Moving localized modes in nonlinear lattices

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An analytical approach based on the perturbed discrete Ablowitz-Ladik equation is applied to investigate intrinsic localized modes for two different models of one-dimensional anharmonic lattices, namely, for a chain with nonlinear interatomic interaction and a chain with nonlinear on-site potential. It is shown that the motion of the localized modes is strongly affected by an effective periodic (Peierls-Nabarro) potential, but for the former model moving localized modes may still exist in a wide region of the mode parameters, whereas for the latter one they will be always captured by the lattice discreteness if the amplitude of the mode exceeds a certain threshold value.

As is well known, spatially localized modes can exist in a linear lattice with impurities.[1] The localized mode has a maximum at the impurity site, and it decreases exponentially as a function of the distance from the impurity. Recently interest in localized modes for strongly anharmonic lattices has grown mostly due to the paper by Sievers and Takeno,[2] who proposed a kind of localized mode in nonlinear lattices. Because the lattice is *without* impurities, they called this mode *an intrinsic localized mode* in order to distinguish it from the impurity-induced localized mode. Different properties of the intrinsic localized mode have been discussed in a number of papers (see, e.g., Refs. 3–11). The original model showing the main properties of the intrinsic localized mode is a chain with anharmonic interatomic interaction, the so-called Fermi-Pasta-Ulam (FPU) model. It describes a one-dimensional lattice composed of atoms with masses m, in which each atom interacts only with its nearest neighbors. If $u_n(t)$ is the displacement of the nth atom from its equilibrium position and k_2 and k_4 are nearest-neighbor harmonic and quartic anharmonic force constants, respectively, the equations of motion are given by

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

The Sievers-Takeno (ST) mode pattern is $u_n(t) = A(\ldots,0,-\frac{1}{2},1,-\frac{1}{2},0,\ldots)\cos\omega t$, where A is the mode amplitude and the approximation is valid for large $(k_4/k_2)A^2$. The mode frequency ω lies above the nonlinear cutoff frequency of the spectrum band. Another type of a spatially localized mode, the so-called even-parity mode, was introduced by Page,[4] and the pattern of the Page (P) stationary mode is $u_n(t) = A(\ldots,\frac{1}{6},-1,1,-\frac{1}{6},\ldots)\cos\omega t$ (see Ref. 10 for more details). As has been recently proved in Ref. 10, the ST mode shows a dynamical instability, whereas the P mode has been found to be extremely stable.

Other types of nonlinear models to analyze properties of intrinsic localized modes are those with nonlinearity produced by an on-site potential,[3,11] e.g., as in the nonlinear Klein-Gordon (KG) chain,

$$m\frac{d^2u_n}{dt^2} = K(u_{n+1}+u_{n-1}-2u_n) - m\omega_0^2u_n + \frac{1}{3}\beta u_n^3. \quad (2)$$

Here highly localized modes exist with the frequencies lying (for $\beta > 0$) *below* the frequency gap ω_0 or (for $\beta < 0$) *above* the cutoff frequency. The structures of these modes are $u_n(t) = A(\ldots,0,\xi,1,\xi,0,\ldots)\cos\omega t$ for $\beta > 0$ or $u_n(t) = A(\ldots,0,-\xi,1-\xi,0,\ldots)\cos\omega t$ for $\beta < 0$; the approximation is better for smaller values of the coupling parameter $\xi = (4K/|\beta|A^2)$.[11]

Because the intrinsic localized modes can be easily exited from localized initial conditions,[5] they are considered to be important objects to contribute to transport properties of nonlinear discrete systems. However, one of the main problems in analyzing such an influence is to demonstrate the stability properties of the modes and also to prove the existence of moving intrinsic localized modes. Since there is no analytical expression for *moving intrinsic localized modes*, in a recent paper by Bickham, Sievers, and Takeno[9] (see also Ref. 10) this study has been carried out numerically, and the authors made measurements of the shape and the dispersion relation for moving anharmonic modes in the model (1). However, these measurements did not show *why* the moving intrinsic localized modes are possible even under the strong influence of discreteness effects and *which kind* of relations exists between different types of models for intrinsic localized modes. Recently, Sandusky, Page, and Schmidt[10] have shown that for the case of interatomic quartic anharmonicity (the FPU chain) the ST localized mode is in fact unstable, but the P mode is extremely stable. Moreover, that reference reports the observation of intrinsic localized modes *trapped* by discreteness similar to the trapping by an impurity (see also discussions

in Ref. 8).

The purpose of this paper is to apply a simple analytical approach to investigate stability properties of localized modes and to discuss the existence of moving intrinsic localized modes in the models (1) and (2) comparing similar results for both types of the models. One of the most important issues of our analysis is to show that nonintegrability of the discrete models (1) and (2) gives rise to an effective periodic Peierls-Nabarro (PN) potential (see, e.g., Ref. 12 and references therein), which may capture the mode at the atom site or between the sites. In particular, we show that the unstable ST mode, which is centered *at* a particle site, corresponds to *a maximum* of the PN potential, so that it does show the instability observed in Ref. 10. We also show that the P mode, which is centered *between* the nearest particle sites, corresponds to *a minimum* of the PN potential, and the latter explains why the P mode is extremely stable and the trapping between the nearest particle sites is observed.[10] Nevertheless, in spite of the strong discreteness effects and the trapping, the model (1) may support moving localized modes in a wide region of the mode parameters, even for the case of a very large amplitude. This result differs drastically from that for the model (2). The latter cannot support propagating localized modes if the mode amplitude exceeds a certain threshold value. Then strongly localized modes in the model (2) will be always *captured* by the lattice discreteness.

The main idea of our approach is to use the integrable discrete Ablowitz-Ladik model as a basis to develop a pertubation theory for the models (1) and (2). We make the so-called "rotating-wave approximation"; i.e., only the terms proportional to the main harmonic are taken into account. In the framework of this approach the intrinsic localized modes of the models (1) and (2) are treated as pertubed lattice solitons. The similarity of intrinsic localized modes with envelope solitons has been already established in the continuum limit,[7,8] but here we will explore this idea for the discrete case considering the lattice solitons pertubatively.

Let us start first from the KG chain (2). Substituting the ansatz

$$u_n = e^{-i\omega_0 t}\Psi_n + e^{i\omega_0 t}\Psi_n^* \tag{3}$$

into Eq. (2), where ω_0 is the gap frequency of the linear spectrum of the chain, we keep only the terms $\sim \exp(\pm i\omega_0 t)$ so that, under the assumption $d\Psi_n/dt \ll \omega_0\Psi_n$, Eq. (2) will reduce to the discrete nonlinear Schrödinger (NLS) equation

$$2im\omega_0\frac{d\Psi_n}{dt} + K(\Psi_{n+1} + \Psi_{n-1} - 2\Psi_n) + \beta|\Psi_n|^2\Psi_n = 0. \tag{4}$$

Equation (4) may be written as a pertubed Ablowitz-Ladik equation

$$2im\omega_0\frac{d\Psi_n}{dt} + K(\Psi_{n+1} + \Psi_{n-1} - 2\Psi_n) + \tfrac{1}{2}\beta(\Psi_{n+1} + \Psi_{n-1})|\Psi_n|^2 = R(\Psi_n)\,, \tag{5}$$

where

$$R(\Psi_n) = \tfrac{1}{2}\beta \mid \Psi_n \mid^2 (\Psi_{n+1} + \Psi_{n-1} - 2\Psi_n)\,. \tag{6}$$

As is well known,[13] the Ablowitz-Ladik model given by Eq. (5) with $R = 0$ is exactly integrable and it supports (moving) nonlinear localized exitations in the form of lattice solitons. The latter may be highly localized objects involving only a few particles. The exact soliton solution of the Ablowitz-Ladik model can be presented in the form

$$\Psi_n(t) = \frac{\sinh\mu \exp\left[ik(n - x_0) + i\alpha\right]}{\cosh\left[\mu(n - x_0)\right]}\,, \tag{7}$$

where in the unperturbed case $\dot{\mu} = 0$, $\dot{k} = 0$,

$$\dot{x}_0 = (2/\mu)\sinh\mu\sin k \quad \text{and} \quad \dot{\alpha} = 2[\cosh(\mu)\cos(k) - 1]\,.$$

In Eq. (7) and the subsequent calculations related to Eqs. (5) and (6) we have used the normalized variables $t \to (2m\omega_0/K)t$ and $|\Psi_n|^2 \to (2K/\beta)|\Psi_n|^2$.

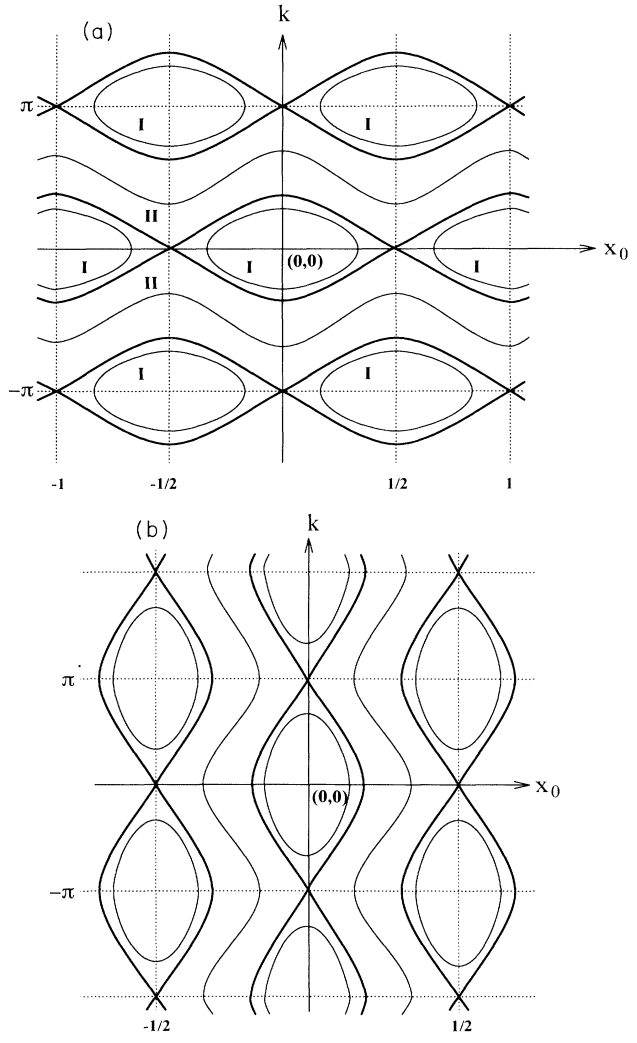

FIG. 1. Phase plane of the soliton parameters (k, x_0) for the KG model: (a) $\mu < \mu_c$ with $\mu_c \approx 3.6862$ and (b) $\mu > \mu_c$.

Considering now the right-hand side of of Eq. (5) as a pertubation (that is certainly valid for not strongly localized modes), we will use the pertubation theory based on the inverse scattering transform.[14] For the case of the Ablowitz-Ladik model the perturbation theory was elaborated in Ref. 15. According to this approach, the parameters of the localized solution (7), i.e., μ, k, α, and x_0, are assumed to be slowly varying in time. The equations describing their evolution in the presence of perturbations may be found in Ref. 15. Substituting (6) into those equations and applying the Poisson formula

$$\sum_{n=-\infty}^{\infty} f(na) = \int_{-\infty}^{\infty} \frac{dx}{a} f(x) \left[1 + 2\sum_{s=1}^{\infty} \cos\left(\frac{2\pi s x}{a}\right)\right]$$

to evaluate the sums appearing as a result of discreteness of our primary model, we obtain two coupled equations for the soliton parameters k and x_0:

$$\frac{dx_0}{dt} = \frac{2}{\mu} \sinh\mu \, \sin k \,, \tag{8}$$

$$\frac{dk}{dt} = -\frac{2\pi^3 \sinh^2\mu \, \sin(2\pi x_0)}{\mu^3 \sinh(\pi^2/\mu)} \,, \tag{9}$$

and also $d\mu/dt = 0$ as above. In Eq. (9) we keep only the contribution of the first harmonic because the higher harmonics of the order s will always appear with the additional multiplier $\sim \exp(-\pi^2 s/\mu)$, which is assumed to be exponentially small (even for $\mu \sim 1$). As μ is constant, the system (8) and (9) may be easily analyzed on the phase plane (k, x_0) considering a parametrical dependence on μ. Small values of the parameter μ correspond to the quasicontinuous approximation when the lattice equations are transformed into the continuous ones, and they may be described by the continuous NLS equation.[7,8] For μ not very small, i.e., in fact for $\mu < \mu_{cr}$, where μ_{cr} is defined below, the phase plane of the dynamical system (8) and (9) is shown in Fig. 1(a). As may be clearly seen from the figure, there are phase trajectories describing moving localized modes [regions II in Fig. 1(a)]. At the same time, there is also possible trapping of solitons with small velocitites ($\sim \sin k$) due to lattice discreteness [regions I in Fig. 1(a)]. The trapping occurs either at the atomic site when $x_0 = 0, \pm 1, \ldots$ (low-frequency modes, small k) or between the neighboring sites when $x_0 = \pm 1/2, \ldots$ (high-frequency modes, k close to π). However, if the parameter μ exceeds the critical value $\mu_{cr} \approx 3.6862$, the phase plane is drastically modified, and it does not have trajectories describing *moving* localized modes [see Fig. 1(b)]. This result simply means that if the nonlinearity (i.e., the mode amplitude) exceeds the threshold value, there are no propagating localized modes in the chain. All such modes will exist only in a trapped state. This nonlinearity-induced global trapping of the localized modes follows from the analysis of the dynamical system (8) and (9) which does not include higher-order harmonics coming from the Poisson formula. The approximation we used is in fact valid for $\exp(\pi^2/\mu) \gg 1$, and this condition is certainly satisfied at $\mu = \mu_{cr}$. Nevertheless, the conclusion is qualitatively valid for a more general case, and such a global trapping may be easily observed by direct numerical simulations.[16]

Let us now consider the similar problem for the FPU chain, being the original model used by Sievers and Takeno.[2] To derive the perturbed Ablowitz-Ladik equation in this case we use the ansatz

$$u_n = (-1)^n \left[e^{i\omega_m t}\Psi_n + e^{-i\omega_m t}\Psi_n^*\right], \tag{10}$$

where $\omega_m = (4k_2/m)^{1/2}$ is the cutoff frequency of the spectrum of the linear chain [in the linear case the spectrum is given by the relation $\omega^2 = \omega_m^2 \sin^2(qa/2)$]. Substituting the ansatz (10) into Eq. (1) and keeping again only the terms proportional to the first harmonic, under the same assumption as above, i.e., $d\Psi_n/dt \ll \omega_m \Psi_n$, we obtain the equation

$$2im\omega_m \frac{d\Psi_n}{dt} + k_2(\Psi_{n+1} + \Psi_{n-1} - 2\Psi_n) + 24k_4 \mid \Psi_n \mid^2 (\Psi_{n+1} + \Psi_{n-1}) = R(\Psi_n), \tag{11}$$

where the term

$$R(\Psi_n) = -3k_4 \{|\Psi_{n+1}|^2\Psi_{n+1} + |\Psi_{n-1}|^2\Psi_{n-1} + 2|\Psi_n|^2\Psi_n + (\Psi_{n+1}^2 + \Psi_{n-1}^2)\Psi_n^* + 2\Psi_n(|\Psi_{n+1}|^2 + |\Psi_{n-1}|^2) + \Psi_n^2(\Psi_{n+1}^* + \Psi_{n-1}^*) - 6|\Psi_n|^2(\Psi_{n+1} + \Psi_{n-1})\} \tag{12}$$

is an effective perturbation to the Ablowitz-Ladik model.

Applying again the soliton perturbation theory,[14,15] we derive the system of *three* coupled equations for the soliton parameters,

$$\frac{dx_0}{dt} = \frac{2}{\mu} \sinh\mu \sin k, \tag{13}$$

$$\frac{dk}{dt} = -\frac{2\pi^3 \sinh^2\mu \, \sin(2\pi x_0)}{\mu^3 \sinh(\pi^2/\mu)} \, g(k,\mu), \tag{14}$$

$$\frac{d\mu}{dt} = \frac{2\pi^3 \sinh^2\mu \, \sin(2\pi x_0)}{\mu^3 \sinh(\pi^2/\mu)} \tanh\mu \;\; f(k,\mu), \tag{15}$$

with

$$g(k,\mu) = \frac{\cos k}{\cosh\mu} - 2\cos(2k),$$

and

$$f(k,\mu) = \frac{\sin k}{\cosh\mu} + 2\sin(2k).$$

To write Eqs. (13)–(15), we have normalized Eq. (11) as follows: $t \to (2m\omega_m/k_2)t$ and $|\Psi_n|^2 \to (k_2/24k_4)|\Psi_n|^2$.

Considering the system (13) and (14) for fixed μ we can use again the phase plane (k, x_0) to show different types of the nonlinear dynamics. As has been seen in the previous case, the phase plane (k, x_0) describes two kinds of the soliton dynamics: soliton trapping by the lattice discreteness for small velocities (regions I) and propagating solitons (regions II and III). The phase plane (k, x_0) does allow one to come to a conclusion about the stability properties of the stationary localized modes. Indeed, the approximation (10) we used to derive the perturbed Ablowitz-Ladik equation corresponds to the high-frequency ST and P localized modes provided k small, when the particles in the chain oscillate with opposite phases. As follows from Fig. 2, for $k = 0$ the points $x_0 = 0, \pm 1, \ldots$ are unstable points (saddles), whereas the points $x_0 = \pm 1/2, \ldots$ are stable points (centers). The high-frequency intrinsic localized mode centered *at* a particle site is known to be the ST mode,[2] so that our Fig. 2 clearly indicates that such modes are unstable. This conclusion has been recently made in Ref. 10 on the basis of other (analytical and numerical) arguments. As for the P mode, it is centered *between* the particle sites, and the corresponding critical points on the phase plane (k, x_0) are stable (see Fig. 2). The existence of these two kinds of stationary modes, i.e., stable and unstable ones, simply follows from the equilibrium points of the effective potential energy to the modes, $U = -U_m \cos(2\pi x_0)$, where the value

$$U_m = \frac{\pi^2 \sinh^2 \mu}{\mu^3 \sinh(\pi^2/\mu)} |g(0, \mu)| \tag{16}$$

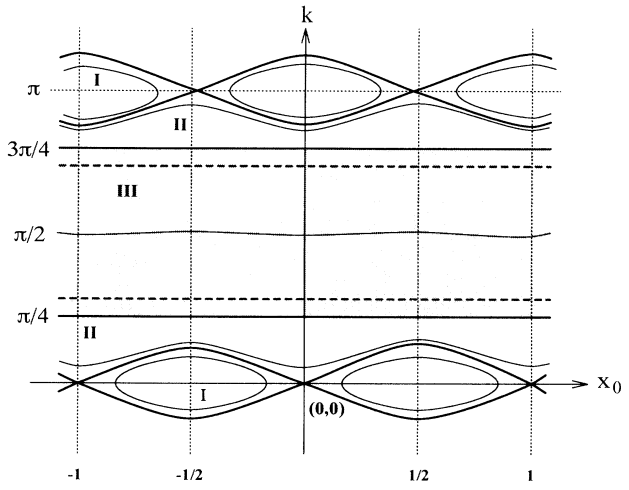

FIG. 2. Same as in Fig. 1 but for the FPU model. The solid straight lines correspond to the case $\mu \neq 0$; the dashed lines are their asymptotic positions for $\mu \to \infty$. All the curves shown are breathing when the evolution of μ given by Eq. (15) is taken into consideration.

may be treated as a trapping energy of the mode to the effective periodic potential (the height of the PN potential; see, e.g., Ref. 12).

The important difference between the KG and FPU models is the presence of *two straight lines* in Fig. 2 for each value of the parameter μ which separate two different kinds of the soliton dynamics and they *never* disappear, even for the cases of very large μ. The dashed lines in Fig. 2 correspond to the case $\mu \to \infty$, but the analysis presented is valid only for not very large μ, i.e., in fact until the inequality $\exp(\pi^2/\mu) \gg 1$ is satisfied. Within the region separated by the straight lines the FPU model *always* admits moving localized modes (lattice solitons), and this result confirms numerical observations of moving localized modes reported earlier (see, e.g., Ref. 9). For the complete model (13)–(15) we have found that in region III (see Fig. 2) the solutions depend *very weakly* on the variation of μ, at least in the middle part of this region. As a result, the main conclusion for moving intrinsic localized modes remains valid even if the evolution of μ (small in the numerical results) is taken into consideration.

In conclusion, the moving intrinsic localized modes have been investigated analytically for two different nonlinear models using an approach based on the perturbed Ablowitz-Ladik equation. Considering nonintegrable terms as perturbation, we have obtained the evolution equations describing propagation of nonlinear localized modes, i.e., lattice solitons, in a chain with nonlinear on-site potential (the Klein-Gordon chain) and in a chain with nonlinear interatomic interaction (the Fermi-Pasta-Ulam model). We have shown that nonintegrability of the discrete models manifests itself in an effective periodic Peierls-Nabarro potential to the soliton motion, the potential being naturally absent in the integrable Ablowitz-Ladik model. The properties of the potential allow one to make a conclusion about the stability of the different localized modes, showing that the ST mode is unstable because it corresponds to a maximum of the effective PN potential. Comparing the two models for the dynamics of the intrinsic localized modes we have shown that they are drastically different with respect to discreteness effects. In particular, intrinsic localized modes in a chain with nonlinear interparticle interaction may *always* exist as moving excitations for a certain region of parameters, in spite of the fact that their motion is affected by the Peierls-Nabarro potential and they may be captured by the lattice discreteness for small velocities. However, for intrinsic localized modes in a chain with nonlinear on-site potential, there is a threshold value of the nonlinearity parameter above which the modes will be *always* captured by the lattice discreteness; i.e., they cannot move along the chain.

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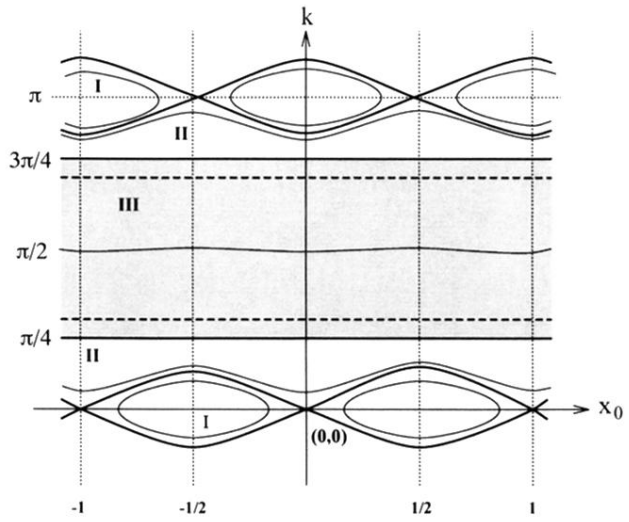

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