Dynamics of Fermi resonance solitary waves propagating along two interfaces

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The dynamics of Fermi resonance solitary waves propagating along two parallel interfaces in a layered organic semiconductor system is investigated both analytically and numerically. It is shown that the interaction between solitary waves leads to their attraction or repulsion, depending on their initial phase difference. In the case of attraction the solitary waves create a bound state, and their centers oscillate in time with respect to their common mass center. The corresponding period of oscillations is calculated. It is found that the amplitudes and widths of the solitary waves also oscillate in time. [S0163-1829(98)01604-X]

I. INTRODUCTION

The search for organic materials for nonlinear optics, photonics, and electronics promoted the development of methods for the preparation of a class of organic structures, namely, organic crystalline superlattices (OCS). The latest achievements in this field were demonstrated in a number of publications.[1–5] At present, investigations in this direction are developing further, therefore the analysis of qualitatively new properties of OCS is very topical and important. The interaction of OCS with light is a fundamental physical problem, as well as of importance for future applications. Papers[6–10] have been devoted to just such an analysis of these properties of OCS. In particular, different kinds of nonlinear excitations propagating through the superlattice have been discussed (Fermi resonance interface modes,[7] Fermi resonance interface solitary waves[9,10]). Here we want to consider the dynamics of two Fermi resonance solitary waves located on two different interfaces of a three-layer system. For convenience, instead of the term ''solitary waves'' in the following we use the shorter term ''solitons,'' as frequently done in the literature. These solitons interact with each other due to the penetration of the vibrational field of one of them into the location region of the other one. As we shall see, such ''tunnel'' coupling results in a considerable change of the dynamics of the solitons as compared to a single soliton.

Let us consider a system consisting of three layers of organic semiconductors with two interfaces. We suppose that a film with $N+1$ b-molecular layers lies between two ''half-infinite'' crystals made of c molecules. The molecules are labeled as follows: sites $(n_x, n_y, n_z \leqslant -1)$ are occupied by c molecules, sites $(n_x, n_y, 0 \leqslant n_z \leqslant N)$ are occupied by b molecules, and sites $(n_x, n_y, N+1 \leqslant n_z)$ are occupied by c molecules again. As in Refs. 7–10, we assume Fermi resonance between c and b harmonic vibrations, i.e., $\omega_c \simeq 2\omega_b$. For this case the main anharmonic interaction occurs across the interfaces, and has the form

$$\hat{H}_{\rm int} = \Gamma[c_{n_x,n_y,-1}(b^\dagger_{n_x,n_y,0})^2 + c_{n_x,n_y,N+1}(b^\dagger_{n_x,n_y,N})^2 + \text{H.c.}], \quad (1)$$

where Γ is the interaction constant, and $b^\dagger(b)$ and $c^\dagger(c)$ are the creation (annihilation) operators for b and c excitations.

In the limit of strong pumping, i.e., at large excitation occupation numbers, we can neglect the quantum fluctuations and use a classical approximation where all operators are replaced by their mean values $\langle b_{n_x n_y n_z}\rangle = B_{n_x n_y n_z}$ and $\langle c_{n_x n_y n_z}\rangle = C_{n_x n_y n_z}$, where B and C are classical complex vibration amplitudes. These variables corresponding to molecules nearest to the interfaces satisfy the following equations:

$$i\partial C_{n_x,n_y,-1}/\partial t - \omega_c C_{n_x,n_y,-1} - V_{c\perp} C_{n_x,n_y,-2} - V_{c\parallel}(C_{n_x-1,n_y,-1} + C_{n_x+1,n_y,-1} + C_{n_x,n_y-1,-1} + C_{n_x,n_y+1,-1}) - \Gamma B^2_{n_x,n_y,0} = 0, \quad (2)$$

$$i\partial C_{n_x,n_y,N+1}/\partial t - \omega_c C_{n_x,n_y,N+1} - V_{c\perp} C_{n_x,n_y,N+2} - V_{c\parallel}(C_{n_x-1,n_y,N+1} + C_{n_x+1,n_y,N+1} + C_{n_x,n_y-1,N+1} + C_{n_x,n_y+1,N+1}) - \Gamma B^2_{n_x,n_y,N} = 0, \quad (3)$$

$$i\partial B_{n_x,n_y,0}/\partial t - \omega_b B_{n_x,n_y,0} - V_{b\perp} B_{n_x,n_y,1} - V_{b\parallel}(B_{n_x+1,n_y,0} + B_{n_x-1,n_y,0} + B_{n_x,n_y+1,0} + B_{n_x,n_y-1,0}) - 2\Gamma B^*_{n_x,n_y,0} C_{n_x,n_y,-1} = 0, \quad (4)$$

$$i\partial B_{n_x,n_y,N}/\partial t - \omega_b B_{n_x,n_y,N} - V_{b\perp} B_{n_x,n_y,N-1} - V_{b\parallel}(B_{n_x+1,n_y,N} + B_{n_x-1,n_y,N} + B_{n_x,n_y+1,N} + B_{n_x,n_y-1,N}) - 2\Gamma B^*_{n_x,n_y,N} C_{n_x,n_y,N+1} = 0, \quad (5)$$

where the parameters $V_{b\perp}$ and $V_{b\parallel}$ ($V_{c\perp}$ and $V_{c\parallel}$) describe the intermolecular interactions between the b (c) molecules in directions perpendicular and parallel to the interface, respectively. The vibrations in the bulk of the crystals obey the usual linear equations (see Refs. 9 and 10). The described system has the following interface solutions,[10] localized near the interface:

$$C_{n_x n_y n_z} = C_1(n_x, n_y) e^{\kappa_c (n_z+1)}, \quad n_z \leqslant -1,$$

$$C_{n_x n_y n_z} = C_2(n_x, n_y) e^{\kappa_c (1+N-n_z)}, \quad n_z \geqslant N+1, \tag{6}$$

and

$$B_{n_x n_y n_z} = \frac{B_1(n_x, n_y)\sinh[\kappa_b(N-n_z)] + B_2(n_x, n_y)\sinh(\kappa_b n_z)}{\sinh(\kappa_b N)} \quad (N \geqslant 0), \tag{7}$$

where κ_b and κ_c are given by

$$e^{\kappa_c} = \frac{\Gamma}{V_{c\perp}} \frac{|B|^2}{|C|}, \quad e^{\kappa_c} = \frac{2\Gamma}{V_{b\perp}} |C|. \tag{8}$$

These expressions hold exactly for the plane-wave solution, but we shall assume their validity for sufficiently wide soliton excitations in the case of strong anisotropy of intermolecular interaction $V_{b,c\perp} \ll V_{b,c\parallel} \equiv V_{b,c}$, too.

We suppose that the variables $B_j(n_x, n_y)$ and $C_j(n_x, n_y)$ do not depend on n_y and have a slow dependence on n_x. In this long wave limit we can replace the finite differences in Eqs. (2)–(5) by derivatives ($n_x \to x$) and arrive at the following system (the dimensionless variable x is measured in units of the lattice constant) of partial differential equations:

$$i\frac{\partial B_j}{\partial t} - \tilde{\omega}_b B_j - V_b \frac{\partial^2 B_j}{\partial x^2} - 2\Gamma B_j^* C_j = \epsilon B_l, \quad j,l = 1,2, \quad j \neq l, \tag{9}$$

$$i\frac{\partial C_l}{\partial t} - \tilde{\omega}_c C_l - V_c \frac{\partial^2 C_l}{\partial x^2} - \Gamma B_l^2 = 0, \quad l = 1,2, \tag{10}$$

where

$$\tilde{\omega}_b = \omega_b + V_b\left(4 + \frac{\sinh[(N-1)\kappa_b]}{\sinh(N\kappa_b)}\right),$$

$$\tilde{\omega}_c = \omega_c + V_c(4 + e^{-\kappa_c}), \tag{11}$$

$$\epsilon = V_{b\perp} \frac{\sinh(\kappa_b)}{\sinh(N\kappa_b)}. \tag{12}$$

When the parameter ϵ, describing the interaction of vibrations located in different interfaces, is small, this interaction can be considered as a perturbation. If we neglect it we arrive at the situation of two independent interfaces. In each of the two interfaces the soliton excitations found in Ref. 9 exist. Exact solutions for such solitons can be obtained in some particular cases. For solitons at rest, we have the expressions

$$B = \frac{|\alpha| e^{-i\omega t/2}}{\cosh^2(\kappa x)}, \quad C = \frac{\alpha|\beta| e^{-i\omega t}}{\cosh^2(\kappa x)}, \tag{13}$$

where

$$\alpha = \frac{3\sqrt{V_b V_c}}{2\sqrt{2}\Gamma} \frac{2\tilde{\omega}_b - \tilde{\omega}_c}{V_c - 2V_b}, \quad \beta = \pm\sqrt{\frac{V_b}{2V_c}},$$

$$\omega = \frac{2(\tilde{\omega}_b V_c - \tilde{\omega}_c V_b)}{V_c - 2V_b} \tag{14}$$

and

$$\kappa = \frac{1}{2}\sqrt{\left|\frac{2\tilde{\omega}_b - \tilde{\omega}_c}{V_c - 2V_b}\right|}. \tag{15}$$

If $V_b = 2V_c$, one can find the particular solution for a mobile soliton

$$B = \frac{|\alpha| \exp(-i\omega t/2 + ikx/2)}{\cosh^2[\kappa(x - vt)]}, \quad C = \frac{\alpha \exp(-i\omega t + ikx)}{\cosh^2[\kappa(x - vt)]}, \tag{16}$$

where now

$$\alpha = \frac{1}{2\Gamma}(\tilde{\omega}_c - 2\tilde{\omega}_b), \quad \omega = \tfrac{2}{3}(2\tilde{\omega}_c - \tilde{\omega}_b) - \frac{V_b}{2}k^2 \tag{17}$$

and

$$\kappa = \sqrt{\left|\frac{\tilde{\omega}_c - 2\tilde{\omega}_b}{6V_b}\right|}, \quad v = -V_b k = -2V_c k. \tag{18}$$

(Analogous solutions, including ''dark'' solitons, have been discussed in the case of a ''cascading nonlinearity'' in Refs. 11–14.) The system of equations (9) and (10) has particular solutions $C_1 = C_2 = C$ and $B_1 = \pm B_2 = B$, where B and C satisfy the equations coinciding with those for the one interface case with shifted value of the frequency $\tilde{\omega}_b \to \tilde{\omega}_b + \epsilon$. Thus the three-layer system under consideration has particular solutions in the form of two solitons with coinciding parameters (up to the sign of the amplitude), and propagating side by side with each other. The case of a monomolecular thin film of B molecules is described by a system of three equations and needs separate discussion (see Ref. 10). In this paper a variational approach will be applied to the investigation of solitons propagating along two interfaces with weak interaction between them [i.e., with small ϵ in Eqs. (9) and (10)].

II. VARIATIONAL EQUATIONS

The variational approach is based on the possibility to represent Eqs. (9) and (10) as Lagrange equations (see, e.g., Refs. 15–18) corresponding to the Lagrangian with the density

$$\mathcal{L} = \mathcal{L}_1 + \mathcal{L}_2 + \mathcal{L}_{\text{int}}, \tag{19}$$

where

$$\mathcal{L}_j = \frac{i}{2}(B_j B_{jt}^* - B_j^* B_{jt}) + \frac{i}{2}(C_j C_{jt}^* - C_j^* C_{jt}) + \tilde{\omega}_b |B_j|^2 + \tilde{\omega}_c |C_j|^2 - V_b |B_{jx}|^2 - V_c |C_{jx}|^2 + \Gamma(C_j B_j^{*2} + C_j^* B_j^2), \quad j = 1,2, \tag{20}$$

$$\mathcal{L}_{int}=\epsilon(B_2B_1^*+B_2^*B_1), \tag{21}$$

$$B_{jt}=\partial B_j/\partial t, \quad B_{jx}=\partial B_j/\partial x, \quad \text{etc.}$$

The action

$$S=\int\int \mathcal{L}\,dx\,dt \tag{22}$$

has its extremal values at the exact solutions of Eqs. (9) and (10). Approximate solutions can be obtained by means of minimizing the action for some trial functions (see analogous investigation for a single soliton in Refs. 17 and 18)

$$B_j=\frac{b_j\exp(i\varphi_j/2)}{\cosh^2[\kappa_j(x-\zeta_j)]}, \quad C_j=\frac{c_j\exp(i\varphi_j)}{\cosh^2[\kappa_j(x-\zeta_j)]}, \tag{23}$$

where

$$\varphi_j=k_j(x-\zeta_j/2)+\delta_j. \tag{24}$$

In contrast to the one-interface case, all parameters b_j, c_j, κ_j, k_j, ζ_j, and δ_j are functions of time due to the interaction of the solitons. Substitution of Eqs. (23) and (24) into Eqs. (19)–(21) yields

$$L=L_1+L_2+L_{\text{int}}=\int \mathcal{L}\,dx, \tag{25}$$

where

$$L_j=\frac{4b_j^2}{3\kappa_j}\left[\tilde{\omega}_b-V_b\left(\frac{k_j^2}{4}+\frac{4}{5}\kappa_j^2\right)-\frac{1}{2}\left(\frac{k_{jt}}{2}\zeta_{jt}-\delta_{jt}\right)+\frac{1}{4}\zeta_jk_{jt}\right]$$
$$+\frac{4c_j^2}{3\kappa_j}\left[\tilde{\omega}_c-V_c\left(k_j^2+\frac{4}{5}\kappa_j^2\right)-\left(\frac{k_{jt}}{2}\zeta_{jt}-\delta_{jt}\right)+\frac{1}{2}\zeta_jk_{jt}\right]$$
$$+\frac{32}{15}\Gamma\frac{b_j^2c_j}{\kappa_j}, \tag{26}$$

$$L_{\text{int}}=2\epsilon b_1b_2\int\frac{\cos\frac{\varphi_1-\varphi_2}{2}dx}{\cosh^2[\kappa_1(x-\zeta_1)]\cosh^2[\kappa_2(x-\zeta_2)]}$$
$$\approx\frac{8\epsilon b_1b_2}{\kappa}\cos\mu\; f(r) \tag{27}$$

and

$$2\mu\equiv\delta_1-\delta_2+\tfrac{1}{2}(k_1\zeta_2-k_2\zeta_1),$$
$$r\equiv\kappa(\zeta_1-\zeta_2), \tag{28}$$

$$f(r)=\frac{r\cosh r-\sinh r}{\sinh^3 r}.$$

In the last calculation of L_{int}, we supposed $\kappa_1=\kappa_2=\kappa$ and $|k_1-k_2|\ll 2\kappa$, $|r|\ll 1$.

Minimizing action (22), we obtain the Lagrange equations for the variables b_j, c_j, δ_j, ζ_j, k_j, and κ, which after some transformations give the following system:

$$2\tilde{\omega}_b-\frac{V_b}{2}k_j^2-\frac{8}{5}V_b\kappa^2-\frac{1}{2}k_j\zeta_{jt}+\frac{1}{2}k_{jt}\zeta_j+\delta_{jt}+\frac{16\Gamma}{5}c_j$$
$$+6\epsilon\cos\mu\; f(r)\frac{b_l}{b_j}=0 \tag{29}$$

$$\tilde{\omega}_c-V_ck_j^2-\frac{4}{5}V_c\kappa^2-\frac{1}{2}k_j\zeta_{jt}+\frac{1}{2}k_{jt}\zeta_j+\delta_{jt}+\frac{4\Gamma}{5}\frac{b_j^2}{c_j}=0, \tag{30}$$

$$\kappa\frac{d}{dt}\left(\frac{b_j^2+2c_j^2}{\kappa}\right)+6(-1)^{j-1}\epsilon b_1b_2\sin\mu\; f(r)=0, \tag{31}$$

$$(b_j^2+2c_j^2)k_{jt}+12\epsilon b_1b_2\cos\mu\frac{\partial f(r)}{\partial\zeta_j}=0, \tag{32}$$

$$(b_j^2+2c_j^2)\zeta_{jt}+(b_j^2V_b+4c_j^2V_c)k_j=0, \tag{33}$$

$$\sum_j[4\kappa^2(b_j^2V_b+c_j^2V_c)-2\Gamma c_jb_j^2]-15\epsilon b_1b_2\kappa\frac{\partial f}{\partial\kappa}\cos\mu=0. \tag{34}$$

For $\epsilon\rightarrow 0$ this system splits into two independent sets of equations corresponding to two isolated interfaces discussed in Ref. 18. Systems (29)–(34) comprises the variational equations describing the dynamics of two solitons. This system is rather complicated and can be considered analytically only under some simplifying assumptions. Here we shall consider the important particular case of the elastic interaction of solitons.

III. ELASTIC INTERACTION OF SOLITONS

Equations (29)–(34) have an obvious integral of motion I_1 defined by

$$2\kappa I_1=b_1^2+2c_1^2+b_2^2+2c_2^2. \tag{35}$$

The expression $(b_j^2+2c_j^2)/\kappa$ characterizes the energy of the soliton and is conserved in the case of a soliton on the isolated interface. In the case of two interacting solitons only the sum of these two quantities is conserved, as we see from Eq. (35). However, in the particular case $\sin\mu=0$, i.e., when $\mu=n\pi$, the energy of each soliton is conserved separately, which corresponds to their elastic interaction. Let us discuss this case in more detail. For its realization it is necessary that $\mu_t=0$ holds all times. As follows from Eqs. (29), (30), (32), and (33), the variable μ is time independent only if

$$c_1=c_2=c, \quad b_1=b_2=b \tag{36}$$

and

$$\text{(i)}\quad k_1+k_2=0 \quad \text{or} \quad \text{(ii)}\quad V_b=2V_c. \tag{37}$$

Conditions (37) correspond to the two particular cases when the exact soliton solutions (13) and (16) are realized.[9]

Equation (32) leads, together with Eqs. (36) and (37), to the conservation of the total momentum

$$k_1+k_2=2k_0=\text{const}, \tag{38}$$

where $k_0 = k_{01} = k_{02}$ is the initial value of k_j. Note that μ is equal to the initial phase difference of the B_j–fields according to the condition $k_{01} = k_{02}$.

Equation (33) gives

$$(\zeta_1 + \zeta_2)_t = -2k_0 \widetilde{V}, \tag{39}$$

where

$$\widetilde{V} = \frac{V_b b^2 + 4V_c c^2}{b^2 + 2c^2}. \tag{40}$$

Hence we conclude that in the case (i) of Eq. (37) the ''center of mass'' does not move, and in case (ii) of Eq. (37) it moves with the constant velocity $-2k_0 V_B$.

Now let us consider the relative motion of the solitons. From Eqs. (32) and (33), we obtain the following systems:

$$I_1(k_1 - k_2)_t + 24\epsilon c^2 \frac{\cos\mu}{\kappa} \frac{\partial f}{\partial \Delta} = 0, \tag{41}$$

$$\Delta_t + \widetilde{V}(k_1 - k_2) = 0, \tag{42}$$

where $\Delta = \zeta_1 - \zeta_2$. After elimination of $k_1 - k_2$, we obtain the equation

$$\Delta_{tt} - \frac{24\epsilon \cos\mu \ \widetilde{V} b^2}{b^2 + 2c^2} \frac{\partial f}{\partial \Delta} = \Delta_t (\ln \widetilde{V})_t. \tag{43}$$

Note that in case (ii) the right-hand side of this equation vanishes since $\widetilde{V} = V_b = \text{const}$, and in case (i) we can also neglect the right-hand side because, as we shall see, it differs from zero only in higher degrees of ϵ. If we neglect the time dependence of the coefficients of this equation, which also arises only in higher degrees of ϵ, then the relative motion can be presented as the motion of the point particle of unit mass with coordinate Δ under the action of force, with the potential

$$U(\Delta) \simeq -\frac{24\epsilon b^2 \widetilde{V} \cos\mu}{\kappa I_1} f(\Delta). \tag{44}$$

Thus at $\mu = \pi$ there is a repulsion of the solitons from each other, and at $\mu = 0$ they attract each other. In the last case the solitons oscillate with respect to their mutual center of mass. At small values of r we obtain, from Eq. (43),

$$\Delta_{tt} + \cos\mu \, \widetilde{\omega}^2 \Delta = 0, \tag{45}$$

where

$$\widetilde{\omega}^2 = \frac{32\epsilon b^2 (V_b b^2 + 4V_c c^2)}{5I_1^2}. \tag{46}$$

The assumption of a time-independent $\widetilde{\omega}^2$ corresponds to the omission of small terms of order ϵ^2 in Eq. (43), so that in the attraction case ($\cos\mu = 1$) we obtain harmonic oscillations of solitons

$$\Delta = \Delta_0 \cos \widetilde{\omega}_0 t, \tag{47}$$

where Δ_0 and $\widetilde{\omega}_0$ are the initial values of Δ and $\widetilde{\omega}$.

Consider now the dependence of the soliton amplitudes b and c on time. We have not yet used two equations: Eq. (34), which can be expressed in the form

$$\frac{8}{I_1^2}(b^2 + 2c^2)^2 (V_b b^2 + V_c c^2) - 4\Gamma c b^2 \simeq 15\epsilon b^2 r f' \cos\mu; \tag{48}$$

and the combination of Eqs. (29) and (30),

$$(2\widetilde{\omega}_b - \widetilde{\omega}_c) + \frac{1}{4}(k_1^2 + k_2^2)(2V_c - V_b) + \frac{4(V_c - 2V_b)}{5I_1^2}(b^2 + 2c^2)^2 + \frac{4\Gamma}{5c}(4c^2 - b^2) = -6\epsilon \cos\mu \ f(r). \tag{49}$$

Note that the soliton width κ is related to the amplitudes through Eq. (35) which was used in the derivation of Eqs. (48) and (49). We also have

$$(k_1 - k_0)^2 = (k_2 - k_0)^2 = k^2 = \left(\frac{\Delta_t}{2\widetilde{V}}\right)^2 \approx \frac{8\epsilon}{15V_b}(r_0^2 - r^2).$$

Let us represent the amplitudes b and c in the forms

$$b = b_0[1 + \epsilon m_1(r)], \quad c = c_0[1 + \epsilon m_2(r)], \tag{50}$$

and substitute Eq. (50) into Eqs. (48) and (49). In zeroth order of the power expansion with respect to ϵ, we obtain equations coinciding with those for the solitons on isolated interfaces. In the next order we have a linear system of two equations for functions m_1 and m_2, which can be transformed to the forms

$$2(5 - 2\beta^2)m_1 + (22\beta^2 - 1)m_2 = \frac{45\cos\mu \ (1 + 2\beta^2)}{4\Gamma c_0} r f'$$

$$4(1 + 5\beta^2)m_1 - (3 + 22\beta^2 + 8\beta^4)m_2 = \frac{45\cos\mu \beta^2 (1 + 2\beta^2)}{2\Gamma c_0} f - \frac{(1 - \beta^2)(1 + 2\beta^2)}{\Gamma c_0}(r^2 - r_0^2), \tag{51}$$

where $\beta^2 = V_b / 2V_c$. Its solutions are

$$m_1 = \frac{D_1}{D}, \quad m_2 = \frac{D_2}{D},$$

$$D = -2(-16\beta^6 + 216\beta^4 + 138\beta^2 + 13), \tag{52}$$

$$D_1 = -\frac{45\cos\mu \ (1 + 2\beta^2)}{2\Gamma c_0}[(8\beta^4 + 22\beta^2 + 3) r f' + 2\beta^2 (22\beta^2 - 1) f] - \frac{(1 - 22\beta^2)(1 + 2\beta^2)(1 - \beta^2)}{\Gamma c_0}(r^2 - r_0^2),$$

$$D_2 = \frac{45\cos\mu\,(1+2\beta^2)}{\Gamma c_0}[\beta^2(5-2\beta^2)f-(1+5\beta^2)rf']$$
$$-\frac{2(5-2\beta^2)(1+2\beta^2)(1-\beta^2)}{\Gamma c_0}(r^2-r_0^2).$$

In case (ii), i.e., for $\beta^2=1$, it follows, for example, that

$$b=b_0+\frac{15\epsilon\cos\mu}{104\Gamma}(14f+11rf')$$
$$\simeq b_0+\frac{15\epsilon\cos\mu}{52\Gamma}\left(\frac{7}{3}+\frac{12}{5}r^2\right),$$

$$c=c_0+\frac{15\epsilon\cos\mu}{26\Gamma}(2rf'-f)\simeq c_0-\frac{15\epsilon\cos\mu}{26\Gamma}\left(\frac{1}{3}+\frac{2}{5}r^2\right), \tag{53}$$

and

$$\kappa\simeq\kappa_0\left(1+\frac{5\epsilon\cos\mu}{26\Gamma c_0}(1-4r^2)\right). \tag{54}$$

Thus we see that the amplitudes b and c and the width κ have different constant shifts and oscillating (for $\mu=0$) components.

Note that taking into account the dependence of b^2 and c^2 on time in Eq. (46), results in a term proportional to $\cos(2\tilde{\omega}_0 t)$ in the expression for $\tilde{\omega}^2$ which could lead to parametric resonance. But with the same order of accuracy the constant part of the frequency shift $\tilde{\omega}-\tilde{\omega}_0\simeq(2/3)\epsilon\tilde{\omega}_0(2m_1+m_2)$ arises, which is greater than the width of the parametric resonance region. Hence, in fact, the parametric resonance does not take place, which justifies taking into account only the terms of order ϵ in Eqs. (45) and (46).

IV. NUMERICAL SIMULATION

The dynamics of two solitons propagating along two different interfaces has been simulated numerically in the case of the simplest physical system described by Eqs. (9) and (10), which consists of four monolayers CBBC. Then we have $\tilde{\omega}_c=\omega_c+2V_c$, $\tilde{\omega}_b=\omega_b+2V_b$, and $\epsilon=V_{b\perp}$. The initial conditions and the parameters of the medium are chosen as follows: $\kappa=0.073$ (this choice corresponds to a soliton with a width of 30 interatomic distances), $\Delta\zeta=6$, $V_b=2V_c=60$, and $\Gamma=1$. Figure 1 shows the distance between solitons centers as a function of time for different values and signs of the interaction constant ϵ. Note that a change of the initial phase difference from $\mu=0$ to π is equivalent to a change of the sign of ϵ. As we see, the simulation confirms the results of our analytic calculations concerning the existence of a bound state of solitons for $\cos\mu=1$, and the repulsion of solitons for $\cos\mu=-1$. It is easy to see that the oscillation frequency is in a good agreement with the formula $\omega=\kappa\sqrt{32\epsilon V_b/15}$, which is a consequence of Eq. (46) for $V_b=2V_c$. The evolution of the fields B_1 and B_2 is shown in Fig. 2 for the same choice of parameters as in Fig. 1(a). The oscillations of the mutual positions and the excellent conservation of the initial sech^2 shape are clearly seen. The time dependences of the amplitudes b_1 and c_1 and of the widths σ_{B_1} and σ_{C_1} are shown in Figs. 3 and 4 respectively, which present the shift of the mean values and oscillations with frequency 2ω of all these parameters according to the formulas (53) and (54). But the numerically observed small difference (about 3%) between the width of the B field and the width of the C field lies beyond the presented analytical theory, which initially assumes the equality of these two widths. The small difference in the soliton widths could be taken into account by an extension of the present analytical approach. However, this would not lead to qualitatively new results, but merely would complicate the analysis.

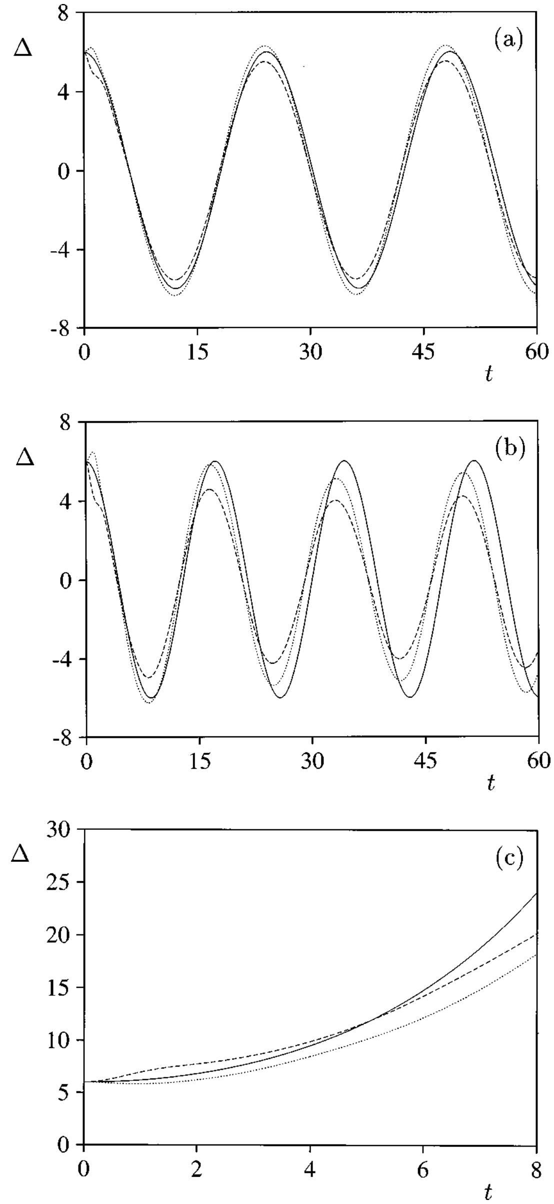

FIG. 1. The distance Δ between the centers of the two solitons as a function of time t for the interaction constants $\epsilon=0.1$ (a) 0.2 (b) and -0.1 (c). Comparison of the result of the anlytical calculation (solid line) with the results of the numerical simulation, where the dashed line shows the distance between the centers of the two B fields, and the dotted line shows the distance between the centers of the two C fields.

Note that for large initial distances between the soliton centers ($r>1$) the quadratic approximation for potential (44)

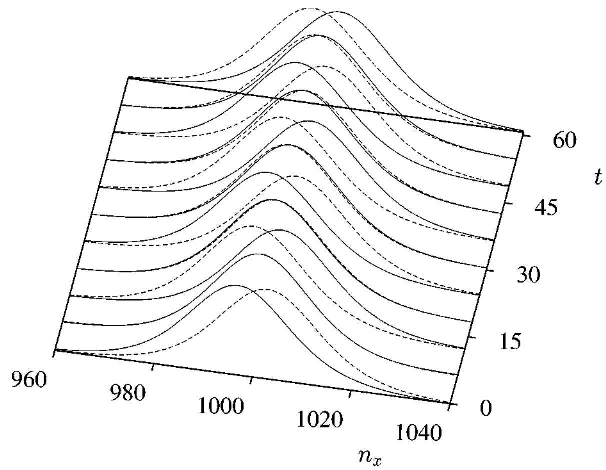

FIG. 2. The evolution of the fields B_1 (solid line) and B_2 (dashed line) with the same parameters as in Fig. 1(a) as a function of the time t and of the site index n_x.

is no longer valid and therefore the oscillations become anharmonic. According to Eq. (44), an increase in Δ_0 causes an increase in the oscillation period, which was observed numerically.

Numerical calculations also demonstrated that a decrease in the soliton widths induces energy emission by the solitons together with a variation of their shapes. If the soliton width approaches ~ 10 interatomic distances, the dynamics of the system changes qualitatively. Such a behavior is not surprising, because in this case the influence of discreteness becomes significant and, as a consequence, the sech^2 shape function is no longer a solution of the governing equations. Details of the dynamics of localized solutions under the influence of discreteness effects represent an extra problem, and lie beyond the scope of this paper.

It is worth mentioning that in the optical context the problem of spatial soliton interaction in bulk media with quadratic nonlinearity was considered in Refs. 19–21. In contrast to the studied case of Fermi resonance solitons, the interaction of optical solitons in bulk media has a nonlinear character. Moreover, initially separated optical solitons which attract each other will overlap completely in the subsequent development, which allows an analytical description only at the initial stage of evolution.[21] Nevertheless, the comparison of numerical results exhibits a qualitative agreement in the behavior of both systems. In particular, a strong dependence of the soliton evolution on the initial phase difference as well as an energy exchange between solitons for $\mu \neq 0,\pi$ have been identified in both scenarios.

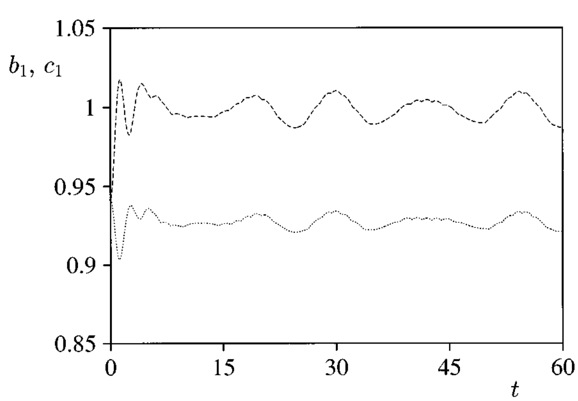

FIG. 3. The dependence on time t of the amplitudes b_1 (dashed line) and c_1 (dotted line) with the same parameters as in Fig. 1(a).

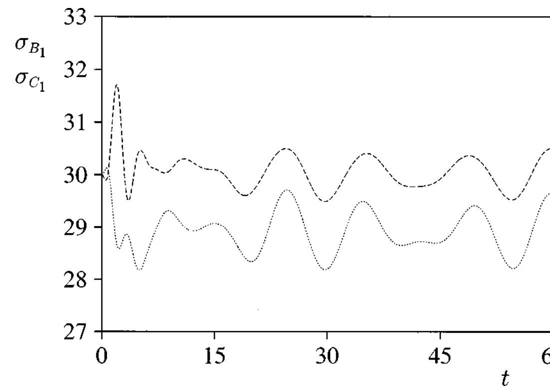

FIG. 4. The dependence on time t of the width σ_{B_1} of the B_1 field (dashed line) and of the width σ_{C_1} of the C_1 field (dotted line), with the same parameters as in Fig. 1(a).

V. CONCLUSION

We considered the problem of the interaction of Fermi resonance solitons propagating along two interfaces of a three-layer structure. The interaction arises due to tunnel penetration of one soliton field in the region of the location of the other one. It is shown that the behavior depends on the initial relative phase of the solitons. In the case of zero initial phase difference $\mu_0 = 0$, the solitons attract each other and create a bound state, and in the opposite case ($\mu_0 = \pi$) they repel each other. An analogous behavior takes place in the case of optical solitons propagating in coupled fiber waveguides, which can be described by a system of coupled nonlinear Schrödinger equations.[16] But in the present case of Fermi resonance solitons the dynamics is much more complicated due to the fact that each soliton contains two fields. As a consequence the system exhibits oscillatory behavior not only in the mutual soliton positions but also in the amplitudes and widths of each excitation field composing the bound state. Note that in the case of weak interaction the dynamics of the solitons does not change qualitatively if the thin film of c molecules is located between semi-infinite layers of b molecules. However, it becomes more sensitive to the change of system parameters, and the oscillatory behavior of soliton interaction becomes less robust. This effect is a consequence of the intrinsic asymmetry of the system with respect to vibration amplitudes B and C. The results obtained can be applied for the analysis of propagation of short excitation pulses along Fermi resonance interfaces in organic multilayer structures.

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