Nonlinear impurity modes in a lattice

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Discreteness effects on nonlinear impurity modes are discussed in the framework of an approximation given by the integrable lattice nonlinear Schrödinger equation (the so-called Ablowitz-Ladik model). It is shown that the nonlinear impurity mode may be treated as an intrinsic localized mode captured by the impurity. Considering a local impurity in the lattice model as a perturbation, analytical results describing interaction of a nonlinear localized mode (as a soliton in the discrete model) with the impurity are presented. It is shown that discreteness may change the character of the soliton-impurity interaction, e.g., the soliton may be trapped by the impurity which is repulsive in the continuum limit.

As is well known, spatially localized oscillations called localized modes can exist in linear lattices with impurities. The localized mode has maximum at the impurity site and it decreases exponentially as a function of the distance from the impurity. Such a localized impurity mode may exist with the frequency lying in the frequency gap or above the cutoff frequency of the linear spectrum (see, e.g., Refs. 1 and 2). A particle in the lattice oscillates out of phase (e.g., for the light mass impurity) or in phase (e.g., for the heavy mass impurity) with its nearest neighbors. In the presence of small nonlinearity there also exist impurity modes of the similar nature (see, e.g., Ref. 3 and references therein), except that their frequencies depend on the amplitude, and these oscillating states are slowly decaying due to emission of radiation.

Recently the interest to localized modes in strongly anharmonic lattices has been increased mostly due to the paper by Sievers and Takeno who have proposed a new kind of localized mode in a homogeneous lattice with harmonic and anharmonic (quartic) forces between particles. 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 modes have been discussed in a number of papers (see, e.g., Refs. 5–13 to cite a few). The intrinsic localized mode by Sievers and Takeno possesses a property similar to the impurity-induced localized mode, that is, the frequency is above the cutoff frequency of the linear lattice and a particle oscillates out of phase with its nearest neighbors. For sufficiently strong anharmonicity, odd-parity localized excitations are possible at any lattice site, with a frequency which may be found by the Green’s-function technique or by the method developed by Page. The localized pattern is \( u_n(t) = A(..., 0, -\frac{1}{2}, 1, -\frac{1}{2}, 0, ...) \cos(\omega t) \), with the approximation being better for a larger nonlinearity parameter. Some authors have proposed another example of a stationary self-localized mode, i.e., the even-parity localized mode, referred to as a p-like mode. In fact, only the mode with the pattern \( A(..., 0, -1, 1, 0, ...) \cos(\omega t) \), which was first introduced by Page, is extremely stable (see Ref. 13 for more details).

As a matter of fact, an intrinsic localized mode in a homogeneous nonlinear chain looks similar to an impurity mode in an inhomogeneous linear system. Then the natural question is: What happens when the intrinsic localized mode will be excited in an inhomogeneous system, namely, in a chain with an isotopic impurity? As has been recently shown in Ref. 11, the nonlinear oscillation around the impurity, i.e., the so-called nonlinear impurity mode, may be treated as an intrinsic localized mode captured by the impurity. Thus, mobility of intrinsic localized modes in a lattice with impurities is a very important problem to conclude about transport properties of the localized modes. However, the problem of the interaction of the localized mode with an impurity is rather complicated because the primary model used in Ref. 4 has no analytical solution for the case of moving localized modes. Nevertheless, in a recent paper the moving highly localized modes in a perfect lattice have been investigated numerically and they do exist. When one considers inhomogeneous lattices, i.e., those with impurities of a different kind, the absence of analytical solutions for a perfect lattice does not allow one to apply even perturbation theory to analyze the interaction of intrinsic localized modes with impurities. However, trying to take into account only a part of the effects produced by discreteness, one may use an integrable discrete lattice, the so-called Ablowitz-Ladik model, where the moving localized mode is known to be described by an exact soliton solution. This model has already been explored as an effective model for studying properties of the intrinsic localized modes. Thus, it is the purpose of this paper to consider the impurity modes in the Ablowitz-Ladik lattice which takes into account discreteness effects explicitly assuming that the (on-site potential) impurity is small enough, and to analyze the soliton-impurity interaction applying the perturbation theory for solitons.

As has been mentioned above, to understand the main physical properties of nonlinear localized modes in dis-
crete models, we will use, as the first step to show how things are going on, the integrable version of the discrete nonlinear Schrödinger (NLS) equation, the Ablowitz-Ladik model,

\[ i\psi_n + (\psi_{n+1} + \psi_{n-1} - 2\psi_n) + |\psi_n|^2(\psi_{n+1} + \psi_{n-1}) = 0. \]  

(1)

Model (1) can be considered as a discrete but approximate version of the model used by Sievers and Takeno but written for the oscillation envelope. In fact, if we try to derive Eq. (1) from the model of Sievers and Takeno making the "rotating-wave" approximation, the resulting (discrete) equation for the oscillation envelope \( \psi_n \) will be similar to Eq. (1) but not the same. As follows from such an approach, the resulting equation differs from Eq. (1) by the soliton dynamics in the regions \( k \ll 1 \) or \( (\pi - k) \ll 1 \), \( k \) being the wave number of the lattice soliton (see below). The difference is displayed as a small-amplitude Pelsers-Nabarro (PN) potential to the soliton motion which is completely absent for discrete integrable models, and this effective periodic potential is responsible for instability of the Sievers-Takeno mode (corresponding to a maximum of the PN potential) and stability of the Page mode (corresponding to a minimum of the PN potential). However, the Ablowitz-Ladik model has an exact soliton solution describing a moving intrinsically localized soliton, so that it might be used to develop a perturbation theory for discrete lattices, ignoring the PN potential which for this model may be surprisingly small.

Substituting the solution \( \psi_n(t) = A \exp(-i\omega t + ikn) \), where \( k (k = qa) \) is the dimensionless wave number, and neglecting the nonlinear terms, we may find the dispersion relation for linear waves in the lattice model,

\[ \omega = 4 \sin^2 \frac{k}{2}. \]  

(2)

i.e., in these notations the linear spectrum is the frequency band \( 0 \leq \omega \leq 4 \), and the cutoff frequency is equal to 4.

We will consider the perturbed version of Eq. (1) in the form when the inhomogeneity changes the on-site potential, i.e.,

\[ i\psi_n + (\psi_{n+1} + \psi_{n-1} - 2\psi_n) + |\psi_n|^2(\psi_{n+1} + \psi_{n-1}) = V_n \psi_n. \]  

(3)

Without perturbations \( (V_n = 0) \), an exact localized solution of Eq. (3) is found to be of the form

\[ \psi_n(t) = \frac{\sinh \beta \exp[i\omega t + 2i(\cosh \beta \cos k - 1) + i\omega_0]}{\cosh(\beta(n - x_0)) \cdot 2\sin \beta \sin k}. \]  

(4)

As may be easily seen, in the limit \( \beta \rightarrow 0 \) the soliton (4) is transformed into the linear wave with the dispersion law (2). Additionally, in the case of small \( \beta \) and \( k \), when the continuum limit is valid, Eq. (4) gives a soliton of the standard NLS equation.

When the potential \( V_n \) describes a local impurity, i.e., \( V_n = \varepsilon \delta_{n,0} \), the stationary solution of Eq. (3) corresponding to a nonlinear impurity mode may be readily found by matching parts of the stationary soliton \((k = 0)\) for \( \varepsilon = 0 \) having the same frequencies \( \Omega = 2(1 - \cosh \beta) \),

\[ \psi_n(t) = \frac{\sinh \beta e^{-i\omega t}}{\cosh(\beta |n - \xi| - \xi)}, \]  

(5)

where, as may be shown at \( n = 0 \), the parameter \( \xi \) is determined by the simple relation

\[ \sinh \beta \tanh \xi = -\frac{\varepsilon}{2}. \]  

(6)

As follows from Eqs. (5) and (6), for the attractive impurity \( (\varepsilon < 0) \) we have \( \xi > 0 \), i.e., solution (5) has a maximum at \( n = 0 \); for the repulsive impurity \( (\varepsilon > 0) \) it has a minimum at \( n = 0 \) between the two maxima at the sites \( \pm n_{\text{max}} \approx \xi / \beta \). The amplitude of the localized oscillation at the impurity site,

\[ |\psi_0| \equiv B = \frac{\sinh \beta}{\cosh \xi} \]  

(7)

may be used as a physical parameter to compare the results with the linear theory. Substituting Eq. (7) into Eq. (6) and using the expression for the frequency, \( \Omega = 2(1 - \cosh \beta) \), we may obtain the dispersion law for the impurity mode,

\[ \Omega = -2 \left( \sqrt{1 + B^2 + \frac{\varepsilon^2}{4}} - 1 \right), \]  

(8)

which shows that the frequency of the impurity mode lies below the linear spectrum band, i.e., \( \Omega < 0 \).

For \( B^2 \ll 1 \) the result (8) is transformed into that of the linear approximation which is valid when the nonlinear term in Eq. (3) is neglected.

It is important to note that above the cutoff frequency of the linear spectrum a localized nonlinear mode also exists and it may be obtained in an analytical form, too. To find such a nonlinear mode, we note, first of all, that if \( \psi_n(t) \) is a solution of Eq. (3), then the function \( \psi_n(t) = (-1)^n e^{i\omega t} \psi_n(-t) \) will also be a solution of Eq. (3) provided the impurity amplitude \( \varepsilon \) will be replaced by \(-\varepsilon \). Therefore, the localized solution describing the nonlinear impurity mode with the frequency lying above the cutoff frequency has the form [cf. Eq. (5)]

\[ \psi_n(t) = (-1)^n \frac{\sinh \beta e^{-i\omega t}}{\cosh(\beta |n - \xi| - \xi)}, \]  

(9)

where the parameter \( \xi \) is defined by [cf. Eq. (6)]

\[ \sinh \beta \tanh \xi = \frac{\varepsilon}{2}, \]  

(10)

and the dispersion relation for the frequency is also changed to be [cf. Eq. (8)]

\[ \Omega = 2 \left( \sqrt{1 + B^2 + \frac{\varepsilon^2}{4}} + 1 \right), \]  

(11)

where the amplitude at the impurity site, \( B \), is given by the same equation (7). It is clear that \( \Omega > 4 \), i.e., the frequency of the localized mode lies above the cutoff frequency.
The localized solutions similar to those given by Eqs. (5) and (9) were first mentioned by Scharf and Bishop\textsuperscript{16} for another (renormalized) version of the discrete NLS equation. However, they did not investigate the stability of such nonlinear impurity modes. Indeed, if we look at the key formulas we get for the nonlinear impurity modes, Eqs. (8) and (11), we cannot detect any dependence on the sign of the parameter $\epsilon$. However, the localized nonlinear modes have different shapes for $\epsilon > 0$ and $\epsilon < 0$, so that, as will be seen from the analysis given below, this point is the main one for the stability properties of the modes.

To demonstrate the stability properties of the nonlinear impurity modes, we will apply the perturbation theory for solitons\textsuperscript{17} which, for the case of Eq. (3), were elaborated in Ref. 18. The main idea of this approach is to look for a soliton solution in the presence of perturbations using its adiabatic form:

$$
\psi_n(t) = \frac{\sinh \beta \exp[i k (n - x_0) + i \alpha]}{\cosh[\beta (n - x_0)]},
$$

(12)

where the parameters $\beta$, $k$, $x_0$, and $\alpha$ are assumed to be functions of time. General equations describing the perturbation-induced dynamics of the soliton parameters may be found in Ref. 18. Substituting the perturbation $\epsilon f(\psi_n) = V_n \psi_n = \epsilon \delta_{n,0} \psi_n$ into those equations, we conclude that $d \beta / dt = 0$, and the dynamics may be reduced to the following system of two equations:

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

$$
dk \over dt = \frac{\epsilon \sinh^2 \beta \tan h(\beta x_0)}{\cosh^2(\beta x_0) + \sinh^2 \beta}. \tag{14}
$$

In the limit $\beta^2 \ll 1$ and $k^2 \ll 1$, Eqs. (13) and (14) describe the scattering of the NLS soliton in the continuum limit approximation\textsuperscript{17} as a classical particle, and this scattering is characterized by the effective potential

$$
U_{\text{eff}}(x_0) = \frac{2 \epsilon \beta}{\cosh^2(\beta x_0)}. \tag{15}
$$

Therefore, in the continuum limit the interaction of the soliton with the attractive impurity ($\epsilon < 0$) gives rise a bound state with the energy $2 \epsilon \beta$. The frequency of the bound state is negative, i.e., it lies below the linear spectrum band, $\Omega \approx -\beta^2$. In the opposite case, i.e., when $\epsilon > 0$, it may be concluded from Eq. (15) that the stationary solution is unstable and the nonlinear impurity mode does not exist in this limit.

In a general case, when discreteness effects are taken into account by Eqs. (13) and (14), the stationary states are defined by the equations $dx_0 / dt = 0$, $dk / dt = 0$, that yield the critical points $x_0 = 0$ and $\sin k = 0$. The case $k = 2 m \pi$ ($m$ is an integer) corresponds to the localized states which are stable for the attractive impurity ($\epsilon < 0$). The other case, $k = \pi + 2 m \pi$ ($m$ is an integer) corresponds to the local states which are stable only for the repulsive case ($\epsilon > 0$). Looking at solution (12) in the two limit cases, i.e., for $k \ll 1$ and $\pi - k \ll 1$, we may conclude that the first type of equilibrium states is related to the impurity mode (5) which has the frequency lying below the linear spectrum band, so that this mode is stable only for $\epsilon < 0$. The second type of equilibrium states corresponds to the impurity mode (9) having the frequency above the cutoff frequency of the linear spectrum and this nonlinear mode is in fact stable only for $\epsilon > 0$. It is important to note that in this latter case there is no analogy with the continuum limit approximation so that the soliton may be trapped by the repulsive impurity as a result of discreteness effects. It is also necessary to mention here that in the linear theory of impurity modes such a localized state may also exist with the frequency lying above the cutoff frequency provided $\epsilon > 0$.

In conclusion, it has been demonstrated that discreteness effects play an important role in the theory of nonlinear impurity modes. Taking the discrete integrable NLS model as an example, it has been shown analytically that discreteness may change the character of the soliton-impurity interaction allowing the soliton trapping in the case when the impurity is repulsive in the continuum limit. Numerical investigations of the soliton-impurity interactions in the discrete Ablowitz-Ladik lattice are now in progress.\textsuperscript{19}

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