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Modulational Instability and Multiple Scales Analysis of Davydov's Model

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The modulational instability (MI) of some discrete nonlinear evolution equations, representing approximations of Davydov's model of α-helix in protein, is studied. In a multiple scales analysis the dominant amplitude usually satisfies the nonlinear Schrödinger equation (NLS), or the Zakharov–Benney equations (ZB), if a long wave-short wave resonance takes place. The MI is studied from a statistical point of view, where a new phenomenon, similar with the Landau damping in plasma physics, can appear for a Lorentzian distribution of the unperturbed Fourier transform of the two-point correlation function.

1 Introduction

Many quasi-one-dimensional molecular systems, especially those of biological interest, are very complicated structures, built from complexes of atoms connected by hydrogen bonds. A typical example is the complex structure of α-helix in protein. It consists of three coupled chains, helically distorted, with hydrogen bonds between the groups of atoms along the chain. It is hard to imagine that a model can be elaborated which could take into account all this complexity. A very simple, but still useful approximation consists in replacing of the three coupled chains by a single straight one. Further from the multitude of the inter- and intra-molecular excitations, only one, corresponding to the amide I oscillations, is taken into account. This is considered to be the "basket" where the energy released in the adenosine triphosphate hydrolysis is stored. The existing dipole-dipole interactions between them provides the mechanism for the transport of these excitonic excitations along the chain. Such an exciton generates a local distortion and a nonlinear coupling between excitons and the acoustic phonon field (describing the harmonic oscillations of the molecules along the chain) appears. The consequence of this nonlinear interaction is generation of robust self-trapped excitations that can transport the energy along the chain. Such a model for storage and transport of energy along the α-helix structure was proposed thirty years ago by Davydov [1–7].

2 Davydov's model

In its simplest form, Davydov's model considers a linear chain of aminoacids – named afterward "molecules" – connected between by hydrogen bonds. If $B_n^+(B_n)$ is the creation (annihilation) operator of the intra-molecular excitation in the n-th cell, the excitonic Hamiltonian can be described by an excitonic Hamiltonian of the form

$$H_{ex} = E_0 \sum B_n^+ B_n - \frac{1}{2} \sum_{mn} J_{mn} B_n^+ B_m,$$

where E_0 is the vibration energy of the $C = O$ group, and J_{mn} the dipole-dipole interaction between two such excitations in the n- and m-th cells. Usually only nearest neighbour interaction is taken into account ($m = n \pm 1$), but also a long range interaction like Kac–Baker model can be considered.

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

The acoustic mode of vibration of the molecules along the chain are described by harmonic Hamiltonian

$$H_{ph} = \frac{1}{2}\sum_n \left(\frac{1}{M}\hat{p}_n^2 + w(\hat{u}_{n+1} - \hat{u}_n)^2\right).$$

M being the mass of the molecule, and w the elastic spring between two neighbouring molecules. The nonlinearity enters in the interaction Hamiltonian

$$H_{int} = \chi \sum_n (\hat{u}_{n+1} - \hat{u}_n) B_n^+ B_n$$

with χ being the phonon-exciton coupling constant. The total Hamiltonian is

$$H = H_{ex} + H_{\text{ph}} + H_{\text{int}}.$$

A coherent state approximation is suitable for describing extended localized states in such systems. For the state vector we shall consider (Davydov ansatz)

$$|\Psi(t)\rangle = \sum_n a_n(t) B_n^+ \exp\left[-\frac{1}{\hbar}\sum_{n'}(\beta_{n'}(t)\hat{p}_{n'} - \pi_{n'}(t)\hat{u}_{n'})\right]|0\rangle,$$

where $a_n(t)$, $\beta_n(t)$, $\pi_n(t)$ are time dependent c-numbers, and $|0\rangle$ is the vacuum state both for excitons and phonons. Using the average value of $\hat{H}$ in the classical equations of motion, one gets

$$i\hbar\dot{a}_n = Ea_n - \sum_p J(a_{n+p} + a_{n-p}) + \chi(\beta_{n+1} - \beta_n)a_n,$$
$$M\ddot{\beta}n - w(\beta_{n+1} - 2\beta_n + \beta_{n-1}) = \chi(|a_n|^2 - |a_{n-1}|^2).$$

With introduction of the relative displacement ρ_n by $\rho_n = \beta_{n+1} - \beta_{n-1}$, the previous equations become

$$i\hbar\dot{a}_n = Ea_n - \sum_{p=1} J_p(a_{n+p} + a_{n-p}) + \chi\rho_n a_n,$$
$$M\ddot{\rho}_n - w(\rho_{n+1} - 2\rho_n + \rho_{n-1}) = \chi(|a_{n+1}|^2 - 2|a_n|^2 + |a_{n-1}|^2).$$

3 Multiple scales method

The multiple scales method is an adequate mathematical method to study long-time evolution of this nonlinear system of coupled equations [8,9]. The classical excitonic variable is written as a Taylor expansion in a small parameter ϵ

$$a_n = e^{i(kln - \omega t)}\epsilon^\alpha \sum_j \epsilon^j A_j(\xi, t_2, t_3, \ldots),$$

where the amplitudes A_j depend only on "slow variables" $(\xi, t_2, t_3, \ldots)$, defined as

$$\xi = \epsilon(ln - v_g t), \quad t_2 = \epsilon^2 t, \quad t_3 = \epsilon^3 t, \quad \ldots.$$

As we shall see and explain below in the non-resonant case $\alpha = 0$, the dominant amplitude A_1 will satisfy the well known nonlinear Schrödinger equation (NLS equation), while in the resonant case we have to take $\alpha = \frac{1}{2}$ and the dominant amplitudes A_1, P_1 will satisfy the Zakharov–Benney equations [10, 11]. For the phononic variable ρ_n we assume an expansion of the form

$$\rho_n = \sum_j \epsilon^{j+1} P_j(\xi, t_2, \dots).$$

Introducing these expansions in the equations of motion for a_n and ρ_n in different orders of ϵ we get:

In order $\epsilon^{1+\alpha}$ we get the dispersion relation

$$\hbar\omega = E - 2\sum_j J_j \cos klj$$

for the linearized system.

In order $\epsilon^{2+\alpha}$ the velocity v_g in the expression of ξ is given by the group velocity (we denote $\omega_n = \frac{1}{n!}\frac{d^n\omega(k)}{dk^n}$)

$$v_g = \omega_1 = \frac{\partial\omega}{\partial k}.$$

The next orders will represent constraints on the amplitudes A_1, P_1, … namely

$$i\frac{\partial A_1}{\partial t_2} + \omega_2 \frac{\partial^2 A_1}{\partial \xi^2} - \frac{\chi}{\hbar} P_1 A_1 = 0 \tag{1}$$

in order $\epsilon^{3+\alpha}$ and

$$(v_g^2 - c_p^2)\frac{\partial^2 P_1}{\partial \xi^2} = \frac{\chi}{M} l^2 \frac{\partial^2}{\partial \xi^2}|A_1|^2 \tag{2}$$

in order ϵ^4. Here by $c_p = \sqrt{\frac{w}{M}}\, l$ we have denoted the sound velocity of the acoustic field.

The non-resonant case will correspond to the situation when $v_g \neq c_p$. Then from (2)

$$P_1 = -\frac{\chi}{w}\frac{1}{1 - \frac{v_g^2}{c_p^2}}|A_1|^2$$

that after substitution into (1) gives

$$i\frac{\partial A_1}{\partial t_2} + \omega_2 \frac{\partial^2 A_1}{\partial \xi^2} + \nu |A_1|^2 A_1 = 0, \tag{3}$$

where $\nu = \frac{\chi^2}{\hbar M}\frac{1}{1-\frac{v_g^2}{c_p^2}}$. This is the well-known NLS equation, a completely integrable system. For $\nu > 0$ (focusing case) it has solitonic solutions. This happens if $v_g < c_p$, and consequently the soliton is a subsonic excitation.

The resonant case corresponds to $v_g \simeq c_p$, and the condition can be realized if the group velocity in the optical branch (excitonic branch) is equal to the phase velocity in the acoustic one. In the multiple scales method we have to go to the order ϵ^5 in the phonon variable, and one obtains

$$\frac{\partial P_1}{\partial t_2} = -\frac{\chi}{2Mv_g} l^2 \frac{\partial |A_1|^2}{\partial \xi}. \tag{4}$$

The system of equations (1) and (4) represents the completely integrable Zakharov–Benney system [10, 11].

In the non-resonant case ($\alpha = 0$), by going to higher order of approximation (ϵ^4) the following equation is obtained [12–19]

$$i\frac{\partial A_2}{\partial t_2} + \omega_2 \frac{\partial^2 A_2}{\partial \xi^2} + \nu(A_1^2 A_2^* + 2|A_1|^2 A_2) = -i\frac{\partial A_1}{\partial t_3} + i\omega_3 \frac{\partial^3 A_1}{\partial \xi^3}. \tag{5}$$

This is a linear non-homogeneous equation for the next amplitude A_2. In the left-hand side we recognize the linearized NLS equation, and the non-homogeneity in the right hand side depends only on the dominant amplitude A_1. It contains the unknown derivative of A_1 with respect to the next slow time t_3. A secular behaviour of this equation is possible if in the rhs we identify some members of the null space (symmetries) of the linearized NLS equation. It is easily seen that the following symmetry appears in the rhs of (5).

$$\sigma_3 = -\left(\frac{\partial^3 A_1}{\partial \xi^3} + 6c|A_1|^2 \frac{\partial A_1}{\partial \xi}\right), \qquad c = \frac{\nu}{2\omega_2}.$$

The secular behaviour is eliminated if the t_3 dependence of A_1 is determined by the equation

$$-\frac{\partial A_1}{\partial t_3} + \omega_3 \left(\frac{\partial^3 A_1}{\partial \xi^3} + 6c|A_1|^2 \frac{\partial A_1}{\partial \xi}\right) = 0 \tag{6}$$

that is the complex modified KdV equation, the next equation in NLS hierarchy. We remain with

$$i\frac{\partial A_2}{\partial t_2} + \omega_2 \frac{\partial^2 A_2}{\partial \xi^2} + \nu\left(A_1^2 A_2^* + 2|A_1|^2 A_2\right) = -6i\omega_3 c|A_1|^2 \frac{\partial A_2}{\partial \xi} \tag{7}$$

which now is a linear non-homogeneous equation free of secularities [18]. In the Appendix both equations (6) and (7) will be solved when A_1 is given by one-soliton solution.

4 Statistical approach of the modulational instability

The modulational instability, also known as the Benjamin–Feir instability [20–23], has proved to be a general process occurring in a large variety of physical situations. The phenomenon is characteristic both for continuous and discrete systems and describes the exponential growth of the amplitude of a (quasi) monochromatic wave propagating in a weakly nonlinear dispersive medium. It is generally believed to be responsible for the formation of robust localized coherent structures in these systems. We shall mainly focus our attention to the NLS equation (3), where $A(X,T)$ is the slowly varying amplitude – considered as a random variable (here X and T are the slow variables of the multiple scales method) and ω_2, ν are the parameters associated with the dispersion (ω_2) and the cubic nonlinearity (ν). One constructs a kinetic equation for the correlation function [24, 25]

$$\rho(X_1, X_2) = \langle A(X_1) A^*(X_2)\rangle,$$
$$\bar{a}^2(X) = \langle A(X) A^*(X)\rangle,$$

namely

$$i\frac{\partial \rho}{\partial t} + \omega_2 \left(\frac{\partial^2}{\partial X_1^2} - \frac{\partial^2}{\partial X_2^2}\right)^2 \rho + 2\nu\left[\bar{a}^2(X_1) - \bar{a}^2(X_2)\right]\rho = 0.$$

Further a Wigner–Moyal transform is used [26, 27]. One introduces the new variables

$$X = \frac{1}{2}(X_1 + X_2), \qquad x = (X_1 - X_2)$$

and the Fourier transform

$$F(k, X, T) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} e^{-ikx}\rho(x, X, T)dx.$$

We obtain

$$\frac{\partial F}{\partial T} + 2\omega_2 k\frac{\partial F}{\partial X} + 4\nu\sum_{n=0}^{\infty}\frac{(-1)^n}{2^{2n+1}(2n+1)!}\frac{\partial^{2n+1}F}{\partial k^{2n+1}}\frac{\partial^{2n+1}\bar{a}^2}{\partial X^{2n+1}} = 0.$$

A linear stability analysis is done considering

$$F(k, X, Y) = F_0(k) + \epsilon F_1(k, X, T),$$
$$\bar{a}^2(X, T) = \bar{a}_0^2 + \epsilon\bar{a}_1^2(X, T),$$
$$\bar{a}_0^2 = \int F_0(k)dk, \qquad \bar{a}_1^2 = \int F_1(k, X, T)dk.$$

The linearized equation for F_1 writes

$$\frac{\partial F_1}{\partial T} + 2\omega_2 k\frac{\partial F_1}{\partial X} + 4\nu\sum_{n=0}^{\infty}\frac{(-1)^n}{2^{2n+1}(2n+1)!}\frac{\partial^{2n+1}F_0}{\partial k^{2n+1}}\frac{\partial^{2n+1}\bar{a}_1^2}{\partial X^{2n+1}} = 0.$$

If a plane wave solution for $F(k, X, T)$ is considered

$$F_1(k, X, T) = f_1(k)e^{i(KX-\Omega T)}.$$

the following integral stability equation is easily found

$$1 + \frac{\nu}{K\omega_2}\int_{-\infty}^{+\infty}\frac{F_0(k+\frac{K}{2}) - F_0(k-\frac{K}{2})}{k - i\lambda}dk = 0. \tag{8}$$

Here we assumed Ω purely imaginary, $\Omega = i\Omega_i$, and $\lambda = \frac{\Omega_i}{2K\omega_2}$. If we assume $\rho_0(x)$ to be an even function of x the previous equation is easily transformed into

$$1 + \frac{i\nu}{K\omega_2}\int_0^x \rho_0(x)e^{-\lambda x}\left(e^{i\frac{K}{2}x} - e^{-i\frac{K}{2}x}\right)dx = 0.$$

Several forms for the initial condition F_0 will be analyzed. As a first example let us consider a δ-spectrum

$$F_0(k) = \bar{a}_0^2\delta(k).$$

It corresponds to a constant initial $\rho_0(x)$. The integration in (8) is straightforward giving

$$\Omega_i = K\omega_2\left(\frac{4\nu}{\omega_2}\bar{a}_0^2 - K^2\right)^{\frac{1}{2}}.$$

An instability exists if both ω_2 and ν have the same sign (this situation corresponds to the focusing case of the NLS equation) and if $K < 2\left(\frac{\nu}{\omega_2}\bar{a}_0^2\right)^{\frac{1}{2}}$. As $\bar{a}_0^2$ is a small quantity this condition corresponds to a "long wave limit". The first condition on the sign of ω_2 and ν is a general one, and we assume it to be satisfied in all the cases we shall discuss. Also we can consider $\nu = 2\omega_2 = 1$, a condition which corresponds to reduction of the NLS equation to the canonical form

$$i\frac{\partial A}{\partial T} + \frac{1}{2}\frac{\partial^2 A}{\partial X^2} + |A|^2 A = 0.$$

The next example is a Lorentzian spectrum

$$F_0(k) = \frac{\bar{a}_0^2}{\pi}\frac{p}{p^2+k^2}, \qquad \rho_0(x) = \bar{a}_0^2 e^{-px}.$$

It is straightforward to show that in this case

$$\Omega_i = K\left(\sqrt{2-\frac{K^2}{4}} - p\right).$$

In this expression it is easily seen that the instability depends also on the correlation length p of the initial distribution, not only of the wave number K. If p is greater than $\sqrt{2-\frac{K^2}{4}}$ the system becomes stable. This is similar with the well-known phenomenon of Landau damping in plasma physics [28].

5 Conclusions

In summary the main conclusions of the present paper are:

- The multiple scales method is used for the analysis of the 1-D Davydov model. It is shown that in the non-resonant case the NLS equation is obtained while in the resonant case the Zakharov–Benney system is found.
- In a higher order approximation, for the non-resonant case, in order for the **secular behavior** to be eliminated the dominant amplitude **has to satisfy** the next equation in the NLS hierarchy (complex mKdV equation).
- The MI of the NLS equation was studied using a statistical approach. As is seen from the Lorentzian case, the statistical properties have a great influence on the development of MI. If the width of the initial 2-point correlation function is too small (p is too large) then the MI is suppressed.

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Appendix

The equation (6) and (7) will be solved when A_1 is the one-soliton solution. With a suitable scaling of the amplitude and the temporal variable ($T = 2\omega_2 t_2$, $\Psi = \sqrt{\frac{\nu}{2\omega_2}}A_1$) the NLS equation (3) can be written in the canonical form

$$i\frac{\partial \Psi}{\partial T} + \frac{1}{2}\frac{\partial^2 \Psi}{\partial \xi^2} + |\Psi|^2\Psi = 0. \tag{A.1}$$

Also with scaling the t_3 variable as $\tau = \omega_3 t_3$ the complex mKdV equation (6) writes

$$-\frac{\partial \Psi}{\partial \tau} + \frac{\partial^3 \Psi}{\partial \xi^3} + 6|\Psi|^2\frac{\partial \Psi}{\partial \xi} = 0.$$

It is convenient to scale the amplitude A_2 in the same way as A_1 ($\phi = \sqrt{\frac{\nu}{2\omega_2}}A_2$) and then equation (7) becomes

$$i\frac{\partial\phi}{\partial T} + \frac{1}{2}\frac{\partial^2\phi}{\partial\xi^2} + (\Psi^2\phi^* + 2|\Psi|^2\phi) = -i\alpha|\Psi|^2\frac{\partial\phi}{\partial\xi}, \qquad \alpha = 3\frac{\omega_3}{\omega_2}. \tag{A.2}$$

The one-soliton solution of the NLS equation (A.1) is

$$\Psi = 2v\frac{e^{-i\Phi}}{\cosh\theta},$$

where

$$\Phi = 2u\xi + 2(u^2 - v^2)T + \Phi_0,$$
$$\theta = 2v(X - X_0 + 2uT).$$

Here u, v are the real and imaginary parts of the eigenvalue of the spectral problem, and they characterize the velocity and the amplitude of the soliton respectively.

As all the equations in the NLS hierarchy have the same spectral problem, the τ dependence in Ψ can appear only in the initial positions and phases, characterizing the unperturbed solution. For the one-soliton solution, only X_0 and Φ_0 will become dependent on τ. It is easy to show that

$$\frac{d\Phi_0}{d\tau} = 8u(u^2 - 3v^2),$$
$$\frac{dX_0}{d\tau} = 4(3u^2 - v^2)$$

leading to a linear dependence of Φ_0 and X_0 on the slow-time variable τ.

Concerning the solution of (A.2), let us consider the case of the solution at rest ($u = 0$). With the new variable $\rho = \tanh 2v\xi$ the equation (A.2) transforms into the equation for the associated Legendre polynomials, with a non-homogeneity in the right hand side, which can be solved exactly [16].

In the simple case of the one-soliton solution we see that in the next order of approximation the initial phase and position of the soliton will depend on the next slow time variable t_3, the effect which cannot be obtained by a perturbation treatment. Also the second amplitude can be determined exactly, and can be expressed through associate Legendre polynomials.

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