Peierls-Nabarro potential barrier for highly localized nonlinear modes

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We consider two types of strongly localized modes in discrete nonlinear lattices. Taking the lattice nonlinear Schrödinger (NLS) equation as a particular but rather fundamental example, we show that (1) the discreteness effects may be understood in the "standard" discrete NLS model as arising from an effective periodic potential similar to the Peierls-Nabarro (PN) barrier potential for kinks in the Frenkel-Kontorova model; (2) this PN potential *vanishes* in the completely integrable Ablowitz-Ladik variant of the NLS equation; and hence (3) the PN potential arises from the *nonintegrability* of the discrete physical models and determines the stability properties of the stationary localized modes.

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I. INTRODUCTION

Many problems in the nonlinear dynamics of spatially extended physical systems involve continuous media, so that nonlinear coherent excitations ("solitons") are naturally described as solutions to partial differential equations. However, models describing microscopic phenomena in solid-state physics are inherently discrete, with the lattice spacing between the atomic sites being a fundamental physical parameter. For these systems, an accurate microscopic description involves (a large set of) coupled ordinary differential equations, and discreteness effects may modify drastically the dynamics of the localized, nonlinear excitations even in the framework of the simplest models (see, e.g., Refs. [1]–[7] to cite a few).

Recently, interest in localized modes in anharmonic lattices has been heightened by the identification of a new kind of strongly localized mode in a homogeneous nonlinear lattice [3]. Since the lattice is *without* impurities, this mode has been termed an *"intrinsic localized mode"* in order to distinguish it from the impurity-induced localized modes well known in the linear theory of crystal lattices (see, e.g., Ref. [8]). Properties of the intrinsic localized modes have subsequently been widely discussed in the literature (see, e.g., Refs. [9]–[18]). For the model describing a chain of particles of equal masses m interacting via harmonic ($\sim k_2$) and quartic anharmonic ($\sim k_4$) forces, the highly localized nonlinear modes may be found by a Green's-function technique [3] or by a simple method developed in [10]. The "Sievers-Takeno" (ST) mode pattern is [3] $u_n(t) = A(..., 0, -\frac{1}{2}, 1, -\frac{1}{2}, 0, ...) \cos(\omega t)$, where A is the mode amplitude and the approximation is better for larger $(k_4/k_2)A^2$. The mode frequency ω lies above the nonlinear cutoff frequency of the spectrum band, and the particles oscillate out of phase with their nearest neighbors, as one would expect for a high-frequency, optical-type excitation [see Fig. 1(a)]. Another type of a spatially localized mode was introduced by Page [10], and the pattern of the Page (P) stationary mode is; $u_n(t) = A(..., \frac{1}{6}, -1, 1, -\frac{1}{6}, ...) \cos(\omega t)$ [see Ref. [18] for more details and Fig. 1(b) for the mode structure]. As has been recently proved in [18], the ST mode shows a dynamical instability whereas the P mode has been found to be extremely stable.

One of the principal problems in the theory of nonlinear localized modes is the description of their motion or propagation through the discrete lattice. When moving along the chain, a mode changes its position and, correspondingly, its structure. Comparison of the two stationary localized modes shown in Figs. 1(a) and 1(b) suggests that they are related by translations of 1/2 lattice spacing and therefore they should both "occur" as two "states" of a single mode transiting through the lattice. Our present study confirms that these two stationary states can indeed be viewed as belonging to a single localized mode and that the difference in their energies may be attributed to *an effective periodic potential* generated by the lattice discreteness and similar to the "Peierls-Nabarro" (PN) potential for kinks in the Frenkel-Kontorova (FK) model (see, e.g., [1]). The PN potential, first discussed in classic papers on the continuum theory (and corrections thereto) of dislocations [19], reflects the fact that the discreteness of the underlying lattice in solid state systems breaks the continuous translation invariance of a continuum model and generates a

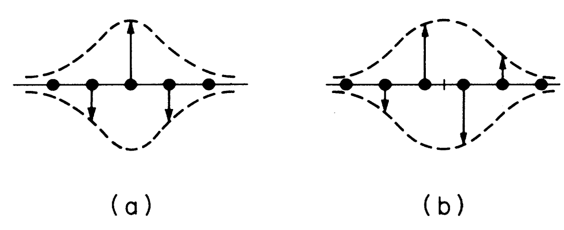

FIG. 1. Shapes of *high-frequency* localized modes in a nonlinear chain when (a) centered on a site and (b) centered between sites. Note that in each case the mode shows the out-of-phase oscillation of neighboring sites that is associated with an opticallike excitation, as one would expect for a high-frequency mode. Case (b) has lower energy than case (a).

periodic potential which affects the continuum dislocations. From the physical point of view, the amplitude of the PN potential may be viewed as the minimum barrier which must be overcome to translate the dislocation by one lattice period.

Although this result holds for many different kinds of localized modes and various nonlinear models, in the present article we focus on the discrete nonlinear Schrödinger (NLS) equation. We consider two variants of this equation, the "standard" discretization and the completely integrable Ablowitz-Ladik [20] version. To motivate the specific choice of the NLS equation, we recall that the analytical approach used to find the shape of the intrinsic localized modes in a lattice is based on the so-called "rotating-wave" approximation, which assumes that only the terms proportional to $\cos(\omega t)$ are taken into account to derive the equation for the spatial structure of the mode (see, e.g., [3, 10]). Therefore, this approach is based, in fact, on the single-frequency approximation, for which an effective NLS equation may be derived in the continuum limit [12, 13].

II. THE "STANDARD" DISCRETE NLS EQUATION

We begin our investigation with the "standard" *lattice* NLS equation

$$i\frac{d}{dt}\psi_n + K(\psi_{n+1} + \psi_{n-1} - 2\psi_n) + \lambda|\psi_n|^2\psi_n = 0. \qquad (1)$$

This equation has been widely used to describe self-trapping phenomenon in a variety of systems, from vibronic modes in natural and synthetic biomolecules [21, 22] to the dynamics of a linear array of vortices [23]. Equation (1) may also be treated as a special limit of the discrete Ginzburg-Landau equation (see, e.g., [23]). In Eq. (1) the parameter K can be viewed as the coupling constant, and the anharmonicity parameter λ describes the nonlinearity. We shall see below that the two different signs of the nonlinearity parameter λ lead to two different kinds of strongly localized modes, with $\lambda < 0$ yielding high-frequency and $\lambda > 0$ yielding low-frequency modes.

Linear oscillations of the lattice (1) of frequency ω and wave number q are described by the dispersion relation, $\omega = 4K\sin^2(q/2)$, with the lattice spacing taken as 1. The spectrum lies in a band $(0, \omega_{\max})$ which is limited by the cutoff frequency $\omega_{\max} = 4K$ due to discreteness: i.e., the lattice can support no oscillation of wavelength shorter than its fundamental lattice spacing and $\omega_{\max}$ is the frequency corresponding to these shortest wavelength oscillations. The *nonlinear* oscillations of the lattice model (1) may exhibit an instability that leads to a self-induced modulation of the spatially constant state as a result of an interplay between nonlinear and dispersive effects. This phenomenon, referred to as *modulational instability*, leads to the existence of inhomogeneous, localized states and is responsible for energy localization.

For the discrete or lattice NLS equation (1), the modulational instability is readily analyzed (see, e.g., [6]). Equation (1) has an exact constant amplitude solution

$$\psi_n(t) = \psi_0 e^{i\theta_n} \quad \text{with} \quad \theta_n = qn - \omega t, \qquad (2)$$

where the frequency ω obeys the *nonlinear* dispersion relation

$$\omega = 4K\sin^2\left(\frac{q}{2}\right) - \lambda|\psi_0|^2 . \qquad (3)$$

The linear stability of the wave form given by (2) and (3) can be investigated by seeking a solution of the form $\psi_n(t) = (\psi_0 + b_n)\exp(i\theta_n + i\chi_n)$, where both $b_n = b_n(t)$ and the differences $\chi_{n+1} - \chi_n = \chi_{n+1}(t) - \chi_n(t)$ are assumed to be small in comparison with the parameters of the carrier wave. In the linear approximation, the two coupled equations for these functions yield the dispersion relation

$$[\Omega - 2K\sin Q\sin q]^2 = 4K\sin^2\left(\frac{Q}{2}\right)\cos q\left[4K\sin^2\left(\frac{Q}{2}\right)\cos q - 2\lambda|\psi_0|^2\right] \qquad (4)$$

for the wave number Q and frequency Ω of the linear modulation waves. Equation (4) determines the condition for the stability of a plane wave with wave number q in the lattice. In contrast to the result in the continuum limit, the stability depends on q, and an instability region exists for $\lambda\cos q > 0$. For positive λ and $q < \pi/2$, a plane wave will be *unstable* to modulations in all this region provided $|\psi_0|^2 > (2K/\lambda)$.

A. Positive λ and low-frequency localized modes

One of the main effects of modulational instability is the creation of localized pulses (see, e.g., Ref. [24]). In the present case this means that for $\lambda > 0$ the small q region is unstable, and, therefore, nonlinearity can induce the formation of localized modes *below* the smallest frequency allowed for constant amplitude nonlinear excitations given by (3). Such localized modes can be obtained directly from the lattice NLS equation (1) following the method of Ref. [10]. We seek stationary solutions of Eq. (1) in the form, $\phi_n(t) = Af_n e^{-i\omega t}$, obtaining a set of coupled algebraic equations for the real function f_n,

$$\omega f_n + K(f_{n+1} + f_{n-1} - 2f_n) + \lambda A^2 f_n^3 = 0. \qquad (5)$$

Based on our earlier remarks, we seek *two* types of strongly localized solutions of Eq. (5), centered respectively at and between the particle sites. First, we assume the mode to be centered at the site $n = 0$ and take $f_0 = 1$, $f_{-n} = f_n$, and $|f_n| \ll f_1$ for $|n| > 1$. Simple calculations yield the pattern of the so-called A modes [see Fig. 2(a)],

$$\phi_n^{(A)}(t) = A(..., 0, \xi_1, 1, \xi_1, 0, ...)e^{-i\omega t}, \qquad (6)$$

where the parameter $\xi_1 = K/\lambda A^2$ is assumed to be small (i.e., terms of order ξ_1^2 are neglected). The frequency ω in Eq. (6) is determined in the *lowest* order in ξ_1 to

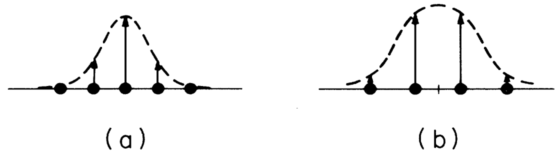

FIG. 2. Shapes of *low-frequency* localized modes in a nonlinear chain when (a) centered on a site and (b) centered between sites. Note that in each case the mode shows the in-phase oscillation of neighboring sites that is associated with an acousticlike excitation, as one would expect for a low-frequency mode. For these modes, case (a) has lower energy than case (b).

be $\omega \approx -\lambda A^2$, and it indeed lies below the lowest band frequency.

The second type of the localized modes, the B modes, may be found assuming that the mode oscillation is centered *symmetrically* between two neighboring particles [see Fig. 2(b)],

$$\phi_n^{(B)}(t) = B(...,0,\xi_2,1,1,\xi_2,0,...)e^{-i\omega t}, \tag{7}$$

where the values ω and ξ_2 are defined as $\xi_2 = K/\lambda B^2$ and $\omega \approx -\lambda B^2$, respectively. Note that both these A- and B-type modes show the "in-phase" oscillations of neighboring sites that one associates with acousticlike modes that occur at low frequencies.

If one imagines a localized wave form *of fixed shape*—for simplicity, think of a Gaussian—being translated rigidly through the lattice, it is clear that when the peak is centered on a lattice site, the symmetry is of the A form, whereas when the peak is centered halfway between sites, the symmetry is of the B form. This observation motivates our ansatz that the A and B modes can be viewed as two stationary configurations corresponding to the moving mode at (different) fixed instants in time *provided* that the amplitudes are adjusted properly. To compare these amplitudes, we fix the discrete analog of the integral of motion (N) having the sense of "the number of particles" in the continuum NLS equation, $N = \sum_n |\phi_n|^2$. The comparison of the integrals N calculated for A and B modes gives the relations between the amplitudes A and B (to lowest order in the small parameter $\xi_1 = K/\lambda A^2$),

$$A^2 = 2B^2. \tag{8}$$

With this condition on A and B, we can interpret now the two modes as stationary states of *the same* localized mode. Using the relation (8), we may now calculate the difference in energy between these two stationary states. From the familiar expression for the energy of the lattice NLS model,

$$H = -K\sum_n [\phi_n(\phi_{n+1}^* - \phi_n^*) + \phi_n^*(\phi_{n+1} - \phi_n)] - \tfrac{1}{2}\lambda \sum_n |\phi_n|^4,$$

we find in the lowest order in the parameter ξ_1 the result that

$$\Delta E_{AB} = E_A - E_B = -\tfrac{1}{2}\lambda A^4 + \lambda B^4 = -\tfrac{1}{4}\lambda A^4 \neq 0. \tag{9}$$

From (9) follows the important conclusion that there is an effective energy barrier (the height of the effective PN potential) between these two stationary states of the lattice NLS equation, so that the A mode has *lower* energy than the B mode in this chain. Recalling our ansatz that the A and B modes may be viewed as *states of the same moving localized mode, simply viewed at different times*, this result means that the motion of the nonlinear localized modes will be affected by a periodic energy relief. In particular, the velocity of the moving mode should show oscillations, and, further, a localized mode may be *captured* by the potential, or may be scattered by it, emitting phonons.

B. Negative λ and high-frequency localized modes

The above analysis of modulational instability in the lattice NLS equation shows that, for $\lambda < 0$, this instability will occur for *large* wave numbers, namely for $q > \pi/2$. Thus, for negative λ, localized modes in the lattice NLS equation are possible with the frequencies lying *above* the cutoff frequency of the nonlinear spectrum band (3). Both the approach developed above and the main conclusions remain valid for these *high-frequency* modes. Consistent with the large wave numbers, these modes show oscillations on the scale of the lattice and their structures are found to be similar to the ST and P modes in a chain with anharmonic interaction [see Figs. 1(a) and 1(b)], i.e.,

$$\phi_n^{(A)}(t) = A(...,0,-\nu_1,1,-\nu_1,0,...)e^{-i\omega t}, \tag{10}$$

and

$$\phi_n^{(B)}(t) = B(...,0,-\nu_2,1,-1,\nu_2,0,...)e^{-\omega t}, \tag{11}$$

where $\nu_1 = K/|\lambda|A^2$, $\nu_2 = K/|\lambda|B^2$, and the frequencies are $\omega \approx 4K + |\lambda|A^2$ and $\omega \approx 4K + |\lambda|B^2$, respectively. All the results for the high-frequency localized modes may be obtained via manipulations similar to those in the case of the low-frequency modes. However, this time the result for the PN energy barrier is just reversed: $\Delta E_{AB} = E_A - E_B = \frac{1}{4}|\lambda|A^4$, i.e., the energy of the B mode is now *smaller* than that of the A mode.

Note that the above analysis also determines the stability properties of the nonlinear localized modes: the stationary localized mode corresponding to a local *maximum* of the PN potential will show an instability whereas the mode corresponding to a *minimum* will be linearly stable. This simple observation made on the basis of the analysis of the PN barrier is in agreement with the recent work by Sandusky, Page, and Schmidt [18], who have shown numerically and analytically (using other arguments and not referring to the PN potential) that for the case of interatomic quartic anharmonicity the ST localized mode [shown in Fig. 1(a)] is in fact unstable, but the P mode [shown in Fig. 1(b)] is extremely stable. Exactly the same conclusion for the high-frequency localized modes follows from our simple analysis. Moreover, the observation of intrinsic localized modes *trapped* by discreteness [18] can be interpreted as trapping by the effective PN potential. Thus the existence of these two kinds of stationary modes, i.e., stable and unstable ones, simply follows from the equilibrium points of an effective PN potential for the localized modes, and this phenomenon is rather general to be valid for different types of nonlinear models.

III. THE ABLOWITZ-LADIK INTEGRABLE DISCRETE NLS EQUATION

It is interesting to compare the results obtained for the "standard" discrete NLS model (1) with those of the completely integrable discrete Ablowitz-Ladik (ALNLS) variant of the NLS equation [20] [cf. Eq. (1)],

$$i\frac{d}{dt}\psi_n + K(\psi_{n+1} + \psi_{n-1} - 2\psi_n) + \tfrac{1}{2}\lambda|\psi_n|^2(\psi_{n+1} + \psi_{n-1}) = 0 \ . \quad (12)$$

Although the models (1) and (12) have the same *linear properties* and lead to *the same NLS equation* in the continuum limit, their *nonlinear* properties are very different. For the model (12), the dispersion relation for modulations around the constant amplitude solution is

$$[\Omega - (2K + \lambda\psi_0^2)\sin Q \sin q]^2 = 4(2K + \lambda\psi_0^2)\sin^2(Q/2)\cos^2 q[(2K + \lambda\psi_0^2)\sin^2(Q/2) - \lambda\psi_0^2]$$

instead of Eq. (4). Therefore, for the ALNLS model, as for the continuum NLS equation, *the modulational instability does not depend on q*. For $Q < Q^*$ determined by $\sin^2(Q^*/2) = \lambda\psi_0^2/(2K + \lambda\psi_0^2)$, *all* the carrier waves are unstable, while for $Q > Q^*$ they are all stable. As a consequence, for a fixed positive value of λ, the ALNLS model (12) can have simultaneously nonlinear modes localized either above or below the linear spectrum band.

A. Intrinsic localized modes

Solving for the A and B modes in the low-frequency limit, we find the A mode to have the same form as Eq. (6) but with the mode frequency given in the lowest order by $\omega \approx -2\sqrt{\lambda K A^2}$, whereas the B mode has precisely the same form as Eq. (7). To compare these two types of the localized modes, we can use the integrals of the ALNLS model, which may be found, for example, in Ref. [5]. Comparing the A and B modes at the fixed integral of motion N having again the sense of "the number of particles" yields $A^2 = \lambda B^4/4K$, and hence $\Delta E_{AB} = E_A - E_B = 4A\sqrt{K/\lambda} - 2B^2 = 0$, i.e., the energy barrier for these two modes vanishes. This result is a direct consequence of the integrability properties of the ALNLS model which supports steady-state propagation of localized pulses—the "discrete solitons"—for any relation between the model parameters λ and K.

B. Perturbative calculation of the PN barrier

One of the simplest ways to calculate the shape of the PN potential in the case of the "standard" NLS equation is to use the integrable version of the lattice NLS equation, i.e., the Ablowitz-Ladik model, and to treat the difference between these two models as a perturbation. To do so, we rewrite the standard discrete NLS equation (1) in the form

$$i\frac{d}{dt}\psi_n + K(\psi_{n+1} + \psi_{n-1} - 2\psi_n) + \tfrac{1}{2}\lambda(\psi_{n+1} + \psi_{n-1})|\psi_n|^2 = R(\psi_n), \quad (13)$$

where

$$R(\psi_n) = \tfrac{1}{2}\lambda \mid \psi_n \mid^2 (\psi_{n+1} + \psi_{n-1} - 2\psi_n) \ . \quad (14)$$

We start from the exact soliton solution of the ALNLS model [20] at $R = 0$ which we take in the form

$$\psi_n(t) = \frac{\sinh\mu \exp[ik(n - x_0) + i\alpha]}{\cosh[\mu(n - x_0)]} \ , \quad (15)$$

where in the unperturbed case $d\mu/dt$=0, dk/dt= 0, dx_0/dt= $(2/\mu)\sinh\mu\sin k$, and $d\alpha/dt$= $2[\cosh(\mu)\cos(k) - 1]$. In Eq. (15) and the subsequent calculations related to Eqs. (13) and (14) we use the normalized variables $t \to t/K$ and $|\psi_n|^2 \to (2K/\lambda)|\psi_n|^2$.

Considering now the right-hand side of Eq. (13) as a perturbation, we can use the perturbation theory based on the inverse scattering transform [25]. For the case of the ALNLS model, the perturbation theory is elaborated in [26]. According to this approach, the parameters of the localized solution (15), 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. [26]. Substituting (14) into those equations and applying the Poisson formula to evaluate the sums appearing as a result of discreteness of our "standard" model, we obtain two coupled equations for the soliton parameters k and x_0:

$$\frac{dx_0}{dt} = \frac{2}{\mu}\sinh\mu \, \sin k \ , \quad (16)$$

$$\frac{dk}{dt} = -\frac{2\pi^3 \sinh^2\mu \, \sin(2\pi x_0)}{\mu^3 \sinh(\pi^2/\mu)} \ , \quad (17)$$

and also $d\mu/dt = 0$. In Eq. (17) we keep only the contribution of the first harmonic because the higher harmonics of the order s will always appear with the additional multipliers $\sim \exp(-\pi^2 s/\mu)$, which are assumed to be small.

The system (16), (17) is Hamiltonian, with

$$H = -\frac{2}{\mu}\sinh\mu \, \cos k - \frac{\pi^2\sinh^2\mu}{\mu^3}\frac{\cos(2\pi x_0)}{\sinh(\pi^2/\mu)} \ ,$$

where the parameters x_0 and k have the sense of the generalized coordinate and momentum, respectively. The first term is the kinetic energy of the effective particle, the second one is a periodic potential, which is, in fact, the periodic PN relief. For consistency with our perturbative approach, we assume the difference between the two models is small, i.e., the parameter μ is assumed to be small, so that the amplitude of the PN potential defined as

$$U_{\mathrm{PN}} = \frac{\pi^2 \sinh^2 \mu}{\mu^3 \sinh(\pi^2/\mu)} \tag{18}$$

is exponentially small in the parameter μ^{-1}. As we can see, the dependence (18) and the periodic potential $U_{\mathrm{PN}} \cos(2\pi x_0)$ are similar to those in the problem for the topological kink in the FK model [1]. As a result, all types of motion of the effective particle are the same as in the case of the FK kink, in particular, the nonlinear mode may be trapped by discreteness, similar to a trapping of a kink [1].

IV. CONCLUSIONS

In conclusion, we have analyzed effects of discreteness on nonlinear localized modes in the lattice NLS models that arise naturally when one studies the analogs of envelope solitons in solid-state applications. We have pointed out that the two kinds of the highly localized nonlinear modes may be viewed as two different states of the same mode being centered either at the particle site or between two neighboring sites. This interpretation allowed us to understand the numerical results on propagating localized modes [16] and results of the stability analysis given in [18]. In particular, we have demonstrated that the discreteness effects on the nonlinear localized modes may be understood as arising from an effective periodic potential similar to the well-known PN potential for topological kinks in the FK model. This PN potential also explains the stability properties of localized modes; in particular, the results that the stable high-frequency mode is centered between neighboring particle sites, whereas the stable low-frequency mode is centered at a particle site. Our analysis further suggests that the existence of this PN-like potential is linked to the nonintegrability of the "standard" NLS model. By studying the discrete *integrable* ALNLS model we have been able to support this suggestion analytically.

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