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Beyond Nonlinear Schrödinger Equation Approximation for an Anharmonic Chain with Harmonic Long Range Interactions

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Abstract

Multi-scales method is used to analyze a nonlinear differential-difference equation. In the order ϵ^3 the NLS eq. is found to determine the space-time evolution of the leading amplitude. In the next order this has to satisfy a complex mKdV eq. (the next in the NLS hierarchy) in order to eliminate secular terms. The zero dispersion point case is also analyzed and the relevant equation is a modified NLS eq. with a third order derivative term included.

Many one-dimensional systems of biological interest are very complicated structures, formed from complexes of atoms — we shall call them "molecules" — connected by hydrogen bounds. It is usually assumed that only one of the intra-molecular excitations plays an active role in the storage and transport of energy in these systems. In the case of α-helix structure in protein this corresponds to the amide I vibration ($C = O$ stretching). We shall call this intra-molecular excitation the vibronic field. Localized excitations of solitonic type can exist in these systems, due to a nonlinear interaction between the vibronic field and the acoustic phonon field, describing the molecule oscillations along the chain. The simplest model starts from a Fröhlich Hamiltonian and with an ansatz — coherent state approximation — for the state vector describing this type of localized excitation ([1]–[3] and references therein).

After eliminating phonon variables a nonlinear differential (time) — difference (space) equation for the vibronic coordinate is obtained;

$$L(\{y_n\}) = G(\{y_n\}), \tag{1}$$

where L is the linear part and G the nonlinear one. For the specific example we have in mind, originating from Takeno's model [2], L and G are given by

$$L(\{y_n\}) = \frac{d^2 y_n}{dt^2} + \omega_0^2 y_n - \sum_{m \neq n} J_{mn} y_m, \tag{2}$$

$$G(\{y_n\}) = \frac{1}{2} A y_n \left(y_{n+1}^2 + y_{n-1}^2\right) - B y_n^3. \tag{3}$$

In the linear part the last term is a long range interaction between vibrons, and we shall assume that J_{mn} decreases exponentially (Kac–Baker model)

$$J_{mn} = J_{|m-n|} = \omega_{LR}^2 \frac{1-r}{2r} e^{-\gamma|m-n|}, \qquad r = e^{-\gamma}. \tag{4}$$

The first term in r.h.s. of G results from the nonlinear interaction between vibrons and phonons, while the second one from a quartic anharmonicity in the vibron Hamiltonian.

The linear equation admit plane wave solutions $e^{i\theta}$, $\theta = kan - \omega t$, where $\omega(k)$ is given by the dispersion relation

$$\begin{aligned} D(\omega k) &= \omega^2(k) - \left(\omega_0^2 - 2\sum_{p=1}^{\infty} J_p \cos kap\right) \\ &= \omega^2 - \left(\omega_0^2 - \omega_{LR}^2 \frac{1-r}{2r}\left(\frac{\sinh\gamma}{\cosh\gamma - \cos ka} - 1\right)\right) \end{aligned} \tag{5}$$

describing an optical vibrational branch with $\omega^2(k)$ a monotonously increasing function of k from $\omega^2(0) = \omega_0^2 - \omega_{LR}^2$ to $\omega^2\left(\frac{\pi}{a}\right) = \omega_0^2 + \omega_{LR}^2 \frac{1-r}{1+r}$. We shall assume that a no-resonance condition takes place

$$D_\nu = D(\nu\omega, \nu k) \neq 0, \qquad \nu \in N^*, \quad \nu \neq 1. \tag{6}$$

It is well known that the effect of a weak nonlinearity occurs at large space-time scales, determining a redistribution of energy on higher harmonics, and a modulation of amplitude. In order to investigate these effects we shall use the multi-scales method (reductive perturbation method) [4]. The method starts by introducing slow space-time variables

$$x = \epsilon an, \qquad t_j = \epsilon^j t \tag{7}$$

and expanding y_n in an asymptotic perturbative series, which due to the form (3) of the nonlinearity G is given by

$$y_n = \sum_{\nu=1}^{odd} e^{i\nu\theta} \sum_{p=\nu}^{\infty} \epsilon^\nu Y_{p,\nu}(x; t_1, t_2, \ldots) + \text{c.c.} \tag{8}$$

Recently several papers have used this method to discuss the propagation of quasi-monochromatic waves in weakly nonlinear media [5]–[8], or of long surface waves in shallow waters [9]. Very interesting are the conclusions concerning the role played by the NLS hierarchy [8], or the KdV hierarchy [9] in eliminating the secular terms which would destroy the asymptotic character of the perturbative series. Of special interest for the present paper is the reference [8], which will be followed as close as possible.

In calculating the time derivative we have to take into account that t appears in θ as well as in the slow time variables $t_1, t_2, \ldots$. Also in writing the expressions for $y_{n\pm1}, y_m$ we have to expand the corresponding amplitudes around the point n. Taken these precautions the calculations are straightforward (although quite tedious in the higher orders): the asymptotic expansion is introduced in (1), (2), (3) and the coefficient of each power of ϵ and each harmonic $e^{i\nu\theta}$ is equated with zero.

In the first order in ϵ we re-obtain the dispersion relation (5). In the order ϵ^2 the amplitude $Y_{1,1}$ has to satisfy the equation

$$L_+ Y_{1,1} = \left(\frac{\partial}{\partial t_1} + v_g \frac{\partial}{\partial x}\right) Y_{1,1} = 0 \tag{9}$$

and consequently $Y_{1,1}$ will depend only on the variable $\xi = x - vt$, where $v_g = \frac{d\omega}{dk} = \omega_1$ is the group velocity.

In the next order ϵ^3, from the terms proportional with $e^{i\theta}$ we get

$$L_+ Y_{2,1} = \frac{\partial Y_{1,1}}{\partial t_2} - K_2(Y_{1,1}), \tag{10}$$

$$K_2(Y_{1,1}) = i\omega_2 \left(\frac{\partial^2 Y_{1,1}}{\partial \xi^2} \right) + iq|Y_{1,1}|^2 Y_{1,1}. \tag{11}$$

Here $\omega_n = \frac{1}{n!}\frac{d^n\omega}{dk^n}$ and $q = \frac{A}{2\omega}\left(2 + \cos 2ka - 3\frac{B}{A}\right)$. As the r.h.s. of (10) is in the null space of $L_+, Y_{2,1}$ will blow up linearly in t_1 unless the r.h.s. is strictly equal with zero, i.e. $Y_{1,1}$ has to evolve in t_2 according to the cubic nonlinear Schrödinger equation $\left(c = \frac{q}{2\omega_2}\right)$

$$\frac{\partial Y_{1,1}}{\partial t_2} = i\omega_2 \left(\frac{\partial^2 Y_{1,1}}{\partial \xi^2} + 2c|Y_{1,1}|^2 Y_{1,1} \right). \tag{12}$$

In this case $Y_{2,1}$ will depend also on the characteristic coordinate ξ only. From terms proportional with the third harmonic $e^{3i\theta}$ one obtains

$$D_3 Y_{3,3} + (A\cos 3ka - B) Y_{1,1}^3 = 0 \tag{13}$$

and due to the no-resonance condition (6) it is an algebraic equation giving $Y_{3,3}$ in terms of $Y_{1,1}$. The same thing happens for all the higher harmonics and the corresponding amplitudes $Y_{p,\nu}$ can be explicitly written in terms of $Y_{p,1}$ and their derivatives. Therefore we shall concentrate our attention to the amplitudes $Y_{p,1}$, related to the first harmonic $e^{i\theta}$.

The solution of the NLS eq. (12) depends on the sign of ω_2 and q. As ω_1 vanishes at $k = 0$ and $k = \frac{\pi}{a}$, there is a point $k_c \in (0, \pi)$ for which $\omega_2(k_c) = 0$. If $k < k_c (k > k_c)$ we have $\omega_2 > 0 (\omega_2 < 0)$. The sign of q depends on the constants A and B. For $A > 0$ and $B < \frac{A}{3}$ it is always positive, while for $B > A$ it is negative. Depending on the sign of ω_2 and q the NLS eq. (12) can have bright or dark soliton solutions.

In the order ϵ^4 from the terms proportional with $e^{i\theta}$ we get

$$\frac{\partial Y_{2,1}}{\partial t_2} - K_2'(Y_{2,1}) = -\frac{\partial Y_{1,1}}{\partial t_3} + \omega_3 \frac{\partial^3 Y_{1,1}}{\partial \xi^3} - 2c\frac{\omega_1\omega_2}{\omega} Y_{1,1} \frac{\partial |Y_{1,1}|^2}{\partial \xi} + q_1 |Y_{1,1}|^2 \frac{\partial Y_{1,1}}{\partial \xi}. \tag{14}$$

Here

$$K_2'(Y_{1,1}) = i\omega \left(\frac{\partial^2 Y_{2,1}}{\partial \xi^2} + 2c(Y_{1,1}^2 Y_{2,1}^* + 2|Y_{1,1}|^2 Y_{2,1}) \right) \tag{15}$$

is the Frechet derivative of K_2, and $q_1 = \frac{dq}{dk}$. The l.h.s. of (14) is the linearized NLS eq. It is well known that the commuting symmetries σ_j of the NLS eq. are solutions of this equation. As they are important for our further discussion we remained the expression of the first ones (by Ψ we shall denote a solution of the NLS eq.)

$$\begin{aligned} &\sigma_0 = -i\Psi, && \sigma_1 = \frac{\partial \Psi}{\partial \xi}, \\ &\sigma_2 = i\left(\frac{\partial^2 \Psi}{\partial \xi^2} + 2c|\Psi|^2 \Psi \right), && \sigma_3 = -\left(\frac{\partial^3 \Psi}{\partial \xi^3} + 6c|\Psi|^2 \frac{\partial \Psi}{\partial \xi} \right). \end{aligned} \tag{16}$$

The eq. (14) is a forced linear equation for $Y_{2,1}$. It is necessary to identify secular terms in the r.h.s. of (14) and then to fix the t_3 dependence of $Y_{1,1}$ in such a way to eliminate their effect. These secular terms have to be found between the members of the null space of linearized NLS eq., i.e. between the commuting symmetries σ_j. Indeed if such a symmetry σ would exists it will generate a $t_2\sigma$ contribution to $Y_{2,1}$, and the asymptotic character of the expansion (8) would be destroyed in a time $t_2 = O\left(\epsilon^{-1}\right)$. One such symmetry (σ_0, σ_3) is easily seen in the r.h.s. of (14), if it is written in the form

$$-\frac{\partial Y_{1,1}}{\partial t_3}+\omega_3\left(\frac{\partial^3 Y_{1,1}}{\partial\xi^3}+6c|Y_{1,1}|^2\frac{\partial Y_{1,1}}{\partial\xi}\right)+N(Y_{1,1}), \tag{17}$$

where

$$N(Y_{1,1}) = -2c\frac{\omega_1\omega_2}{\omega}Y_{1,1}\frac{\partial|Y_{1,1}|^2}{\partial\xi}+(q_1-6c\omega_3)|\Psi_{1,1}|^2\frac{\partial\Psi_{1,1}}{\partial\xi}.$$

In order to avoid this secular behaviour we require that the t_3 dependence of $Y_{1,1}$ is given by the following complex modified KdV equation

$$-\frac{\partial Y_{1,1}}{\partial t_3}+\omega_3\left(\frac{\partial^3 Y_{1,1}}{\partial\xi^3}+6c|Y_{1,1}|^2\frac{\partial Y_{1,1}}{\partial\xi}\right) = 0 \tag{18}$$

which is the next equation in the NLS hierarchy. The influence of the rest $N(Y_{1,1})$ on $Y_{2,1}$ can be further treated using a Green function formalism [10].

Let us consider a single soliton solution [11]

$$\Psi = 2\frac{P_1}{\sqrt{c}}\frac{e^{-i\phi}}{\cosh z}, \tag{19}$$

$$\phi(\xi,t_2) = 2S_1\xi+4\omega_2\left(S_1^2-P_1^2\right)t_2+\phi_0, \qquad z(\xi,t_2) = 2P_1(\xi-\xi_0+4\omega_2 S_1 t_2),$$

where S_1, P_1 are the real and imaginary part of the complex eigenvalue $\zeta_1 = S_1 + iP_1$ in the inverse scattering transform method, and ϕ_0, ξ_0 are the initial phase and the initial position of the soliton. Applying the above procedure, in order to eliminate the possible secularities, the soliton parameters must be t_3-dependent. This dependence can be found introducing (19) in (18). The complex eigenvalue will remain unchanged, while for ϕ_0, ξ_0 the following linear equations are found [8]

$$\frac{d\phi_0}{dt_3} = -8\omega_3 S_1\left(S_1^2-3P_1^2\right), \qquad \frac{d\xi_0}{dt_3} = -8\omega_3 P_1\left(3S_1^2-P_1^2\right). \tag{20}$$

A similar analysis was given by Kodama [12], and the same results are obtained using the direct perturbation method of Keener and McLaughlin [10]. More complex situations and details will be published elsewhere.

Let us consider now the situation when $\omega_2 = 0$, i.e. the propagation of a wave with the wave vector k_c. As ω_1 has a maximum at this point it represents the wave propagating with the highest group velocity. A similar situation is encountered in the case of pulse propagation in nonlinear optical fibers where this point is known as the "zero dispersion point" (ZDP) [13]–[15]. The power required to generate an optical soliton is minimal in this point, and its evolution in space and time is governed by a modified NLS eq., with a third order derivative included. We shall show that a similar situation appears in the present case.

In applying the multiple scale method we shall use the same asymptotic expansion (8) for the vibronic variable. Then the nonlinearity contribution begins with terms of order ϵ^3. To have contributions of the same order from third order derivatives we have to change the scaling of the ξ variable, namely

$$\xi = \epsilon^{\frac{2}{3}}(an - \omega_1 t). \tag{21}$$

We have to take into account also a dependence of the phase θ of the propagating wave on the slow variable ξ. Defining the local wave number k as the derivative of the phase θ with respect to (an) we find that k is slightly different from k_c, and the simplest choice is

$$k = k_c \left(1 + \epsilon^{\frac{2}{3}}\right). \tag{22}$$

Expanding all the quantities depending on k around the point k_c in the order ϵ^3 the following equation is found for the leading amplitude $Y_{1,1} \to \Psi$,

$$i\Psi_T + 3\Psi_{XX} + i\Psi_{XXX} + Q|\Psi|^2\Psi = 0, \tag{23}$$

where $X = k_c\xi$, $T = \Omega t_2$, $\Omega = \omega_3 k_c^3$ and $Q = \frac{q}{\Omega}$. It has the same form as the equation describing the propagation of nonlinear pulses in optical fibers in the ZDP region [13]–[15]. In our case it makes the transition between the two regions, where bright and dark solitons exist. It seems that it is not completely integrable, but some analytical and numerical results suggest that some long-living localized excitations exist [15]. Further investigations are necessary.

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