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# Soliton dynamics in chiral molecular chains with first- and third-neighbour interactions

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**Abstract.** We investigate the propagation and interaction of solitons associated with circularly polarized vibrations in gyrotropic media. The chirality of the structure yields different dispersion laws and hence different phase and group velocities for the left- and right-handed modes. The helical arrangement of the monomers is modelled through first- and third-neighbour interactions. The dynamics of the excitations is governed by a system of coupled discrete nonlinear Schrödinger equations which is studied both analytically and numerically. Depending on the initial conditions and the interaction constants, different evolutionary patterns are obtained corresponding to unbound or bound one- and two-soliton solutions. The results can be applied to the process of energy transfer in helical polymers.

**PACS.** 63.20.Ry Anharmonic lattice modes – 78.20.Ek Optical activity

## 1 Introduction

Solitons in molecular chains have been widely investigated with the aim to explain the mechanism of energy transport in biological systems [1–3]. Complicated models have been considered, involving different nonlinear [4,5] and long-range [6–8] interactions. In [9] a theory of the nonlinear dynamics of pulses of conjugate circularly polarized intramolecular vibrations in gyrotropic molecular crystals was developed. It was shown that the gyrotropy associated with the chiral structure tends to separate the pulses, while the attractive nonlinear cross-interaction tends to lock them together. In the present paper we extend the investigations of [9] taking into account both first- *and* third-neighbour interactions. This model is appropriate for the description of the soliton dynamics in some helical polymers [10].

## 2 Analytical solutions

We start with the Hamiltonian for circularly polarized vibrations in gyrotropic crystals corresponding to the Heitler-London approximation [9]:

$$\begin{aligned} H = {} & \hbar\omega_0 \sum_n (A_n^\dagger A_n + B_n^\dagger B_n) \\ & + \sum_{n,m} [(M_{nm}^s + \mathrm{i}M_{nm}^{as}) A_n^\dagger A_m + (M_{nm}^s - \mathrm{i}M_{nm}^{as}) B_n^\dagger B_m] \\ & + (g_1/2) \sum_n (A_n^\dagger A_n^\dagger A_n A_n + B_n^\dagger B_n^\dagger B_n B_n) \\ & + g_2 \sum_n A_n^\dagger A_n B_n^\dagger B_n \end{aligned} \tag{1}$$

where $\hbar\omega_0$ is the energy of the intramolecular excitation, $A_n^\dagger, A_n$ and $B_n^\dagger, B_n$ are the Bose creation and annihilation operators for right and left circular vibrations at site $n$. $M_{nm}$ are the matrix elements of the intermolecular interaction operator, which contain a symmetric part $M_{nm}^s$ corresponding to the dipole-dipole interaction and an antisymmetric part $M_{nm}^{as}$ emerging from the dipole-quadrupole interaction. Within our model, the latter is responsible for the gyrotropic properties of the system. It can be seen that the intermolecular-interaction terms associated with exchange of right and left circularly polarized vibrations are different and this leads to different phase and group velocities of the two conjugate modes. The anharmonic part of the Hamiltonian contains two terms: the first one $\sim g_1$describes the nonlinear interaction between quasiparticles of the same type and the

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second $\sim g_2$ – an elastic interaction between conjugate quasiparticles in which the energy of each mode (the individual number of quasiparticles) is conserved.

Writing down the equations of motion for the operators $A_n$ and $B_n$, averaging them with the help of on-site coherent states of Glauber-type [9] and introducing first- and third-neighbour interactions

$$\begin{aligned} &M^s_{nn+1} = M^s_{n+1n} = M_1\,, \quad M^{as}_{nn+1} = -M^{as}_{n+1n} = -\gamma_1 \\ &M^s_{nn+3} = M^s_{n+3n} = M_3\,, \quad M^{as}_{nn+3} = -M^{as}_{n+3n} = -\gamma_3 \\ &M_1, M_3, \gamma_1, \gamma_3 - real \end{aligned} \tag{2}$$

the following set of equations for the averaged vibrational amplitudes $\langle A_n\rangle \equiv \alpha_n$ and $\langle B_n\rangle \equiv \beta_n$ has been obtained:

$$\begin{aligned} \mathrm{i}\hbar\frac{\partial\alpha_n}{\partial t} &= \hbar\omega_0\alpha_n + M_1(\alpha_{n+1}+\alpha_{n-1}) - \mathrm{i}\gamma_1(\alpha_{n+1}-\alpha_{n-1}) \\ &\quad + M_3(\alpha_{n+3}+\alpha_{n-3}) - \mathrm{i}\gamma_3(\alpha_{n+3}-\alpha_{n-3}) \\ &\quad + (g_1|\alpha_n|^2 + g_2|\beta_n|^2)\alpha_n\,, \\ \mathrm{i}\hbar\frac{\partial\beta_n}{\partial t} &= \hbar\omega_0\beta_n + M_1(\beta_{n+1}+\beta_{n-1}) + \mathrm{i}\gamma_1(\beta_{n+1}-\beta_{n-1}) \\ &\quad + M_3(\beta_{n+3}+\beta_{n-3}) + \mathrm{i}\gamma_3(\beta_{n+3}-\beta_{n-3}) \\ &\quad + (g_1|\beta_n|^2 + g_2|\alpha_n|^2)\beta_n\,. \end{aligned} \tag{3}$$

The soliton dynamics is determined completely by the system of coupled discrete nonlinear Schrödinger equations (3) which we have studied both analytically and numerically.

Analytical solution of (3) in the case of weak anharmonicity and long pulses, are sought in the form of amplitude-modulated waves with slowly-varying envelopes

$$\begin{aligned} \alpha_n(t) &= \mathrm{e}^{\mathrm{i}(k_1 n - \omega_1 t)}\varphi_n(t) \\ \beta_n(t) &= \mathrm{e}^{\mathrm{i}(k_2 n - \omega_2 t)}\psi_n(t) \end{aligned} \tag{4}$$

where $k_i$ and $\omega_i$ are the wave numbers and the frequencies of the carrier waves (the lattice constant equals unity). Within this semi-discrete approach [6] the system (3) reduces to

$$\begin{aligned} \mathrm{i}\hbar\frac{\partial\varphi}{\partial t} &= (\epsilon_1 - \hbar\omega_1)\varphi + b_1\frac{\partial^2\varphi}{\partial x^2} - \mathrm{i}\frac{\partial\epsilon_1}{\partial k_1}\frac{\partial\varphi}{\partial x} \\ &\quad + (g_1\varphi^2 + g_2\psi^2)\varphi \\ \mathrm{i}\hbar\frac{\partial\psi}{\partial t} &= (\epsilon_2 - \hbar\omega_2)\psi + b_2\frac{\partial^2\psi}{\partial x^2} - \mathrm{i}\frac{\partial\epsilon_2}{\partial k_2}\frac{\partial\psi}{\partial x} \\ &\quad + (g_1\psi^2 + g_2\varphi^2)\psi \end{aligned} \tag{5}$$

where

$$\begin{aligned} \epsilon_i &= \hbar\omega_0 + 2(M_1\cos k_i - (-1)^i\gamma_1\sin k_i \\ &\quad + M_3\cos 3k_i - (-1)^i\gamma_3\sin 3k_i) \\ b_i &= M_1\cos k_i - (-1)^i\gamma_1\sin k_i \\ &\quad + 9(M_3\cos 3k_i - (-1)^i\gamma_3\sin 3k_i)\,, \quad i = 1,2 \end{aligned} \tag{6}$$

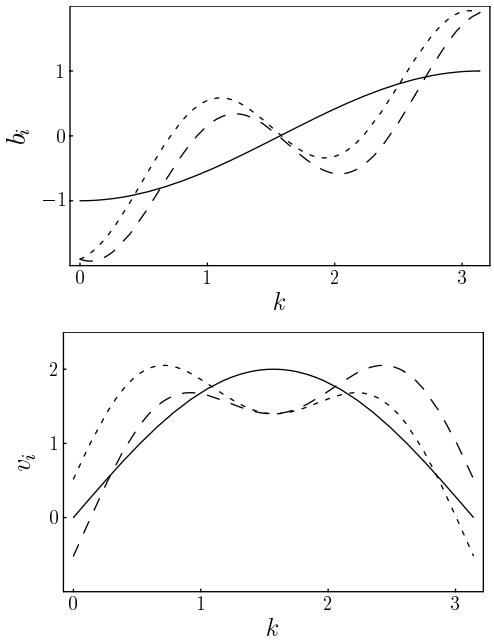


**Fig. 1.** Group-velocity dispersion $b_i$ and velocity $v_i$ for $M_1 = -1$, $M_3 = 0.1M_1$, $\gamma_1 = 0.2$ and $\gamma_3 = 0.1\gamma_1$ ($i = 1$ - dotted line, $i = 2$ - dashed line) and for $M_3 = \gamma_1 = \gamma_3 = 0$ - solid line. The energies are measured in $\hbar\omega_0$, the lengths in lattice constants, and the time in $\omega_0^{-1}$.

are the exciton energy and the group-velocity dispersion, respectively.

Without the cross-interaction terms ($g_2 = 0$), the system (5) decomposes into two uncoupled nonlinear Schrödinger equations for the conjugate circular amplitudes. The sign of the ratio $b_i/g_1$ determines the type of the soliton solutions. In what follows we shall consider positive values which yield bright-soliton solutions of the form:

$$\begin{aligned} \varphi(x,t) &= \varphi_0\mathrm{sech}\frac{x - v_1 t}{L_1}, \qquad \psi(x,t) = \psi_0\mathrm{sech}\frac{x - v_2 t}{L_2} \\ \varphi_0^2 &= \frac{2b_1}{g_1 L_1^2}, \qquad \psi_0^2 = \frac{2b_2}{g_1 L_2^2} \\ \hbar\omega_1 &= \epsilon_1 + \frac{b_1}{L_1^2}\,, \quad \hbar\omega_2 = \epsilon_2 + \frac{b_2}{L_2^2} \\ \hbar v_1 &= -2[M_1\sin k - \gamma_1\cos k + 3(M_3\sin 3k - \gamma_3\cos 3k)] \\ \hbar v_2 &= -2[M_1\sin k + \gamma_1\cos k + 3(M_3\sin 3k + \gamma_3\cos 3k)] \end{aligned} \tag{7}$$

where $\varphi_0, \psi_0$; $L_1, L_2$; and $v_1, v_2$ are the amplitudes, widths and velocities of the two solitons. This solution describes non-interacting conjugate pulses, propagating with equal carrier wave numbers $k_1 = k_2 = k$ and different velocities and shapes.

It is important to note, that due to the factors of, respectively, 9 and 3 in front of the terms $\sim M_3$ and $\sim \gamma_3$ in (6) and (7), the effects of the third-neighbour interactions on the group-velocity dispersion and the velocity are significant (see Fig. 1). This leads to considerable modification of the soliton parameters and even a change of the type of the solution in the regions where this interaction

changes the sign of $b_i$. Comparatively, third-neighbour interactions play a minor role in the exciton energy $\epsilon_i$ (6).

When an attractive elastic nonlinear cross-interaction between the pulses exists ($g_2 < 0$), in the case of small $\Delta k = k_2 - k_1$, the system (5) possesses an analytical solution:

$$\varphi(x,t) = \varphi_0 \mathrm{sech} \frac{x - vt}{L}$$
$$\psi(x,t) = \psi_0 \mathrm{sech} \frac{x - vt}{L} \tag{8}$$

with the following relations between the soliton parameters:

$$\Delta k = 2 \arctan\left(-\frac{\gamma_1 + 3\gamma_3(2\cos 2k_1 - 1)}{M_1 + 9M_3(2\cos 2k_1 - 1)}\right)$$
$$b_1 = b_2 = b\,, \quad \epsilon_1 = \epsilon_2 = \epsilon$$
$$\omega_1 = \omega_2 = \hbar^{-1}\left(\epsilon + \frac{b}{L^2}\right), \quad \varphi_0^2 = \psi_0^2 = \frac{2b}{L^2(g_1 + g_2)}$$
$$v = -2\hbar^{-1}[M_1 \sin k_1 - \gamma_1 \cos k_1 + 3(M_3 \sin 3k_1 - \gamma_3 \cos 3k_1)]\,. \tag{9}$$

The solution (8, 9) describes a soliton bound state which consists of partial pulses with identical shapes and velocities and slightly different carrier wave numbers. Depending on the values of the parameters and on the initial amplitudes, a linearly polarized pulse can evolve to either an unbound or a bound one- or two-soliton solution.

## 3 Numerical results

We have solved numerically the set of discrete equation (3) for different values of the parameters and different initial conditions. Figure 2 illustrates the effects of the discreteness in the case of narrow noninteracting solitons. For $L = 10$ (Fig. 2a) the solution practically coincides with the analytical solution (7). In the case of a shorter pulse however ($L = 5$, Fig. 2b), as the initial condition is not an exact solution, the soliton radiates part of its energy and propagates with a smaller velocity.

In the case of interacting conjugate pulses with $k_1 = k_2 = k$ the evolutionary pattern is controlled by the balance between the kinetic energy of the relative motion of the pulses

$$U_{kin} = -\frac{2(\gamma_1 \cos k + 3\gamma_3 \cos 3k)^2}{M_1 \cos k + 9M_3 \cos 3k} N_e \tag{10}$$

and the potential energy of their elastic interaction

$$U_{pot} = \frac{2}{3} g_2 \varphi_0^2 N_e \tag{11}$$

where

$$N_e = \int_{-\infty}^{\infty} \varphi^2(x,t)\,\mathrm{d}x = \int_{-\infty}^{\infty} \psi^2(x,t)\,\mathrm{d}x \tag{12}$$

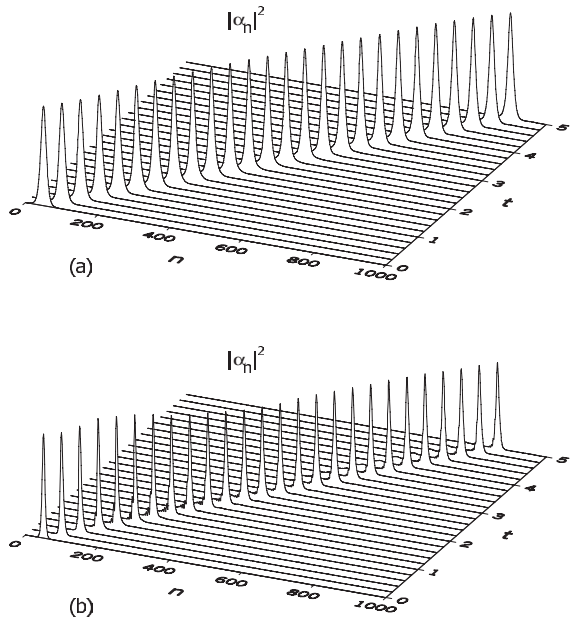


**Fig. 2.** Time evolution of an initial soliton (7) with $M_3 = 0.1M_1$, $M_1 = -0.1$, $\gamma_1 = \gamma_3 = 0$, $g_1 = -0.005$, $g_2 = 0$, and $k = 0.6$ for (a) $L = 10$ and (b) $L = 5$. $t$ is in $1000\omega_0^{-1}$ units.

is the number of excited vibrational quanta of each mode, which has been considered to be one and the same. This corresponds to the physically important case of a linearly polarized initial pulse whose evolution we have studied numerically. The condition for bound soliton states is

$$R = \left|\frac{U_{kin}}{U_{pot}}\right| < 1\,. \tag{13}$$

Due to the third-neighbour interaction terms in the expression for the kinetic energy (10), the condition for bound solutions (13) differs considerably from the corresponding condition for the case of first-neighbour interaction only [9], and the evolutionary patterns in the two cases can be quite different.

In the case of strong gyrotropy and weak elastic cross-interaction, when the kinetic energy dominates over the potential one, an initial linearly-polarized pulse decomposes into two circularly-polarized pulses propagating with different velocities (7). In the opposite case, when the potential energy dominates ($R < 1$), the partial pulses are locked together to form a soliton bound state (Fig. 3). The wave numbers of the pulses are modified according to the analytical solution (9) and the energy in each mode is conserved. The coupling process is accompanied by amplitude and position oscillations of the partial pulses. It can be seen, that third-neighbour interactions (Fig. 3b) modify the shape and the velocity of the coupled soliton solution according to (9).

In the intermediate region ($R \sim 1$), where the kinetic energy nearly equals the potential one, the initial pulse decomposes into two pairs of coupled partial pulses propagating with different relative velocities (Fig. 4). This can be classified as an asymmetric bound two-soliton solution.

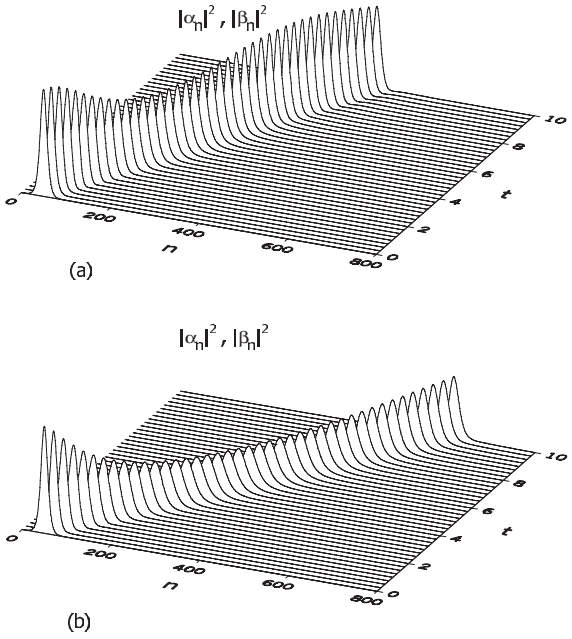


**Fig. 3.** Time evolution of interacting partial pulses with initial $k = 0.2$ into a bound one-soliton state for $\gamma_1 = 0.0035$ and $g_1 = g_2 = -0.005$. (a) $M_3 = \gamma_3 = 0$; (b) $M_3 = 0.05M_1$, $\gamma_3 = 0.05\gamma_1$. $t$ is in $1000\omega_0^{-1}$ units.

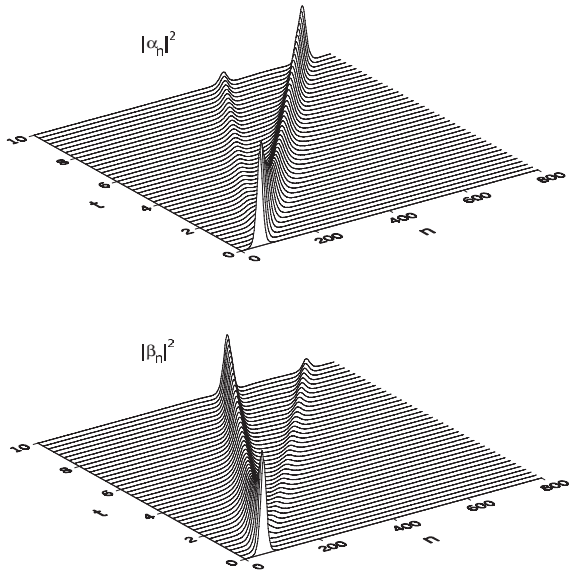


**Fig. 4.** Time evolution of the initial partial pulses into a bound two-soliton state for $\gamma_1 = 0.001$. All other parameters are the same as in Figure 3.

The process can be explained qualitatively in the following way: the potential energy in this case is not sufficient for the coupling of the pulses into a single bound-soliton state and a walk-off effect takes place. However, due to the nonlinear cross-interaction, part of each partial pulse splits off the main pulse in the form of a small-amplitude soliton which is locked to the conjugate large-amplitude soliton. The relative velocity of the two pairs is smaller than that of the uncoupled solution. Weaker initial amplitudes lead to weaker coupling and strongly asymmetric two-soliton bound states and for $R \gg 1$ the evolution corresponds to the uncoupled soliton solution (7).

## 4 Conclusion

We have shown that third-neighbour interactions, which are important in some helical polymers, change significantly the unbound soliton solutions and their parameters. They also modify the condition for bound soliton solutions and their parameters. Depending on the geometry of the helix, second-neighbour interactions may also be important and should be taken into account. In general, the long-range interactions increase effectively the size of the unit cell and the role of the discreteness for narrow solitons. The dynamics of wide solitons is governed by the nonlinear Schrödiger equations in the continuum limit and our results in this case are similar to those for optical solitons in birefringent optical fibers [11].

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## References

1. A.S. Davydov, *Solitons in Molecular Systems* (Reidel, Boston, 1985)
2. A.C. Scott, Phys. Rep. **217**, 1 (1992)
3. T. Dauxois, M. Peyrard, A.R. Bishop, Phys. Rev. E **47**, 684 (1993)
4. X. Wang, D.W. Brown, K. Lindenberg, Phys. Rev. B **39**, 5366 (1989)
5. S. Takeno, J. Phys. Soc. Jpn **59**, 3127 (1990)
6. N. Flitzanis, St. Pnevmatikos, M. Remoissenet, J. Phys. C **18**, 4603 (1985)
7. M. Johansson, Yu.B. Gaididei, P.L. Christiansen, K.Ø. Rasmussen, Phys. Rev. E **57**, 4739 (1998)
8. S.F. Mingaleev, Yu.B. Gaididei, F.G. Mertens, Phys. Rev. E **58**, 3833 (1998)
9. K.T. Stoychev, M.T. Primatarowa, R.S. Kamburova, J. Phys. Cond. Matt. **12**, 10429 (2000)
10. T. Miyazawa, J. Chem. Phys. **32**, 1647 (1960)
11. C.R. Menyuk, J. Opt. Soc. Am. B **5**, 392 (1988); Y.S. Kivshar, J. Opt. Soc. Am. B **7**, 2204 (1990)