Nonlinear effects in molecular chains with two types of intramolecular vibrations

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The influence of a nonlinear spring and nonlinearity in exchange integrals in molecular chains are theoretically investigated in the presence of intramolecular vibrations of two different types. Considering a cubic term in the potential, we show that the anharmonic effect leads to a set of three coupled nonlinear equations (one Boussinesq equation and two nonlinear Schrödinger equations) for which we propose an exact soliton solution. The nonlinearity in the exchange integrals results in two coupled nonlinear Schrödinger equations with saturable nonlinearity. [S1063-651X(96)00306-6]

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I. INTRODUCTION

Interest in physical and mathematical modeling of the molecular systems has been steadily increasing during the last 30 years as it is noticed that solitary waves exist in such system. It was shown that these solitary waves are bound states of the intramolecular excitations (excitons) and the lattice deformation [1,2]. We have proposed a model of two-dimensional molecular crystals [3]. Here, a spatial soliton with a sech profile has been derived in the continuum limit. In a preceding work, the present authors [4] have also studied the influence of a nonlinear spring and nonlinearity in exchange integrals on solitary excitations in one-dimensional molecular chains, in the presence of only one intramolecular coordinate A_n for each molecule. If we were to think about generalizing this model, we would need A_n, B_n, C_n, ... and all these would need to be coupled with each other as well as with the displacements Q_n of the molecules from their equilibrium positions. The purpose of this paper is to extend the treatment of the preceding paper [4], to the case where there exist two different coordinates A_n and B_n which we can solve exactly and propose a soliton solution.

We considered a system where n vibrational excitons belonging to two frequencies of the spectrum are created. In the next section, we introduce an anharmonic cubic potential, we present the basic equations governing the system, and we derive an exact soliton solution. Considering a nonlinearity in exchange integrals, we demonstrate in Sec. III that the system can be described by two coupled nonlinear Schrödinger (NLS) equations with saturable nonlinearity.

II. PHONONS ANHARMONICITY

The Hamiltonian for phonons and excitons interacting in the crystal is given by [1–6]

$$H=H_{\rm ph}+\sum_n J_nA_n^+A_n+\sum_n \tilde{J}_nB_n^+B_n-4I\sum_n A_n^+A_nB_n^+B_n$$
$$+\sum_n M_{n-1n}(A_n^+A_{n-1}+\text{H.c.})$$
$$+\sum_n \tilde{M}_{n-1n}(B_n^+B_{n-1}+\text{H.c.}). \quad (1)$$

In this representation, J_n and $\tilde{J}_n$ are the energies of the two different types of the intramolecular vibrations (excitons) at the nth molecule. M_{n-1n} and $\tilde{M}_{n-1n}$ characterize the interaction between adjacent molecules, due to the two types of excitons, respectively. Otherwise, A_n^+ (B_n^+) and A_n (B_n) denote the creation and annihilation operators of a quantum of A type (B type) excitons at the nth molecule. These operators satisfy the Bose commutation relation.

Taking into account the dipole character of the interactions, we expand the quantities J_n, $\tilde{J}_n$, M_{n-1n}, and $\tilde{M}_{n-1n}$ as follows:

$$J_n\cong J_0-[J_{1L}(Q_n-Q_{n-1})+J_{1R}(Q_{n+1}-Q_n)],$$

$$J_{1L}\equiv\frac{-\partial J_n}{\partial(Q_n-Q_{n-1})},\quad J_{1R}\equiv\frac{-\partial J_n}{\partial(Q_{n+1}-Q_n)},$$

$$\tilde{J}_n\cong\tilde{J}_0-[\tilde{J}_{1L}(Q_n-Q_{n-1})+\tilde{J}_{1R}(Q_{n+1}-Q_n)], \quad (2a)$$

$$\tilde{J}_{1L}\equiv\frac{-\partial \tilde{J}_n}{\partial(Q_n-Q_{n-1})},\quad \tilde{J}_{1R}\equiv\frac{-\partial \tilde{J}_n}{\partial(Q_{n+1}-Q_n)}, \quad (2b)$$

$$M_{nn-1}\cong M_0-M_1(Q_n-Q_{n-1}),\quad M_1\equiv\frac{-\partial M_{nn-1}}{\partial(Q_n-Q_{n-1})}, \quad (2c)$$

$$\tilde{M}_{nn-1}\cong\tilde{M}_0-\tilde{M}_1(Q_n-Q_{n-1}),\quad \tilde{M}_1\equiv\frac{-\partial \tilde{M}_{nn-1}}{\partial(Q_n-Q_{n-1})}. \quad (2d)$$

The form of the Hamiltonian Eq. (1) gives an idea of the behavior of the system. The physical system is a collection of molecules in an orderly array, oscillating about equilibrium position with coordinate Q_n. This type of term gives rise to acoustic modes in the excitation spectrum. In addition, the molecules are capable of internal vibrations described by the second quantized operators A_n and B_n. This second type of motion gives rise to so-called optical modes in the spectrum. The two basic motions are then decorated with various nonlinearities.

Following Zolotaryuk, Spatschek, and Kluth [7], we restrict ourselves only to the symmetric case when $J_{1L}=J_{1R}=J_1$ and $\tilde{J}_{1L}=\tilde{J}_{1R}=\tilde{J}_1$.

Now, the Hamiltonian (1) takes the form

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$$H = H_{\rm ph} + H_{\rm ex} + H_{\rm int}, \tag{3}$$

with

$$H_{\rm ex} = \sum_n (J_0 A_n^+ A_n + \tilde{J}_0 B_n^+ B_n) + \sum_n M_0 (A_n^+ A_{n+1} + \text{H.c.}) + \sum_n \tilde{M}_0 (B_n^+ B_{n+1} + \text{H.c.}) - 4 I A_n^+ A_n B_n^+ B_n, \tag{3a}$$

$$H_{\rm int} = -J_1 \sum_n (Q_{n+1} - Q_{n-1}) A_n^+ A_n + \tilde{J}_1 (Q_{n+1} - Q_{n-1}) \times B_n^+ B_n - M_1 \sum_n (Q_{n+1} - Q_n)(A_n^+ A_{n+1} + \text{H.c.}) - \tilde{M}_1 \sum_n (Q_{n+1} - Q_n)(B_n^+ B_{n+1} + \text{H.c.}). \tag{3b}$$

Equation (3b) describes the interaction, coupling molecular center-of-mass motion and internal vibration amplitudes: the terms $Q_{n(+1)} A_n$ and $Q_{n(+1)} B_n$ describe the mixing of acoustic and optical modes. The terms $Q_{n(+1)} A_n^+ A_{n+1}$ and $Q_{n(+1)} B_n^+ B_{n+1}$ are the higher order terms which have the effect of changing propagation of intramolecular excitations as Q_n amplitudes change. The term $A_n^+ A_n B_n^+ B_n$ in Eq. (3b) describes the coupling between the two coordinates.

In the anharmonic approximation, the energy of the molecules in the chain is

$$H_{\rm ph} = \sum_n \left[\frac{p_n^2}{2M} + \frac{M\omega_0^2}{2!} (Q_{n+1} - Q_n)^2 + \frac{\alpha_0}{3!} (Q_{n+1} - Q_n)^3 \right]. \tag{3c}$$

Let us consider state vectors which are the products of a normalized exciton state and a coherent phonon state

$$|\Psi(t)\rangle = \sum_n [\psi_n(t) A_n^+ + \beta_n(t) B_n^+] |0\rangle_{\rm ex} \exp[-S(t)] |0\rangle_{\rm ph}, \tag{4}$$

with

$$S(t) = \frac{i}{\hbar} \sum_n [u_n(t) p_n - \pi_n(t) Q_n]. \tag{5}$$

The displacements $u_n(t)$ and the amplitudes $\psi_n(t)$ and $\beta_n(t)$ are determined from the Hamiltonian equations

$$i\hbar \frac{\partial \psi_n(t)}{\partial t} = J_0 \psi_n + M_0 (\psi_{n+1} + \psi_{n-1}) - J_1 (u_{n+1} - u_{n-1}) \psi_n - M_1 [(u_{n+1} - u_n) \psi_{n+1} + (u_n - u_{n-1}) \psi_{n-1}] - 4 I \beta_n \beta_n^* \psi_n, \tag{6}$$

$$i\hbar \frac{\partial \beta_n(t)}{\partial t} = \tilde{J}_0 \beta_n + \tilde{M}_0 (\beta_{n+1} + \beta_{n-1}) - \tilde{J}_1 (u_{n+1} - u_{n-1}) \beta_n - \tilde{M}_1 [(u_{n+1} - u_n) \beta_{n+1} + (u_n - u_{n-1}) \beta_{n-1}] - 4 I \psi_n \psi_n^* \beta_n, \tag{7}$$

$$M \frac{\partial^2 u_n(t)}{\partial t^2} = (u_{n+1} + u_{n-1} - 2u_n) \left[M\omega_0^2 + \frac{{}^{\alpha}0}{2} \times (u_{n+1} - u_{n-1}) \right] - M_1 [\psi_n^* (\psi_{n+1} - \psi_{n-1}) + \psi_n (\psi_{n+1}^* - \psi_{n-1}^*)] - \tilde{M}_1 [\beta_n^* (\beta_{n+1} - \beta_{n-1}) + \beta_n (\beta_{n+1}^* - \beta_{n-1}^*)] - J_1 [|\psi_{n+1}|^2 - |\psi_{n+1}|^2] - \tilde{J}_1 [|\beta_{n+1}|^2 - |\beta_{n+1}|^2]. \tag{8}$$

In the continuum limit, these Eqs. (6)–(8) are transformed into

$$i\psi_t = -A_0 \psi_{xx} - \mu \psi + g u_x \psi - \lambda |\beta|^2 \psi, \tag{9}$$

$$i\beta_t = -\tilde{A}_0 \beta_{xx} - \tilde{\mu} \beta + \tilde{g} u_x \beta - \lambda |\psi|^2 \beta, \tag{10}$$

$$u_{tt} = (C_0/M) u_{xx} + (D_0/M)(u_x^2)_x + (E_0/M) u_{4x} + (g_1/M)(|\psi|^2)_x + (\tilde{g}_1/M)(|\beta|^2)_x, \tag{11}$$

with

$$A_0 = -\frac{M_0 a^2}{\hbar}, \quad \mu = -\frac{(J_0 + 2M_0)}{\hbar}, \quad g = -\frac{(M_1 + J_1) a}{\hbar}, \tag{12}$$

$$\tilde{A}_0 = -\frac{\tilde{M}_0 a^2}{\hbar}, \quad \tilde{\mu} = -\frac{(\tilde{J}_0 + 2\tilde{M}_0)}{\hbar}, \quad \tilde{g} = -\frac{(\tilde{M}_1 + \tilde{J}_1) a}{\hbar}, \tag{13}$$

$$E_0 = \frac{M\omega_0^2 a^4}{12}, \quad D_0 = \frac{{}^{\alpha}0 a^3}{2}, \quad C_0 = M\omega_0^2 a^2, \tag{14}$$

$$g_1 = -2(M_1 + J_1) a, \quad \tilde{g}_1 = -2(\tilde{M}_1 + \tilde{J}_1) a, \quad \lambda = \frac{4I}{\hbar}. \tag{15}$$

Differentiating Eq.(11) once with respect to x, and substituting $\eta = u_x$, one obtains the nonlinear master system of equations

$$i\psi_t = -A_0 \psi_{xx} - \mu \psi + g \eta \psi - \lambda |\beta|^2 \psi, \tag{16}$$

$$i\beta_t = -\tilde{A}_0 \beta_{xx} - \tilde{\mu} \beta + \tilde{g} \eta \beta - \lambda |\psi|^2 \beta, \tag{17}$$

$$\eta_{tt} = (C_0/M) \eta_{xx} + (D_0/M)(\eta^2)_{xx} + (E_0/M) \eta_{4x} + (g_1/M)(|\psi|^2)_{xx} + (\tilde{g}_1/M)(|\beta|^2)_{xx}. \tag{18}$$

Let us now look for a solution for this new system of coupled equations. The solutions of (16)–(18) are taken in the form

$$\psi(x,t) = \phi(s) \exp[i(kx - \omega t)], \tag{19}$$

$$\beta(x,t)=\rho(s)\exp[i(\tilde{k}x-\tilde{\omega}t)], \tag{20}$$

$$s=x-vt, \tag{21}$$

where v is the soliton velocity. Inserting Eqs. (19)–(21) into Eqs. (16)–(18), we get

$$\omega\phi=-A_0\phi_{ss}+(A_0k^2-\mu)\phi+g\eta\phi-\lambda\rho^2\phi, \tag{22}$$

$$\tilde{\omega}\rho=-\tilde{A}_0\rho_{ss}+(\tilde{A}_0\tilde{k}^2-\tilde{\mu})\rho+\tilde{g}\eta\rho-\lambda\phi^2\rho, \tag{23}$$

$$\left(v^2-\frac{C_0}{M}\right)\eta=(D_0/M)\eta^2+(E_0/M)\eta_{ss}+(g_1/M)\phi^2+(\tilde{g}_1/M)\rho^2, \tag{24}$$

$$2kA_0-v=0, \tag{25}$$

$$2\tilde{k}\tilde{A}_0-v=0. \tag{26}$$

We assume η to be of the form

$$\eta=N\,\mathrm{sech}^2\left(\frac{s}{\Delta}\right) \tag{27}$$

where N is the amplitude of the pulse soliton and Δ is its width.

The solution is determined by substituting Eq. (27) into Eqs. (22)–(24). We shall suppose M_0, J_1, M_1, $\tilde{M}_0$, $\tilde{J}_1$, and $\tilde{M}_1$ to be negative and restrict our considerations to excitation states lying near the bottom of the vibrational exciton band. We obtain, after some mathematical transformations the following form of the solution:

$$\phi=\phi_0\mathrm{sech}\left(\frac{s}{\Delta}\right), \tag{28}$$

$$\rho=\rho_0\mathrm{sech}^2\left(\frac{s}{\Delta}\right), \tag{29}$$

with

$$\omega+\frac{A_0}{\Delta^2}-A_0k^2+\mu=0, \tag{30a}$$

$$\tilde{\omega}+\frac{4\tilde{A}_0}{\Delta^2}-\tilde{A}_0\tilde{k}^2+\tilde{\mu}=0, \tag{30b}$$

$$\frac{2A_0}{\Delta^2}+gN-\lambda\rho_0^2=0, \tag{30c}$$

$$\frac{6\tilde{A}_0}{\Delta^2}+\tilde{g}N-\lambda\phi_0^2=0. \tag{30d}$$

On the other hand, the normalization condition

$$\int_{-\infty}^{+\infty}(|\psi(x,t)|^2+|\beta(x,t)|^2)\,\frac{dx}{a}=n \tag{31}$$

yields

$$2\phi_0^2+\frac{4}{3}\rho_0^2=\frac{na}{\Delta}, \tag{32}$$

n appears because the whole solitary formation consists of n intramolecular excitations of A and B types.

The expression of the amplitude can be deduced from Eqs. (30c) and (30d)

$$\phi_0^2=\frac{1}{\lambda}\left(\frac{6\tilde{A}_0}{\Delta^2}+\tilde{g}N\right), \tag{33}$$

$$\rho_0^2=\frac{1}{\lambda}\left(\frac{2A_0}{\Delta^2}+gN\right). \tag{34}$$

Combining (33), (34), and (32), we arrive at the following value of the width Δ:

$$\Delta=\frac{2\left(\frac{8A_0}{3}+12\tilde{A}_0\right)}{n\lambda a+\left[n^2\lambda^2a^2-4\left(\frac{8A_0}{3}+12\tilde{A}_0\right)\left(\frac{4gN}{3}+2\tilde{g}N\right)\right]^{1/2}}. \tag{35}$$

The expression of k, $\tilde{k}$, ω, $\tilde{\omega}$ are given by the Eqs. (25) and (26) and (30a) and (30b), respectively.

This solution occurs upon fulfillment of the inequalities

$$2A_0+Ng\Delta^2>0,\quad 6\tilde{A}_0+N\tilde{g}\Delta^2>0,\quad N<0$$
$$\text{and}\ \ n^2\lambda^2a^2>4N\left(\frac{8A_0}{3}+12\tilde{A}_0\right)\left(\frac{4g}{3}+2\tilde{g}\right). \tag{36}$$

This solution is of a great interest for biological systems because it represents soliton of lattice contraction ($\eta<0$). Another possible solution is

$$\phi=\phi_0\mathrm{sech}^2\left(\frac{s}{\Delta}\right),\quad \rho=\rho_0\mathrm{sech}\left(\frac{s}{\Delta}\right),$$

the profile remains the same, the only difference appears in the expression of the parameters of the solution.

The energy which is transferred by a soliton (28) and (29) is expressed by

$$E=E_{\mathrm{ph}}+E_{\mathrm{int}}+E_{\mathrm{ex}}. \tag{37}$$

In the continuum limit, we have

$$E_{\mathrm{ph}}=\int_{-\infty}^{+\infty}\langle\Psi(t)|H_{\mathrm{ph}}|\Psi(t)\rangle\,\frac{dx}{a}, \tag{37a}$$

$$E_{\mathrm{ex}}=\int_{-\infty}^{+\infty}\langle\Psi(t)|H_{\mathrm{ex}}|\Psi(t)\rangle\,\frac{dx}{a}, \tag{37b}$$

$$E_{\mathrm{int}}=\int_{-\infty}^{+\infty}\langle\Psi(t)|H_{\mathrm{int}}|\Psi(t)\rangle\,\frac{dx}{a}. \tag{37c}$$

Substitution of (3a), (3b), (3c) and (4) into (37a), (37b), (37c) yields

$$E_{\rm ph}=\int_{-\infty}^{+\infty}\left[\frac{M}{2}\,(v^2+a^2\omega_0^2)\,\eta^2+\frac{M\omega_0^2}{2}\left(-a^3\,\eta\,\eta_x+\frac{a^4}{3}\,\eta\,\eta_{xx}+\frac{a^4}{4}\,\eta_x^2\right)+\frac{\alpha}{6}\left(a^3\,\eta^3-\frac{3}{2}\,a^4\,\eta^2\,\eta_x\right)\right]\frac{dx}{a}, \tag{38a}$$

$$E_{\rm ex}=\int_{-\infty}^{+\infty}[(J_0+2M_0)|\psi|^2+(\widetilde{J}_0+2\widetilde{M}_0)|\beta|^2-M_0a^2|\psi_x|^2-\widetilde{M}_0a^2|\beta_x|^2-I|\psi|^2|\beta|^2]\,\frac{dx}{a}, \tag{38b}$$

$$E_{\rm int}=-M_1\int_{-\infty}^{+\infty}[2a\,\eta|\psi|^2+a^3(\tfrac{1}{2}\{\eta(|\psi|^2)_x\}_x-\eta|\psi_x|^2+\tfrac{1}{3}\,\eta_{xx}|\psi|^2)]\,\frac{dx}{a}-\widetilde{M}_1\int_{-\infty}^{+\infty}[2a\,\eta|\beta|^2+a^3(\tfrac{1}{2}\{\eta(|\beta|^2)_x\}_x-\eta|\beta_x|^2+\tfrac{1}{3}\,\eta_{xx}|\beta|^2)]\,\frac{dx}{a}-J_1\int_{-\infty}^{+\infty}\left[a\,\eta|\psi|^2+\frac{a^3}{6}\,\eta_{xx}|\psi|^2)\right]\frac{dx}{a}-\widetilde{J}_1\int_{-\infty}^{+\infty}\left[a\,\eta|\beta|^2+\frac{a^3}{6}\,\eta_{xx}|\beta|^2)\right]\frac{dx}{a}. \tag{38c}$$

After integrating these expressions of the energies, we arrive at

$$E_{\rm ph}=\frac{2}{3a}\,(v^2+a^2\omega_0^2)MN^2\Delta+\frac{8\alpha}{45}\,a^2N^3\Delta-\frac{2}{45\Delta}\,MN^2a^3\omega_0^2, \tag{39a}$$

$$E_{\rm ex}=\frac{2}{a}\left[J_0+2M_0-M_0a^2k^2-\frac{64}{15}\,I\Delta\rho_0^2\right]\Delta\,\phi_0^2+\frac{4}{3a}\,[\widetilde{J}_0+2\widetilde{M}_0-\widetilde{M}_0a^2\widetilde{k}^2]\Delta\rho_0^2-\frac{2}{3\Delta}\,M_0a\,\phi_0^2-\frac{16}{15\Delta}\,\widetilde{M}_0a\rho_0^2, \tag{39b}$$

$$E_{\rm int}=\left[\left(\frac{4}{3}\,a^2k^2-\frac{8}{3}\right)\Delta+\frac{28}{45\Delta}\,a^2\right]M_1N\phi_0^2+\left[\left(\frac{16}{15}\,a^2\widetilde{k}^2-\frac{32}{15}\right)\Delta+\frac{64}{63\Delta}\,a^2\right]\widetilde{M}_1N\rho_0^2-\left[\frac{4}{3}\,a\Delta-\frac{8}{45\Delta}\,a^3\right]J_1N\phi_0^2-\left[\frac{16}{15}\,a\Delta-\frac{64}{31\Delta}\,a^3\right]\widetilde{J}_1N\rho_0^2. \tag{39c}$$

Let us now analyze this theory for realistic parameter values. Alpha helix proteins are examples of one-dimensional molecular systems consisting of periodically repeated molecules which interact weakly with one another. Here are the numerical values chosen in this situation when one consider only one type of exciton [8–10].

$$J_0=0.205\ \ \text{eV};\quad M_0=-7.8\ \ \text{cm}^{-1};$$

$$M_1=-10^{-12}\ \ \text{N};\quad J_1=-3.4\times10^{-11}\ \ \text{N}$$

$$M=114\ \ \text{m}_p;\quad v=4.5\times10^3\ \ \text{m/s};\quad v_0=4.6\times10^3\ \ \text{m/s}$$

$$\alpha_0=-4.98\ \ \text{eV/Å}^3;\quad N=-0.789\quad\text{and}\ D=4.5\ \ \text{Å}.$$

To our knowledge, the numerical values associated to the bi-exciton as well as the coupling constant I of the two types of the excitons have not yet been determined. We assume that the parameters of the second coordinate B_n differ from the first ones as follows:

$$\widetilde{M}_0=M_0(1+\varepsilon_1),\quad \widetilde{M}_1=M_1(1+\varepsilon_2),$$

$$\widetilde{J}_1=J_1(1+\varepsilon_3),\quad \widetilde{J}_0=J_0(1+\varepsilon_4),$$

with $\varepsilon_i\ll1,\quad (i=1,2,3,4)$. The above relations avoid the hypothesis of important fluctuations between both types of intramolecular vibrations, and allow a better cohesion of the system.

The solution (27)–(29) propagates along an alpha helix chain and assures the muscular contraction, if ε_1, ε_2, ε_3 and the anharmonicity parameter I are subject to the constraint

$$4{,}5(291.64I^2\times10^{32}+3.14(436.48\times10^{-28}-230.52\times10^{-6}\varepsilon_1)(49.8\times10^{-33}-8.54\times10^4)\{\varepsilon_3+\varepsilon_2\}))^{1/2}+76.85I\times10^{16}-515.84\times10^{-8}+230.52\times10^{14}\varepsilon_1\ll0.$$

This condition arises from the requirement of the continuum approximation $(\Delta\gg D)$.

III. NONLINEARITY IN EXCHANGE INTEGRALS

Now we consider nonlinear effects due to the following expansion of the resonance interactions:

$$M_{nn-1}\cong M_0-M_1(Q_n-Q_{n-1})+M_2(Q_n-Q_{n-1})^2,$$

$$M_1\equiv\frac{-\partial M_{nn-1}}{\partial(Q_n-Q_{n-1})},\quad M_2\equiv\frac{1}{2}\,\frac{\partial^2M_{nn-1}}{\partial(Q_n-Q_{n-1})^2}, \tag{40}$$

$$\widetilde{M}_{nn-1}\cong\widetilde{M}_0-\widetilde{M}_1(Q_n-Q_{n-1})+\widetilde{M}_2(Q_n-Q_{n-1})^2,$$

$$\widetilde{M}_1\equiv\frac{-\partial\widetilde{M}_{nn-1}}{\partial(Q_n-Q_{n-1})},\quad \widetilde{M}_2\equiv\frac{1}{2}\,\frac{\partial^2\widetilde{M}_{nn-1}}{\partial(Q_n-Q_{n-1})^2}. \tag{41}$$

To underline clearly the effects of this type of nonlinearity, we consider a harmonic potential. The equations of motion for the operators ψ_n, β_n and u_n become

$$i\hbar \frac{\partial \psi_n(t)}{\partial t} = J_0\psi_n + M_0(\psi_{n-1}+\psi_{n+1}) - 4I\beta_n^*\beta_n\psi_n - J_1\psi_n(u_{n+1}-u_{n-1}) - M_1[(u_{n+1}-u_n)\psi_{n+1} + (u_n-u_{n-1})\psi_{n-1}] - M_2[(u_{n+1}-u_n)^2\psi_{n+1} + (u_n-u_{n-1})^2\psi_{n-1}], \tag{42}$$

$$i\hbar \frac{\partial \beta_n(t)}{\partial t} = \widetilde{J}_0\beta_n + \widetilde{M}_0(\beta_{n-1}+\beta_{n+1}) - 4I\psi_n^*\psi_n\beta_n - \widetilde{J}_1\beta_n(u_{n+1}-u_{n-1}) - \widetilde{M}_1[(u_{n+1}-u_n)\beta_{n+1} + (u_n-u_{n-1})\beta_{n-1}] - \widetilde{M}_2[(u_{n+1}-u_n)^2\beta_{n+1} + (u_n-u_{n-1})^2\beta_{n-1}], \tag{43}$$

$$M \frac{\partial^2 u_n(t)}{\partial t^2} = M\omega_0^2(u_{n+1}+u_{n-1}-2u_n) - M_1[\psi_n^*(\psi_{n+1} - \psi_{n-1}) + \text{c.c.}] - \widetilde{M}_1[\beta_n^*(\beta_{n+1}-\beta_{n-1}) + \text{c.c.}] - J_1[|\psi_{n+1}|^2 - |\psi_{n-1}|^2] - \widetilde{J}_1[|\beta_{n+1}|^2 - |\beta_{n-1}|^2] - 2M_2[(u_n-u_{n-1})(\psi_n\psi_{n-1}^* + \text{c.c.}) - (u_{n+1}-u_n)(\psi_n\psi_{n+1}^* + \text{c.c.})] - 2\widetilde{M}_2[(u_n-u_{n-1})(\beta_n\beta_{n-1}^* + \text{c.c.}) - (u_{n+1}-u_n)(\beta_n\beta_{n+1}^* + \text{c.c.})]. \tag{44}$$

The continuum equations of motion ($n \to x$) take the form

$$i\psi_t = -A_0\psi_{xx} - \mu\psi + gu_x\psi + g_2(u_x)^2\psi - \lambda|\beta|^2\psi, \tag{45}$$

$$i\beta_t = -\widetilde{A}_0\beta_{xx} - \widetilde{\mu}\beta + \widetilde{g}u_x\beta + \widetilde{g}_2(u_x)^2\beta - \lambda|\psi|^2\beta, \tag{46}$$

$$Mu_{tt} = C_0u_{xx} + g_1(|\psi|^2)_x + \widetilde{g}_1(|\beta|^2)_x + g_3(u_x|\psi|^2)_x + \widetilde{g}_3(u_x|\beta|^2)_x, \tag{47}$$

where

$$g_2 = \frac{2M_2a^2}{\hbar}, \quad g_3 = 4M_2a^2,$$

$$\widetilde{g}_2 = \frac{2\widetilde{M}_2a^2}{\hbar}, \quad \widetilde{g}_3 = 4\widetilde{M}_2a^2. \tag{48}$$

Other parameters are the same as in Sec. II.

In the quasistationary limit, Eqs. (45)–(47) can be reduced to two coupled nonlinear Schrödinger equations with saturable nonlinearity

$$i\psi_t = -A_0\psi_{xx} - \mu\psi - \frac{(d|\psi|^2 + d_0|\beta|^2)\psi}{1+\alpha_1|\psi|^2 + \widetilde{\alpha}_1|\beta|^2}, \tag{49}$$

$$i\beta_t = -\widetilde{A}_0\beta_{xx} - \widetilde{\mu}\beta - \frac{(\widetilde{d}|\beta|^2 + \widetilde{d}_0|\psi|^2)\beta}{1+\alpha_1|\psi|^2 + \widetilde{\alpha}_1|\beta|^2}, \tag{50}$$

with

$$d = \frac{gg_1}{C_0}, \quad d_0 = \lambda + \frac{g\widetilde{g}_1}{C_0}, \quad \alpha_1 = \frac{g_3}{C_0}, \tag{51}$$

$$\widetilde{d} = \frac{\widetilde{g}\,\widetilde{g}_1}{C_0}, \quad \widetilde{d}_0 = \lambda + \frac{\widetilde{g}g_1}{C_0}, \quad \widetilde{\alpha}_1 = \frac{\widetilde{g}_3}{C_0}. \tag{52}$$

Numerical and analytical resolution of the system of Eqs. (49) and (50) should probably bring different types of soliton solutions. This aspect of the problem is under consideration and will be done in a forthcoming paper.

IV. CONCLUDING REMARKS

Solitary excitations play an important role in molecular mechanisms that take place in biological systems. In such systems, where the degrees of freedom are numerous, coupled and influenced by the environment in which the molecule sits, the problem of solving the equations of molecular motion, becomes intractable. The most feasible way is to isolate the ‘‘dominating coordinates’’ and investigate the coupling between these coordinates. This method has been applied to alpha helical proteins by Davydov, where he considered essentially two degrees of freedom.

The present model is an extension of a previous work where we have also considered only two degrees of freedom (one displacement coordinate and one exciton coordinate). Indeed, there exist more than one type of intramolecular vibrations in a real physical nonlinear system. The intramolecular nuclear vibrations are obviously very significant for the explanation of the energy spectrum of the molecular crystals. Thus we have studied in this paper the crucial problem of nonlinearities when two types of excitons belonging to two different frequencies of the spectrum are created. The results obtained here bring important modifications in the equations governing the dynamics of the system. It should be very interesting to propose an exact soliton solution for the coupled NLS equations with saturable nonlinearities (49) and (50), so, the work is still opened.

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