Internal Modes of Solitary Waves

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We develop an analytical approach for describing a birth of internal modes of solitary waves in nonintegrable nonlinear models. We show that a small perturbation of a proper sign to an integrable model can create a soliton internal mode bifurcating from the continuous wave spectrum. The theory is applied to the double sine-Gordon and discrete nonlinear Schrödinger equations, and an excellent agreement with numerical data is demonstrated. [S0031-9007(98)06329-7]

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As is well known, different nonlinear models can possess spatially localized solutions for solitary waves [1]. In many cases, the solitary waves are analyzed in the framework of integrable models which, however, describe realistic physical systems only with certain approximation [2]. Therefore, the fundamental question is the following: *What kind of novel physical effects can be expected for solitary waves in nonintegrable models?* It is commonly believed that solitary waves of nonintegrable models differ from solitons of integrable models only in the character of the soliton interactions: unlike proper solitons, interaction of solitary waves is accompanied by radiation [2]. In this Letter we demonstrate the existence of nontrivial effects of different nature, generic for nearly integrable and nonintegrable models. We show that a small perturbation to an integrable model may create *an internal mode* of a solitary wave. This effect is beyond a regular perturbation theory, because solitons of integrable models do not possess internal modes. But in nonintegrable models such modes introduce *qualitatively new features* into the system dynamics being responsible for long-lived oscillations of the solitary wave shape and resonant soliton interaction.

Until now, internal modes have been analyzed only for the so-called *kink solitons*, topological solitary waves of the Klein-Gordon type models (see, e.g., Refs. [3,4]). The internal modes of kinks, usually called "shape modes," are known to modify drastically the kink dynamics because they can temporarily store energy taken away from the kink's translational motion and later restore the energy back. This mechanism gives rise to resonant structures in the kink-antikink collisions [3] and kink-impurity interactions [5]. In spite of many (basically numerical) results obtained for the kink's internal modes, the important problem still remains unsolved: *What is the analytical criterion for creating the kink's internal mode?*

As a matter of fact, this problem is much more general, and it can be formulated for many soliton bearing physical models. For example, nonlinear propagation of modulated wave packets is often described with the help of *envelope solitons* of the integrable cubic nonlinear Schrödinger (NLS) equation. However, the analysis of self-focusing and propagation of self-guided spatially localized beams (spatial solitons) in plasmas and optical non-Kerr materials requires one to employ the (usually nonintegrable) models more general than the cubic NLS equation [6]. One of the important common features of these solitary waves observed in numerical simulations is that they display long-lived persistent oscillations of their amplitude [7–9]. The similar phenomenon has been found for nonlinear localized modes in discrete lattices [10], where the basic equations can be approximated by the discrete NLS equation and localized modes resemble the envelope solitons involving only a few lattice cites (the so-called *discrete breathers*). Many of the features observed numerically for different types of envelope solitons can be naturally explained in the framework of the concept of the soliton internal mode, generically similar to the kink's shape mode.

In this Letter we suggest *a general analytical approach* allowing one to predict when a perturbation to an integrable model leads to a birth of the soliton internal mode. We derive the results for two customary models, the perturbed sine-Gordon (SG) and NLS equations, explaining many of the features of the soliton dynamics earlier observed only numerically. The analytical method we suggest is generic, and it should work for all soliton models possessing the following properties: a soliton generates a reflectionless potential in an associated linear problem, and the continuous wave spectrum of the linear problem is separated from the discrete spectrum. We conclude therefore that the internal mode is a *fundamental concept* for many nonintegrable soliton models.

Kinks.—First, we consider kinks of the perturbed SG equation,

$$\frac{\partial^2 u}{\partial t^2} - \frac{\partial^2 u}{\partial x^2} + \sin u + \epsilon \hat{g}(u) = 0\,, \qquad (1)$$

where $\hat{g}(u)$ is an operator standing for perturbation (which describes, e.g., a deformation of the sinusoidal potential or the effect of a higher-order dispersion). Assuming ϵ small, we look for the kink solution $u_k(x)$ of Eq. (1) in

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the form of a Taylor series, $u_k(x) = u_k^{(0)}(x) + \epsilon u_k^{(1)}(x) + O(\epsilon^2)$, where $u_k^{(0)}(x) = 4\tan^{-1} e^x$ is the kink solution of the SG equation. The spatially localized correction $u_k^{(1)}(x)$ to the kink's shape can then be found in an explicit form,

$$u_k^{(1)}(x) = \frac{1}{\cosh x} \int_0^x dx' \cosh^2 x' \int_0^{x'} \frac{\hat{g}(u_k^{(0)})}{\cosh x''}\, dx''.$$

To analyze the small-amplitude modes around the kink $u_k(x)$, we linearize Eq. (1) substituting $u(x,t) = u_k(x) + w(x)e^{i\Omega t} + w^*(x)e^{-i\Omega t}$, where Ω is an eigenvalue and $w(x)$ satisfies the linear equation,

$$\frac{d^2 w}{dx^2} + \left(\frac{2}{\cosh^2 x} - 1\right)w + \Omega^2 w + \epsilon \hat{f}(x) w = 0, \quad (2)$$

where$\hat{f}(x) \equiv u_k^{(1)} \sin u_k^{(0)} - \hat{g}'(u_k^{(0)})$.

In the leading order ($\epsilon = 0$), the eigenvalue problem (2) is described by a standard equation with a solvable potential, so that its general solution is presented through a set of eigenfunctions,

$$w(x) = \alpha_{-1} W_{-1}(x) + \int_{-\infty}^{\infty} \alpha(k) W(x,k)\, dk, \quad (3)$$

where the function $W_{-1}(x) = \operatorname{sech} x$ is the eigenmode of the discrete spectrum corresponding to the eigenvalue $\Omega^2 = 0$ (the so-called neutral mode), whereas the eigenfunction $W(x,k) = e^{ikx}(k + i\tanh x)/(k+i)$ describes the continuous wave spectrum with the infinite band of eigenvalues, $\Omega^2 = \Omega^2(k) = (1 + k^2)$. We note that (i) the continuous wave spectrum bands are separated from the eigenvalues of the discrete spectrum and (ii) the eigenfunctions $W(x,k)$ include only one exponential factor in both the limits $x \to \pm\infty$ meaning that the effective potential in Eq. (2) is reflectionless at $\epsilon = 0$. Under the latter condition, the end point of the continuum spectrum band ($k = 0$) belongs to the spectrum and the limiting (nonoscillating) function $W(x,0) = \tanh x$ is not secularly growing.

Now we analyze the perturbed spectral problem (2) in the first-order approximation in ϵ expanding the function $w(x)$ through the set of eigenfunctions; see Eq. (3). First, a perturbation of the effective potential in Eq. (2) should lead to *a deformation* of the eigenfunctions as well as to *a shift* of the eigenvalues of the discrete spectrum. Second, under the conditions (i) and (ii) the perturbation can lead to a birth of *an additional eigenvalue* of the discrete spectrum which bifurcates from the continuum spectrum band.

To find this new eigenvalue, we notice that in the first order in ϵ, a perturbation may shift the cutoff frequency $\Omega_{\min}$ of the phonon band, $\Omega_{\min}^2 = 1 + \epsilon \hat{g}'(0)$. Therefore, to describe a birth of a novel discrete state, we suppose that its eigenvalue detaches from the cutoff frequency, $\Omega^2 = \Omega_{\min}^2 - \epsilon^2\kappa^2$, where κ is the parameter which determines the location of an additional discrete-spectrum eigenvalue, $k_0 = i\epsilon\kappa$. Then, we convert Eq. (2) by means of Eq. (3) into the following integral equation:

$$a(k) = \frac{\epsilon}{2\pi} \int_{-\infty}^{+\infty} \frac{K(k,k') a(k')\, dk'}{k'^2 + \epsilon^2\kappa^2}, \quad (4)$$

where $a(k) = \alpha(k)(k^2 + \epsilon^2\kappa^2)$ and the integral kernel $K(k,k')$ is defined as

$$K(k,k') = \int_{-\infty}^{\infty} W^*(x,k)[\hat{f}(x) + \hat{g}'(0)] W(x,k')\, dk',$$

where $\hat{f}(x)$ and $\hat{g}(x)$ are, in general, operators. To obtain Eq. (4), we have neglected a nonsingular contribution of the discrete spectrum and also used the orthogonality condition,

$$\int_{-\infty}^{\infty} W^*(x,k') W(x,k)\, dx = 2\pi \delta(k' - k).$$

Because the novel eigenvalue bifurcates from the continuum spectrum band $\Omega = \Omega_{\min}$ at $k = 0$, we can construct an asymptotic solution to Eq. (4) for small k by evaluating a singular contribution of the integral, $a(k) = \operatorname{sgn}(\epsilon)(2|\kappa|)^{-1} K(k,0) a(0)$. As a result, we define the parameter κ from the self-consistency condition,

$$|\kappa| = \frac{1}{2}\operatorname{sgn}(\epsilon) \int_{-\infty}^{\infty} \tanh x [\hat{f}(x) + \hat{g}'(0)] \tanh x\, dx. \quad (5)$$

Therefore, the new eigenvalue $k_0 = i\epsilon\kappa$ of the discrete spectrum appears when the right-hand side of Eq. (5) is positive. It follows from Eq. (3) that the corresponding eigenfunction is exponentially localized, $w(x) \to \pm(\pi/\epsilon\kappa) a(0) \exp(\mp\kappa x)$ as $x \to \pm\infty$. This result confirms the observation that a thresholdless birth of the soliton internal mode from the continuum spectrum becomes possible only in those models where solitary waves generate reflectionless potentials in the associated eigenvalue problem. This property is common for many soliton bearing nonlinear models.

As an example of the application of a general result (5), we consider *the double SG equation* following from Eq. (1) at $\hat{g}(u) = \sin(2u)$. The kink's internal mode exists for $\epsilon > 0$, and it was analyzed numerically by Campbell *et al.* [4]. However, it was noticed that the (basically incorrect) analytical method suggested in Ref. [4] does not provide a good agreement with numerical data (see Fig. 16 in Ref. [4]). Applying the asymptotic method presented above, we find the first-order correction to the kink's profile,

$$u_k^{(1)}(x) = 2\left(\frac{x}{\cosh x} - \frac{\sinh x}{\cosh^2 x}\right),$$

and then, using Eq. (5), calculate the discrete eigenvalue, $k_0 = i(8/3)\epsilon$. Therefore, the kink's internal mode is possible only for $\epsilon > 0$, and its frequency is defined by the expansion

$$\Omega^2 = 1 + 2\epsilon - \frac{64}{9}\epsilon^2 + O(\epsilon^3). \quad (6)$$

Figure 1 presents the kink's internal mode of the double SG equation as a function of ϵ, calculated numerically similar to Ref. [4] (dashed curve) and compared with our asymptotic analytical result (solid curve).

Envelope solitons and breathers.—Similar to the kink of the perturbed SG equation, the criterion for the soliton internal mode can also be derived for many other soliton bearing models. As an important example, we consider the case of envelope solitons of the perturbed NLS equation

$$i\,\frac{\partial\psi}{\partial t} + \frac{\partial^2\psi}{\partial x^2} + 2|\psi|^2\psi + \epsilon\hat{g}(|\psi|^2)\psi = 0\,, \qquad (7)$$

where, in general, $\hat{g}(.)$ is an operator. Localized solution of Eq. (7) for solitary waves can be found in the form $\psi(x,t) = \Phi(x)e^{it}$. The real function $\Phi(x)$ is expressed asymptotically as $\Phi(x) = \Phi_0(x) + \epsilon\Phi_1(x) + O(\epsilon^2)$, where $\Phi_0 = \operatorname{sech} x$ is the soliton of the cubic NLS equation, and Φ_1 is a localized correction defined from Eq. (7). The linearized problem for the perturbed NLS equation arises upon the substitution $\psi(x,t) = \{\Phi(x) + [u(x) - w(x)]e^{i\Omega t} + [u^*(x) + w^*(x)]e^{-i\Omega t}\}e^{it}$, and it has the form,

$$\frac{d^2u}{dx^2} + \left(\frac{6}{\cosh^2 x} - 1\right)u + \Omega w + \epsilon\hat{f}_1(x)u = 0\,, \qquad (8a)$$

$$\frac{d^2w}{dx^2} + \left(\frac{2}{\cosh^2 x} - 1\right)w + \Omega u + \epsilon\hat{f}_2(x)w = 0\,, \qquad (8b)$$

where $\hat{f}_1(x) = \hat{g}(\Phi_0^2) + 2\Phi_0^2\hat{g}'(\Phi_0^2) + 12\Phi_0\Phi_1$ and $\hat{f}_2(x) = \hat{g}(\Phi_0^2) + 4\Phi_0\Phi_1$.

The linear eigenvalue problem (8) can be solved exactly at $\epsilon = 0$ (see, e.g., Ref. [11]). Its spectrum consists of two (symmetric) branches of the continuous modes with the eigenvalues $\Omega = \pm\Omega(k) = \pm(1 + k^2)$, and discrete spectrum modes corresponding to the degenerated eigenvalue $\Omega = 0$. Thus, the linear problem (8) meets the requirements of our analytical method for the bifurcation of the internal mode to occur from the continuum spectrum band. For definiteness, we consider the upper branch of the spectrum and suppose that the cutoff frequencies $\Omega_{\min} = \pm 1$ are not affected by the perturbation. Then, the internal mode frequency can be presented in the form, $\Omega_0 = 1 - \epsilon^2\kappa^2$. Applying the analysis similar to that in the case of the perturbed SG kink, we finally obtain the expression for the parameter $|\kappa|$,

$$|\kappa| = \frac{1}{4}\operatorname{sgn}(\epsilon)\int_{-\infty}^{\infty}\{U(x,0)\hat{f}_1(x)U(x,0) + W(x,0)\hat{f}_2(x)W(x,0)\}\,dx\,, \qquad (9)$$

where the nonoscillatory eigenfunctions are defined in the limit $k \to 0$, i.e., $U(x,0) = 1 - 2\operatorname{sech}^2 x$ and $W(x,0) = 1$.

As an important example, we consider the case of the discrete NLS equation usually used as a simple model for discrete breathers [10],

$$i\,\frac{d\psi_n}{dt} + \frac{1}{h^2}(\psi_{n+1} + \psi_{n-1} - 2\psi_n) + 2|\psi_n|^2\psi_n = 0\,, \qquad (10)$$

where h is the lattice spacing. In the continuum limit when the function ψ_n varies slow on the site number n, we derive the perturbed NLS equation (7) with $\epsilon = h^2/12$ and $\hat{g}(|\psi|^2)\psi = \partial^4\psi/\partial x^4$. The correction $\Phi_1(x)$ has the form,

$$\Phi_1(x) = \frac{1}{2}\left(\frac{x\sinh x}{\cosh^2 x} - \frac{7}{\cosh x} + \frac{8}{\cosh^3 x}\right).$$

Calculating the parameter κ from Eq. (9), we find the result $\kappa = 4/3$. Because $\epsilon = h^2/12 > 0$, this means that due to discreteness effect an additional eigenvalue always bifurcates from the continuum spectrum. The asymptotic result for the mode's frequency is $\Omega = 1 - h^4/81$.

To verify this result, we have found numerically, the localized mode of the discrete NLS equation (10) and its internal mode. The symmetry has been imposed, and lattices up to 250 particles as well as quadruple precision have been considered. The numerical determination of the internal mode frequency required a certain strategy to avoid the finite size effects. The localized mode is supposed to decrease like $e^{\kappa j}$, where $\cosh\kappa = 1 + (1 - \Omega)h^2/2$. Then, we look for a self-consistent value of Ω that is an eigenvalue of the matrix defined by discretized Eqs. (8) with the boundary condition $u_{N+1} = u_n e^{-\kappa(\Omega)}$ to interpolate between free and fixed boundary conditions. Numerical data are presented in Fig. 2, together with the analytical asymptotic result.

Therefore, taking into account even a weak discreteness in the NLS model *always leads to a birth of a soliton internal mode*. That is why in discrete lattices solitary waves (the discrete breathers) are observed in many numerical simulations with long-lived almost periodic variations of their amplitude which correspond to the excitation of "breathing" oscillations due to the internal mode [10].

It is interesting to note that the criterion for the existence of a soliton internal mode has an analogy with the famous Peierls problem in quantum mechanics [12] stating that a

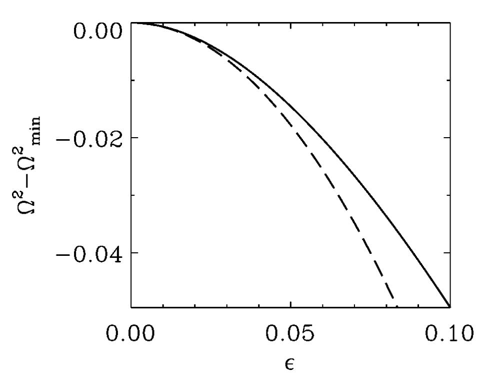

FIG. 1. Frequency Ω^2 of the kink's internal mode in the double SG model. Solid curve: analytical result (6); dashed curve: numerical data. $\Omega_{\min}$ is the cutoff frequency of the continuum spectrum band $\Omega_{\min} = 1 + 2\epsilon$.

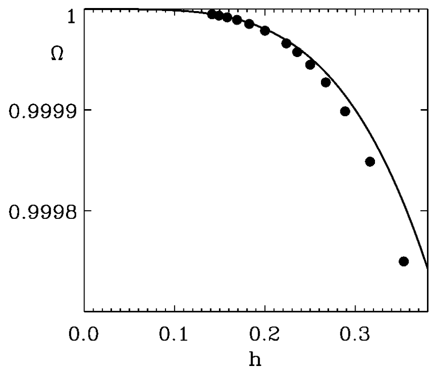

FIG. 2. Frequency Ω of the internal mode for the localized breather of the discrete NLS equation (10) shown as a function of the lattice spacing h. Filled circles: numerical data; solid curve: analytical result.

one-dimensional attractive potential well always possesses at least one discrete eigenvalue. For the case of the soliton internal mode, an additional eigenvalue appears with no threshold provided $\epsilon\kappa > 0$, due to a deformation of the reflectionless soliton potential.

From the viewpoint of the scattering problem, a reflectionless potential corresponds to the transmission coefficient $T(k) = 1/a(k)$ equal to 1 for all k, while in the general case, it tends to zero in the limit $k \rightarrow 0$. This special feature is due to the fact that the zero wave number corresponds to what is called *a half-bound state* and the phase shift of that state is 0. This property is generically not robust against perturbations, and one can expect that a weak perturbation will bring it to a "normal" situation, with a fully reflected zero wave number (with the phase shift π) and, depending on the sign of the perturbation, a bound state under the continuum. This corresponds, in fact, to the problem of the soliton internal mode we have solved above.

Additionally, we would like to mention that the approach suggested above can be readily used to calculate the bifurcations of higher-order soliton modes. As an important physical example, we take into account the discreteness effects in the ϕ^4 model, deriving the perturbed equation of the form, $u_{tt} - u_{xx} - 2u + 2u^3 + \epsilon u_{xxxx} = 0$, where $\epsilon = h^2/12$. Applying our technique, we find that, additionally to the kink shape mode with the frequency $\Omega^3 = 3$, discreteness leads to the emergence of the second localized mode, with the frequency $\Omega^2 = 4 - (4/15)^2 h^4$, that bifurcates from the continuous spectrum band. We have found that this result is in excellent agreement with numerical simulations of the kink spectrum in the discrete ϕ^4 model. The similar result, but in the next order, has been found for the discrete SG model allowing one to explain the mysterious oscillations of the kink shape reported earlier [13].

A birth of the internal mode looks impossible in the cases where the continuum spectrum is not separated from the eigenvalues of the discrete (neutral) modes, as, e.g., in the case of the perturbed Korteweg–de Vries solitons. We expect that in this type of systems the solitary wave dynamics is determined by strong radiation but not by internal modes, unlike the models discussed here.

At last, we would like to mention that the eigenvalues embedded into a continuous spectrum were considered in Refs. [14,15] by means of the Evans function technique. These eigenvalues were shown to lead to real [14] or complex [15] eigenvalues associated with the soliton instabilities. The Evans function technique can also be applied to analyze the problem considered in this Letter.

In conclusion, using two important nonlinear models as characteristic examples, we have shown that there exists *no threshold* for creating an internal mode of a solitary wave. The particular examples display how the internal mode can appear due to either a small deformation of nonlinearity or weak discreteness. We believe the analytical method suggested here is generic, and it can be applied to other problems of this type.

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