phys. stat. sol. (b) **217**, 769 (2000)

Subject classification: 63.20.Kr; 63.20.Ry; 71.35.Aa; S12

Soliton Dynamics in Three Coupled Molecular Chains

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(Received May 14, 1999; in revised form August 10, 1999)

Soliton propagation in three coupled molecular chains is investigated both analytically and numerically. Two different models of initial excitation localized on one or two chains are considered. The condition for a periodic transfer of solitons between the chains is obtained. The dynamics depends on the interchain coupling and the initial number of excitations. The nonlinear interaction stabilizes the soliton evolution.

Die Fortpflanzung von Solitonen in drei gekoppelten Molekülketten wird sowohl analytisch als auch numerisch untersucht. Zwei verschiedene Modelle der Anfangsanregung, wenn sie an einer oder zwei Ketten lokalisiert ist, werden betrachtet. Die Bedingung für eine periodische Übertragung der Solitonen zwischen den Ketten ist abgeleitet. Die Dynamik hängt von der Wechselwirkung zwischen den Ketten und der Anfangsanzahl der Anregungen ab. Die nichtlineare Wechselwirkung stabilisiert die Solitonenevolution.

1. Introduction

Widely investigated are solitary waves in molecular systems with the aim to explain a variety of phenomena. Considerable interest has been devoted to the study of Davydov solitons as a possible mechanism for energy transport in proteins [1 to 10]. It is assumed that the intramolecular excitations form a bound state with the lattice deformation which propagates along the polypeptide chain with constant shape and velocity. More complicated nonlinear interactions including the intramolecular anharmonicity of vibrational excitons (vibrons) have been studied in [3, 8, 9, 11]. Thermal stability [5, 6, 12, 13] and effects of disorder [14, 15] have been considered. The Pauli character of electronic excitons and the resulting kinematical repulsion between them has been taken into account in [3, 16]. Recently, the Davydov approach has been generalized to the propagation of the polaron (self-localized electron) on a two-dimensional lattice in connection to the charge transport in condensed-matter systems [17, 18].

The α-helix structure of protein molecules consists of three spines (chains) of hydrogen bonded peptide groups in the longitudinal direction. Most of the investigations are based on the assumption that they are approximately parallel and independent. The main soliton properties are derived considering the propagation of the amide-I vibration in only one spine. There are suggestions that the coupling between the spines is strong and a model of a dipole–dipole (linear) interchain coupling has been proposed [2]. Analytical and numerical considerations for this case have been performed in [19, 20]. It was pointed out that the three interacting chains can be simulated within a one-chain model with revised parameter values.

In the present paper, we consider a general model for the propagation of intramolecular excitations in a system of three coupled chains. In addition to the linear dipole–dipole interaction a nonlinear interaction between the chains is included. A detailed analysis of the soliton dynamics for different initial excitations is performed. The results can be applied in particular to the propagation of Davydov solitons in proteins.

2. General

We shall consider a system of three parallel chains of molecules described in the Heitler-London approximation by the Hamiltonian

$$H = \hbar\omega_0 \sum_{n,i} A^\dagger_{n,i}A_{n,i} + M \sum_{n,i} (A^\dagger_{n,i}A_{n+1,i} + A^\dagger_{n+1,i}A_{n,i}) + \frac{g_1}{2} \sum_{n,i} A^\dagger_{n,i}A^\dagger_{n,i}A_{n,i}A_{n,i}$$
$$+ d \sum_{n,i} (A^\dagger_{n,i}A_{n,i+1} + A^\dagger_{n,i+1}A_{n,i}) + g_2 \sum_{n,i} A_{n,i}{}^\dagger A^\dagger_{n,i+1}A_{n,i}A_{n,i+1} \,, \tag{1}$$

where $\hbar\omega_0$ is the energy of the intramolecular excitation and $A^\dagger_{n,i}$ ($A_{n,i}$) are the corresponding creation (annihilation) Bose operators at site n on chain i ($i = 1,2$ or 3). M and g_1 are the resonant interaction between neighbouring molecules and the exciton–exciton interaction in the same chain, while d and g_2 describe the linear and nonlinear interactions between the neighbouring chains, respectively.

The form (1) is relevant not only for fixed molecules but also when their motion is taken into account which is important for the Davydov solitons. In this case the Hamiltonian of the system is expressed by [2, 4, 19]

$$H_D = H_{ex} + H_{ph} + H_{int} \,, \tag{2}$$

where H_{ex} is the energy operator for amide-I vibrations including their dipole–dipole interactions, H_{ph} is the operator for the phonon energy and

$$H_{int} = \chi_1 \sum_{n,i} (u_{n+1,i} - u_{n,i})\, A^\dagger_{n,i}A_{n,i} \,, \tag{3}$$

is the exciton–phonon interaction operator, $u_{n,i}$ being the displacement operator for the peptide group at site (n,i). The form (3) gives the change of the amid-I energy located at (n,i) caused by the deformation of the same spine i. We extend the model and include also contributions due to the deformation of the neighbouring spines $i \pm 1$

$$H_{int} = \chi_1 \sum_{n,i} (u_{n+1,i} - u_{n,i})\, A^\dagger_{n,i}A_{n,i} + \chi_2 \sum_{n,i} (u_{n+1,i+1} - u_{n,i+1})\, A^\dagger_{n,i}A_{n,i} \,, \tag{4}$$

supposing that $\chi_2 < \chi_1$. For small displacements of the peptide groups with mass m (harmonic phonon energy H_{ph}) and small soliton velocity v compared with the sound velocity v_0 it holds [19]

$$u_{n+1,i} - u_{n,i} = -\frac{\chi_1}{m(v_0^2 - v^2)}\, A^\dagger_{n,i}A_{n,i} \,. \tag{5}$$

Then substituting (5) in (4) we obtain a Hamiltonian of the form (1), where the nonlinear parameters g_1 and g_2 are proportional to the exciton–phonon coupling constants χ_1 and χ_2, respectively and depend on the soliton velocity.

Using coherent states, the equations of motion for the operators $A_{n,i}$ lead to the following system of coupled nonlinear equations for the vibrational amplitudes $\alpha_{n,i}$:

$$i\hbar \frac{\partial \alpha_{n,i}}{\partial t} = \hbar\omega_0 \alpha_{n,i} + M(\alpha_{n+1,i} + \alpha_{n-1,i}) + d(\alpha_{n,i+1} + \alpha_{n,i-1}) + g_1|\alpha_{n,i}|^2 \alpha_{n,i} + g_2(|\alpha_{n,i+1}|^2 + |\alpha_{n,i-1}|^2)\, \alpha_{n,i} \,. \tag{6}$$

We like to point out that these equations can be obtained by the standard Davydov treatment for zero temperatures where the Hamiltonian (2) is averaged with the wave-function $|D_2\rangle$ [1,4,7]. In this procedure the lattice deformation is considered classically and a set of coupled equations for the vibrational amplitudes $\alpha_{n,i}$ and the average displacements of the peptide groups $\langle u_{n,i}\rangle$ will be obtained. For small soliton velocities (adiabatic approximation) this set can be transform to (6), which allows us to analyze the interchain coupling in greater detail. In the general case of arbitrary soliton velocities one has to consider the whole system of equations.

Note that the interactions between the chains in (6) (linear as well as nonlinear) are symmetrical which is determinated by the arrangement of the spines. The dynamics of the system for $i = 1, 2$ (two-chain model) has been analyzed in details in [21]. The condition for a periodic transfer of a soliton from one chain to the other with a period $t_0 = \pi/d$ was obtained and the influence of the shape of the initial excitation and the nonlinear coupling on the soliton evolution was analyzed. Similar investigations have been performed for optical fibers and waveguide couplers [22,23].

Now we proceed with the three-chain model. First we describe briefly some analytical results. In the continuum limit (6) turns to a system of three coupled nonlinear Schrödinger equations which is completely integrable and has soliton solutions only when $d = 0$ and $g_1 = g_2$ [24]. For $d = g_2 = 0$ the system decomposes into three uncoupled equations which possess separate solutions. The type of the solitons depends on the sign of the ratio M/g_1. In the following part we shall consider the positive sign (bell solitons) which is relevant for the situation in proteins ($M < 0$, $\chi_1 > 0$) and for solitons traveling slowly with respect to the sound speed. For the case $d = 0$ and $g_1 \neq g_2$ (i.e. only the nonlinear coupling between the chains is significant) we find in the semidiscrete approximation the envelope bound state

$$\alpha_1(x,t) = \alpha_2(x,t) = \alpha_3(x,t) = \varphi_0\, e^{i(kx-\omega t)} \operatorname{sech} \frac{x - vt}{L} \tag{7}$$

with

$$\hbar\omega = \hbar\omega_0 + 2M\cos k + \frac{M\cos k}{L^2}\,, \quad \varphi_0^2 = \frac{2M\cos k}{L^2(g_1 + 2g_2)}\,, \quad \hbar v = -2M\sin k\,. \tag{8}$$

This corresponds to a nonlinear excitation with width $2L$ and constant velocity v. The other parameters of the solution: wave number k, energy $\hbar\omega$ and amplitude φ_0 are fully determined by (8).

Further we shall investigate the propagation of solitons for two different initial conditions. The quantity which is conserved in our considerations is the total number of excitations $N_e = N_1(t) + N_2(t) + N_3(t)$, where

$$N_i(t) = \int_{-\infty}^{\infty} |\alpha_i(x,t)|^2 dx \tag{9}$$

is the number of excitations in the i-th chain.

3. One-Soliton Excitation

We investigated numerically the evolution of the soliton formation

$$\alpha_{n,1}(t=0) = \varphi_0 \, e^{ikn} \operatorname{sech} \frac{n}{L}, \qquad \varphi_0 = \frac{1}{L}\sqrt{\frac{2M}{g_1}}, \qquad k = -\frac{\hbar v}{2M} \tag{10}$$

launched initially in one of the chains. Here φ_0 is the amplitude and k the wave number of the fundamental soliton. The quantity N_e has the value $2L\varphi_0^2$. In the linear case the initial excitation jumps periodically to the other two chains with the period $t_0 = 2\pi/3d$ and is equally distributed between them. Note that in contrast to the two-chain model, only a fraction 8/9 of the total excitation number N_e oscillates and the transfer period is shorter.

We performed numerical simulations in the general case ($d \neq 0$, $g_1 \neq g_2$) and studied the conditions for stable soliton transfer. We have obtained that for periodic exchange between the chains the inequality

$$\frac{d_{c1}}{d} \ll 1, \qquad d_{c1} = \left| \frac{5(g_1 - g_2)\, M}{8\sqrt{2}\, g_1 L^2} \right| \tag{11}$$

has to be fulfilled. This means that for a given initial soliton (for a given value of the parameter L) the evolution depends on the linear and nonlinear interchain coupling parameters. For $g_2 = 0$ and small values of d only a part of the particle number N_e smaller than 8/9 is transferred to the other chains. This is insufficient to form solitons and the motion is unstable. If the linear constant exceeds the critical value d_{c1} the exchange between the excited chain and the other two becomes periodic. The transferred number of excitations increases and tends to the value $8/9 N_e$, but this quantity is not enough to form stable solitons. The initial excitation does not retain its shape (Fig. 1). We have chosen the following parameter values $L = 5.75$, $M = -0.1$, $g_1 = -0.005$ for which $d_{c1} = 0.00133$. The length is measured in lattice constants, the time in ω_0^{-1} and the energies in $\hbar\omega_0$.

The inclusion of the nonlinear interaction g_2 stabilizes the soliton dynamics and the period of energy exchange becomes close to t_0. The influence of g_2 in this case is significant and leads to a stable periodic energy redistribution between the three chains.

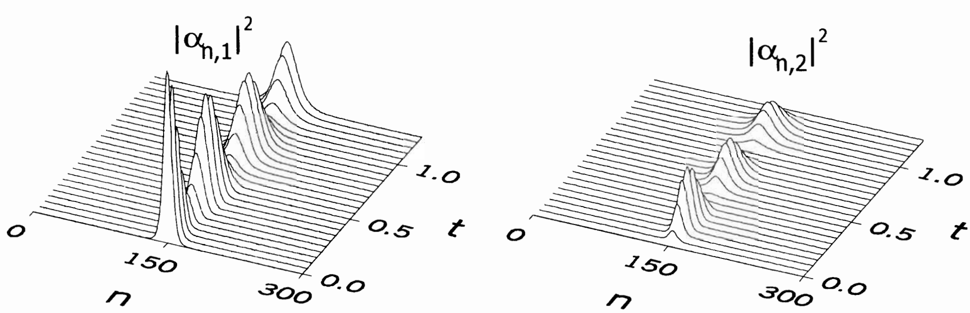

Fig. 1. Time evolution of one soliton excitaton for $d = 0.005$ and $g_2 = 0$. The frame of reference is moving with the soliton velocity v. The picture for $|\alpha_{n,3}|^2$ is identical with that for $|\alpha_{n,2}|^2$. The time t is plotted in $1000\omega_0^{-1}$

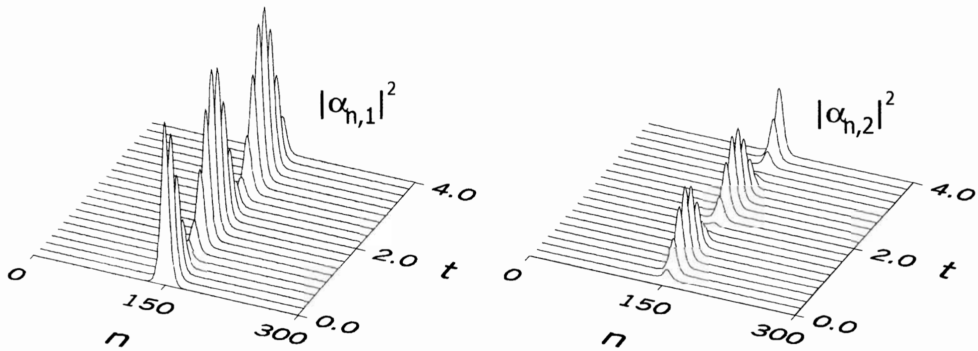

Fig. 2. Stable soliton dynamics for $g_2 = 0.005$ and $d = 0.00125$. The initial condition and the other parameters are the same as in Fig. 1

When $g_1 = g_2$ the inequality (11) is always fulfilled. Independent of the values of the linear coupling coefficient the number of transferred particles from the first chain is $8/9N_e$ and forms two equal solitons in the second and third chains (Fig. 2). The soliton formations are stable and jump back and forth.

The same picture was obtained for arbitrary values of the nonlinear coupling coefficient g_2 and large values of the linear coupling coefficient d. Our numerical results show that for $g_2 = 0.0025$ and $d = 0.005$ the soliton motion is stable also (Fig. 3).

Effects of soliton switching have been observed also in three-core nonlinear fiber couplers [25 to 27]. We would like to point out that this system includes only the linear coupling as the main one between the fibers.

4. Two-Soliton Excitations

We studied the evolution of two-soliton formations

$$\alpha_{n,1}(t = 0) = \alpha_{n,2}(t = 0) = \varphi_0 \, e^{ikn} \operatorname{sech} \frac{n}{L} ,$$
$$\varphi_0 = \frac{1}{L} \sqrt{\frac{2M}{g_1 + g_2}} , \qquad k = -\frac{\hbar v}{2M} , \tag{12}$$

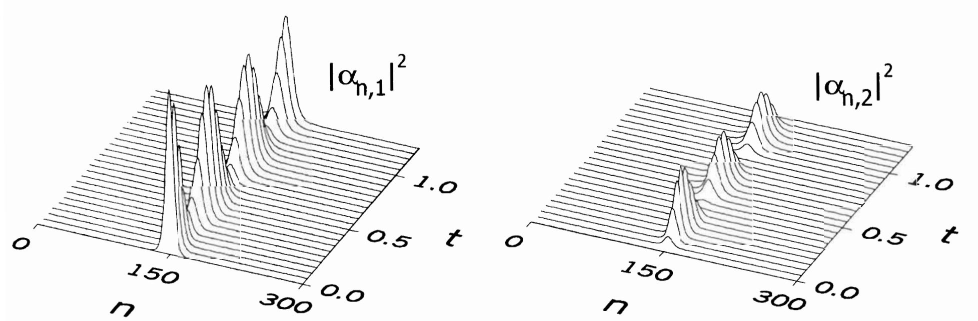

Fig. 3. Stable soliton switching for $g_2 = 0.0025$ and $d = 0.005$. The initial condition and the other parameters are the same as in Fig. 1

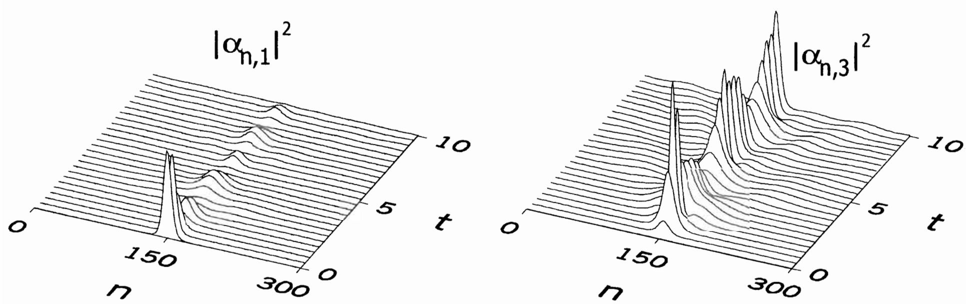

Fig. 4. Evolution of two excited pulses for $g_2 = 0$ and $d = 0.00075$. The pictures for $|\alpha_{n,2}|^2$ and $|\alpha_{n,1}|^2$ are identical. The time t is plotted in $1000\omega_0^{-1}$

which at the initial time are launched in the first and second chains with amplitude φ_0 and wave number k. According to (9) $N_e = N_1(0) + N_2(0)$ with $N_1(0) = N_2(0) = 2L\varphi_0^2$. In the linear case these excitations jump periodically to the third chain with the same period t_0 as in the case of one soliton excitation. Only a portion 8/9 of each excitation $N_1(0)$ and $N_2(0)$ is moved to the third chain and the formed soliton has a particle number $N_3(t_0)$ close to $16/9N_1(0)$, which is bigger than the value for the fundamental soliton and smaller than the value for the two-soliton solution. In the absence of linear coupling and if we have a two-soliton solution it is expected to evolve in a periodic manner with soliton period $t_s = \pi L^2/4|M|$. Such a periodic evolution is destroyed by the linear coupling coefficient and stays unchanged when $d \neq 0$ and t_s coincides with t_0.

As in the early stage for a given value of L the soliton switching results depend on both the linear and the nonlinear interchain coupling parameters. The motion is periodic when the inequality

$$\frac{d_{c2}}{d} \ll 1\,, \qquad d_{c2} = \left|\frac{(g_1 - g_2)\,M}{4\sqrt{2}\,g_1 L^2}\right| \tag{13}$$

is fulfilled.

First we investigate again the case $g_2 = 0$. For values of the linear coupling coefficient near the critical value d_{c2}, almost $8/9N_e$ of the initial number of excitations escapes into the unexcited chain and remains confined there. The main part is localized and the

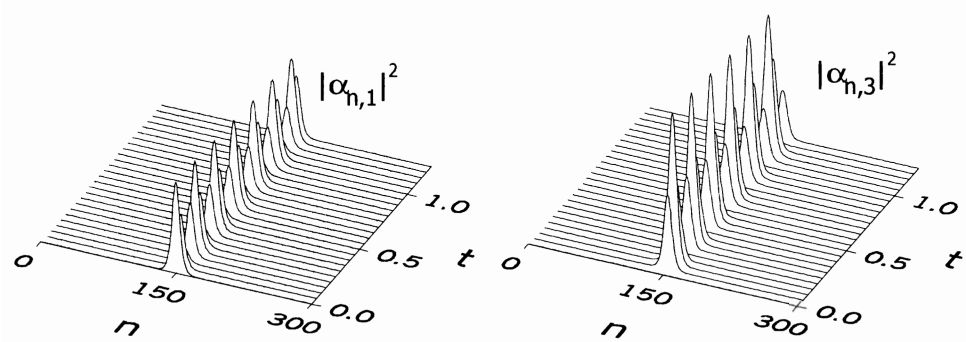

Fig. 5. Soliton switching for $g_2 = 0$ and $d = 0.01$. The initial condition and the other parameters are the same as in Fig. 4

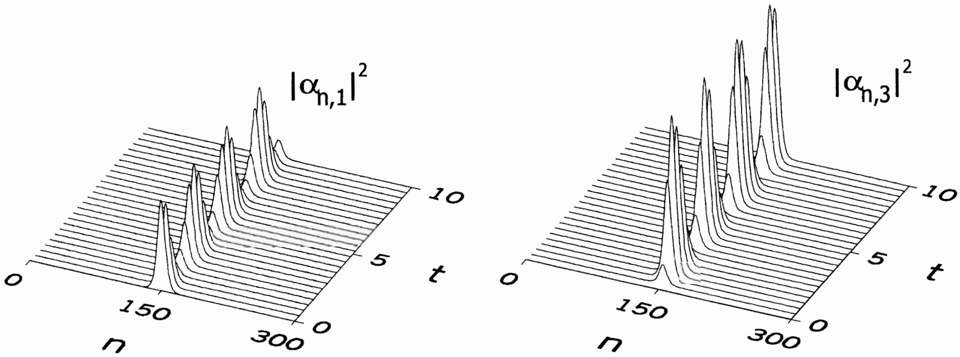

Fig. 6. Stabilized soliton propagation with interchain coupling $d = 0.00075$ and $g_2 = 0.005$. The initial condition and the other parameters are the same as in Fig. 4

rest is radiated. This behaviour is shown in Fig. 4. The numerical simulations are carried out for soliton parameters $L = 5.75$, $M = -0.1$, $g_1 = -0.005$ which lead to $d_{c2} = 0.0005$. The linear coupling coefficient is $d = 0.00075$.

For $d \gg d_{c2}$ the energy couples back and forth between the chains, but radiation is observed again. When d is large and $t_s = t_0$ the total particle number $8/9N_e$ of the third chain goes back to the initial excited chains and we have a stable soliton dynamics (Fig. 5).

As can be seen in Fig. 6 it turns out that the nonlinear interchain coupling stabilizes the evolution picture. For $g_1 = g_2$ in spite of the small value of d and that only portion of the initial N_e is switched, the soliton formations are stable and the motion is periodic.

5. Conclusion

We have investigated the soliton dynamics in three parallel molecular chains for different initial conditions. Depending on the coupling parameters we have different evolution pictures. For relatively small values of the linear coupling coefficient the initial excited solitons can be destroyed with time. For large values of the linear coupling we observe a periodic jump of the solitons between the chains as in [19]. The inclusion of the nonlinear interchain coupling stabilizes significant the soliton dynamics. So for parameter values which are relevant for the α-helix molecule soliton excitations can exist and propagate unchanged.

Acknowledgements We are grateful to Dr. K.T. Stoychev for a critical reading of our manuscript. This work is supported in part by the National Science Foundation of Bulgaria under Grant No. F514 and F810.

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