values inside parentheses are the amplitudes at successive sites, and $\Omega \approx 2\lambda_r A^{2r}$.

I should also note that the result $f_1 \approx \frac{1}{2}$ has a numerically small correction which in the limit $r \gg 1$ tends to zero (see Ref. [2]), $f_1 = \frac{1}{2}[1 + (\frac{1}{2})^{2r+1}]$. At $r = 1$ the correction in the brackets is 0.125, being indeed small. Accordingly, the value f_2 differs from zero, $f_2 \approx \frac{1}{2}f_1^{2r+1}$ that at $r = 1$ yields $f_2 \approx 0.063$.

For the primary field u_n, the localized mode (16) corresponds to the mode pattern proposed by Page [2]. To find the other mode, proposed by Sievers and Takeno [1], in the framework of Eq. (5), I assume that the mode is centered between the neighboring particle sites taking $f_0 = f_1 = 1$. Straightforward calculations which take into account the condition (15) yield the spatially localized structure,

$$\psi_n(t) = Ae^{i\Omega t}(\ldots, 0, \tfrac{1}{3}, 1, 1, \tfrac{1}{3}, 0, \ldots), \tag{17}$$

where this time $\Omega \approx 3\lambda_r A^{2r}$. As a matter of fact, the mode (16) corresponds for the field u_n to the pattern $(\ldots, 0, 1, -1, 0, \ldots)$, whereas the mode (17) corresponds to the u_n pattern $(\ldots, 0, -\frac{1}{2}, 1, -\frac{1}{2}, 0, \ldots)$. As has been recently demonstrated in Ref. [13], the Sievers-Takeno pattern shows a dynamical instability and, according to [5, 6], such an instability may be attributed to an effective periodic potential which appears in result of the lattice discreteness being similar to the well-known Peierls-Nabarro (PN) relief to kinks. Thus the relationship between the localized modes to the models (1) and (5) allows one to conclude that the stationary mode (16) is *absolutely stable*, similar to the Page mode, and it corresponds to a minimum of an effective PN relief.

As a matter of fact, the model (1) assumes the interaction potential symmetric. This is not, however, a general case because it is usually harder to compress a bond than to stretch it, and several studies were performed to take into account the simultaneous effect of cubic and quartic anharmonicity on localized excitations in quasicontinuous [14, 15] as well as in highly discrete [16, 17] cases. Unfortunately, the calculations presented above cannot be expanded to cover the case of a combination of odd and even arbitrary powers. However, for the particular case of the cubic and quartic anharmonicity when the interaction potential is taken as $V(x) = \frac{1}{2}k_2x^2 + \frac{1}{3}k_3x^3 + \frac{1}{4}k_4x^4$ where $x \equiv u_{n+1} - u_n$, this can be done looking for a solution in the form

$$v_n = A[\phi_n + (-1)^n\psi_n e^{i\omega_m t} + \cdots] + \text{c.c.}, \tag{18}$$

and assuming the following scaling for the functions ϕ_n, ψ_n, etc.: $\psi_n \sim \epsilon$, $\phi_n \sim \epsilon^2$, etc. The calculation itself takes into account discreteness and it is similar to that recently done for the case of highly localized modes in a chain with a nonlinear on-site potential [3]. In the main order I obtain the NLS equation (5) at $r = 1$ with the renormalized coefficient in front of the term $(|\psi_{n+1}|^2\psi_{n+1} + |\psi_{n-1}|^2\psi_{n-1} + 2|\psi_n|^2\psi_n)$,

$$\lambda_r \to \frac{A^2}{2m\omega_m}\left(3k_4 - \frac{4k_3^2}{k_2}\right). \tag{19}$$

The condition $3k_4k_2 > 4k_3^2$ which follows from the approximation based on the NLS equation and Eq. (19) determines the region where the discrete NLS equation has localized solutions, so that localized modes may exist only in the case when the cubic nonlinearity does not exceed a certain critical value (see also Refs. [14, 15, 17]).

The effective discrete equation (5) in the continuum limit reduces to the nonlinear Schrödinger equation with arbitrary power nonlinearity,

$$i\frac{\partial\psi}{\partial t} + D\frac{\partial^2\psi}{\partial x^2} + 4\lambda_r|\psi|^{2r}\psi = 0, \tag{20}$$

where $x = an$ is treated here as a continuous variable. For the special case of $r = 1$, Eq. (20) becomes the cubic NLS equation which is exactly integrable [18]. For the so-called subcritical case, $r < 2$, Eq. (20) has a stable soliton solution, but for the critical case, $r = 2$, and the supercritical case, $r > 2$, the soliton becomes unstable displaying blowup (see, e.g., Ref. [19] for a review). The term "blowup" designates the situation where the maximum of $|\psi|$ tends to infinity in a finite time interval, and the pulse width tends to zero. As a matter of fact, blowup in an evolution equation means that the assumptions made in the derivation of the equation break down, and physically the blow-up will be always stoped by dispersion or higher-order nonlinearity. For the system under consideration, the blowup dynamics may give (for the case $r \geq 2$ only) an effective mechanism of the energy localization in discrete lattices, and this phenomenon allows one to predict the characteristic time of such a localization as a blowup time (see, e.g., [19]).

It is clear that additional terms do appear in physical models which may be reduced to the NLS equation with higher-order even-power nonlinearity, and this may prevent the blowup dynamics (see, e.g., Ref. [20]). In particular, taking into account in Eq. (20) the terms $\sim a^2$, one may obtain the *perturbed* NLS equation,

$$i\frac{\partial\psi}{\partial t} + D\frac{\partial^2\psi}{\partial x^2} + \frac{a^2}{12}D\frac{\partial^4\psi}{\partial x^4} + 4\lambda_r|\psi|^{2r}\psi + a^2\lambda_r\frac{\partial^2}{\partial x^2}(|\psi|^{2r}\psi) = 0, \quad (21)$$

with higher-order linear and nonlinear dispersion terms (which are in fact of the same order), and one may naturally expect (especially, taking into account the results of Ref. [20] where the effect of higher-order linear dispersion was analyzed to show suppression of blowup) that these additional dispersive terms may indeed drastically reduce the blowup dynamics. As a matter of fact, a pulse, being compressed due to collapse, cannot become more narrow than the localized mode (16), so that one can expect that *in discrete lattices the blowup dynamics leads not to collapse but rather to localization* of energy being initially distributed in a nonlinear lattice into large amplitude excitations.

The influence of the discreteness effects on blowup has been recently investigated numerically by Bang, Rasmussen, and Christiansen [21] for the case of the standard discrete NLS equation with even-power on-site nonlinearity. In particular, they have found that in a discrete NLS equation a pulse becomes localized in finite time although the degree of nonlinearity is subcritical, $r \approx 1.95$ [21].

In conclusion, in the framework of an effective discrete equation for the wave envelope two possible mechanisms for creating highly localized nonlinear modes in discrete lattices have been discussed analytically. It has been pointed out that in homogeneous nonlinear lattices modulational instability and blowup are likely two possible mechanisms for the generation of energy localization within certain spatially finite regions, and those mechanisms seem to be complimentary to an impurity-induced energy localization in the case of inhomogeneous lattices [7, 8].

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