Solitonic energy transfer in a coupled exciton-vibron system

Dirk Hennig
Freie Universität Berlin, Fachbereich Physik, Institut für Theoretische Physik, Arnimallee 14, 14195 Berlin, Germany
(Received 19 October 1999)

We consider the exciton transfer along a one-dimensional molecular chain. The exciton motion is influenced by longitudinal vibrations evolving in a Toda lattice potential. It is shown how the soliton solutions of the vibron system coupled to the exciton system induce solitonic exciton transfer. To this aim the existence of a regime of suppressed energy exchange between the coupled excitonic and vibrational degrees of freedom is established in the case of which a nonlinear Schrödinger equation for the exciton variable is derived. The nonlinear Schrödinger equation possesses soliton solutions corresponding to coherent transfer of the localized exciton.

PACS number(s): 41.20.Jb, 42.65.Pc, 63.20.Pw, 71.10.−w

I. INTRODUCTION

As is well known the interplay of dispersion and nonlinearity in nonlinear evolution equations may result in localized solutions [1,2]. Solitons are an important prototype of such localized solutions allowing stable storage and coherent transport of a physical quantity. The soliton concept was successfully applied in various physical contexts including nonlinear optics, condensed matter physics, and hydrodynamics [3]. Soliton solutions are regarded to play also an important role in modeling the efficient and loss-free transfer of energy and quasiparticles in biomolecular aggregates [4–9]. Basic to many models of biomolecules is a lattice system the sites of which correspond to the molecular subunits of the chain [10]. The mere excitonic transfer along these molecular sites is usually described by a tight-binding system giving rise to a linear discrete Schrödinger equation for the exciton amplitude. Taking the coupling between the vibrational degrees of freedom of the molecular sites and the exciton motion into account nonlinearity come into play in the coupled exciton vibron equations. In the case of Davydov's model of biomolecular energy transfer [4] the lattice system of coupled exciton and vibron equations was reduced to a single integrable continuum nonlinear Schrödinger equation expressed solely in the excitonic amplitude. The corresponding soliton solutions describe the solitonic exciton movement. In the frame of Davydov's model passing from the discrete system of coupled exciton vibron equations to a single integrable continuum equation was crucial for obtaining exact soliton solutions. On the other hand there are only a few examples of integrable lattice system known, such as the Toda lattice [11] and the Ablowitz-Ladik lattice [12] both possessing soliton solutions. Nonetheless, also nonintegrable discrete systems can provide localized solutions in the form of intrinsically localized modes, also called breathers [13–18]. However, unlike the mobile solitons, most of the intrinsically localized modes are pinned by the discrete structure of the lattice preventing them from transferring excitation energy across the lattice [19–22].

In this paper we address the issue of exciton transfer along a molecular lattice chain where the exciton dynamics is influenced by anharmonic longitudinal lattice vibrations. We demonstrate that for the discrete system of the coupled exciton vibron dynamics solitonlike solutions exist yielding coherent exciton transfer. In particular, different from the Davydov soliton model, our approach does not necessitate the elimination of the vibrational degrees of freedom from the coupled exciton vibron system. Moreover, incorporation of the nonlinear evolution of the vibrations proves to be essential in achieving solitonic exciton dynamics.

In Sec. II we introduce the model of the coupled molecular exciton vibron system and in Sec. III its dynamics with emphasis on soliton solutions is studied. Section IV deals with the energy exchange between the exciton and vibron systems. The energy exchange rate is computed from which we infer on different regimes of interaction between the two subsystems. Finally in Sec. V a brief summary is given.

II. THE COUPLED EXCITON VIBRON SYSTEM

We consider the transfer of an exciton along a one-dimensional molecular chain where the excitonic movement is influenced by longitudinal vibrations of the molecular constituents of the chain. The Hamiltonian is determined by

$$H=H_{\mathrm{exc}}+H_{\mathrm{vib}}, \tag{1}$$

with the excitonic part given by a tight-binding lattice system

$$H_{\mathrm{exc}}=-\sum_{n=-\infty}^{\infty} V_{nn-1}(c_n^* c_{n-1}+c_n c_{n-1}^*), \tag{2}$$

where c_n represents the probability amplitude of the exciton to occupy the site n and V_{nn-1} is the transfer matrix element of the coupling between two molecular lattice sites. The transfer matrix element depends on the intersite relative coordinate q_n-q_{n-1} in an exponential fashion

$$V_{nn-1}=V_0\exp[-\gamma(q_n-q_{n-1})], \tag{3}$$

with q_n being the elongation of the nth molecular unit and γ is the range parameter [23]. The nonlinear dynamics of the longitudinal vibrations of the molecular sites is described through a Toda lattice system with Hamiltonian

$$H_{\mathrm{vib}}=\frac{1}{2}\sum_n p_n^2+\frac{a}{b}\sum_n \{\exp[-b(q_n-q_{n-1})]-1\}, \tag{4}$$

and $a,b>0$. We underline that our anharmonic treatment of the lattice vibrations goes beyond the usual harmonic approximation of the Holstein or Davydov-type Hamiltonians [4,10]. In Ref. [24] a Davydov-type Hamiltonian was considered where the intermolecular vibrations were also treated as a Toda lattice. However, the coupling to the exciton was chosen to be linear in the vibrational coordinates whereas in the current paper it is taken to be nonlinear. It is through Eq. (3) that the coupling between the excitonic and intersite vibrational degrees of freedom is introduced. Since the latter are not constant, the transfer matrix elements are modulated by the motion of the molecular sites relative to each other. When two adjacent units are further apart, the corresponding matrix element diminishes, causing a reduction in the excitonic transfer from one site to the other. Correspondingly, for two neighboring sites being closer to each other the transfer matrix element increases resulting in enhanced excitonic transfer.

The system of coupled exciton vibron equations reads

$$i\dot{c}_n = -V_0\{\exp[-\gamma(q_{n+1}-q_n)]c_{n+1} - \exp[-\gamma(q_n-q_{n-1})]c_{n-1}\} \tag{5}$$

$$\ddot{q}_n = a\{\exp[-b(q_{n+1}-q_n)] - \exp[-b(q_n-q_{n-1})]\} - \gamma V_0\{(c_{n+1}^* c_n + c_{n+1}c_n^*)\exp[-\gamma(q_{n+1}-q_n)] - (c_n^* c_{n-1} + c_n c_{n-1}^*)\exp[-\gamma(q_n-q_{n-1})]\}. \tag{6}$$

For $\gamma=0$ the excitonic and vibrational degrees of freedom decouple. The solutions of the two separate subsystems exhibit markedly different behavior. The linear tight-binding system

$$i\dot{c}_n = -V_0(c_{n+1}+c_{n-1}), \tag{7}$$

does not support any localized solution at all. In fact, when we take as an example an initially strongly localized excitonic state of a single-site excitation $c_n(t=0)=\delta_{n,m}$ it decays in the course of time according to $|c_n(t)|^2 = |\mathcal{J}_{n-m}(2V_0 t)|^2$ ($\mathcal{J}_n$ is the Bessel function of the first kind). Eventually, the excitonic energy becomes spread along the lattice sites. In contrast, the Toda system supports moving localized vibronic states in form of solitons

$$\exp[-b(q_n-q_{n-1})] = 1 + \sinh\kappa\,\mathrm{sech}^2(\kappa n - \beta_T t), \tag{8}$$

with the soliton parameters $\beta_T = \sqrt{ab}\sinh\kappa$ [11]. When the two systems become coupled ($\gamma>0$) an interesting question arises, namely, whether the Toda solitons are preserved, and if so, can they additionally ''infect'' the exciton evolution to behave in a solitonic fashion as well?

III. SOLITONIC EXCITONIC MOTION MEDIATED BY VIBRONIC TODA SOLITONS

In this section we study the dynamics of the coupled exciton vibron system of Eqs. (5) and (6) focusing interest on possible solitonlike excitonic propagation induced by solitonic Toda vibrations. To reduce the number of parameters in our model we assume that $\gamma=b$ and furthermore set $V_0=1$. The system of coupled equations then reads

$$i\dot{c}_n = -\exp[-b(q_{n+1}-q_n)]c_{n+1} - \exp[-b(q_n-q_{n-1})]c_{n-1} \tag{9}$$

$$\ddot{q}_n = a\left[1-\frac{b}{a}(c_{n+1}^* c_n + c_{n+1}c_n^*)\right]\exp[-b(q_{n+1}-q_n)] - a\left[1-\frac{b}{a}(c_n^* c_{n-1} + c_n c_{n-1}^*)\right]\exp[-b(q_n-q_{n-1})]. \tag{10}$$

Considering the case $b/a \ll 1$ we note that the excitonic terms in Eq. (10) have negligible impact on the dynamics of the vibrational system. Therefore, up to terms of the order $\mathcal{O}(b/a)$, the vibrational dynamics is governed by the Toda lattice solutions. Upon inserting the soliton solution of the latter into Eq. (9) one obtains

$$i\dot{c}_n = -[1+\sinh\kappa\,\mathrm{sech}^2(\kappa(n+1)-\beta_T t)]c_{n+1} - [1+\sinh\kappa\,\mathrm{sech}^2(\kappa n-\beta_T t)]c_{n-1}. \tag{11}$$

The structure of this nonlinear Schrödinger equation points to its relationship with the integrable Ablowitz-Ladik (AL) equation given by

$$i\dot{\psi}_n = -[1+|\psi_n|^2](\psi_{n+1}+\psi_{n-1}), \tag{12}$$

which exhibits exact soliton solutions

$$\psi_n^s(t) = \sinh(\beta_{\mathrm{AL}})\mathrm{sech}[\beta_{\mathrm{AL}}(n-ut)]\exp[-i(\omega t - \alpha n + \sigma)] \tag{13}$$

and

$$\omega = -2\cos\alpha\cosh\beta_{\mathrm{AL}}, \quad u = 2\beta_{\mathrm{AL}}^{-1}\sin\alpha\sinh\beta_{\mathrm{AL}}, \tag{14}$$

where $\beta_{\mathrm{AL}} \in [0,\infty)$ and $\alpha \in [-\pi,\pi]$ [12].

In order to establish full contact between Eqs. (11) and (12) we suppose that c_n obeys the soliton solution (13) and adopt the soliton parameters such that $|c_n^s|^2 = \sinh\beta_{\mathrm{AL}}\mathrm{sech}^2[\beta_{\mathrm{AL}}(n-ut)]$ matches the driving term $\sinh\kappa\,\mathrm{sech}^2[\kappa n - \beta_T]$ in Eq. (11) which requires that $\beta_{\mathrm{AL}} = \kappa$ as well as $2\sin\alpha = \sqrt{ab}$ holds. Then we can indeed express Eq. (11) as a modified AL equation

$$i\dot{c}_n^s - (1+|c_n^s|^2)(c_{n+1}^s + c_{n-1}^s) = (|c_n^s|^2 - |c_{n+1}^s|^2)c_{n+1}^s. \tag{15}$$

The derivation of the AL-type equation (15) in terms of the AL soliton solution is justified if the term on the right-hand side (RHS) acts only as a small perturbation of the the genuine AL equation represented by the left-hand side (LHS) of Eq. (15). The strength of the perturbation is measured by the ratio

$$\frac{|(|c_n^s|^2 - |c_{n+1}^s|^2)c_{n+1}^s|}{(1+|c_n^s|^2)|c_{n+1}^s + c_{n-1}^s|} \leqslant \tanh^2\beta_{\mathrm{AL}}, \tag{16}$$

which in fact is small as long as β_{AL} is not very large. (In the forthcoming studies we take $\beta_{\mathrm{AL}} = \kappa \leqslant 0.5$.)

In order to give analytical evidence that Eq. (15) supports slightly modified AL soliton solutions we invoke perturbation theory based on the inverse scattering transform [25,26]. (Perturbed AL equations were also considered in Ref. [27].) Within the frame of this approach it is assumed that the parameters of the exact AL soliton vary slowly in time and the equations describing their evolution affected by the perturbation are given by

$$\dot{\alpha}=-\sinh\beta_{\mathrm{AL}}\sum_{n=-\infty}^{\infty}\frac{\sinh[\beta_{\mathrm{AL}}(n-x_0)]}{\cosh\{\beta_{\mathrm{AL}}[(n+1)-x_0]\}\cosh\{\beta_{\mathrm{AL}}[(n-1)-x_0]\}}\times\mathrm{Re}\{f(c_n^s)\exp[-i\alpha(n-x_0)-i\sigma]\},\tag{17}$$

$$\dot{x}_0=\frac{2\sinh\beta_{\mathrm{AL}}}{\beta_{\mathrm{AL}}}\sin\alpha+\frac{\sinh\beta_{\mathrm{AL}}}{\beta_{\mathrm{AL}}}\sum_{n=-\infty}^{\infty}\frac{(n-x_0)\cosh[\beta_{\mathrm{AL}}(n-x_0)]}{\cosh\{\beta_{\mathrm{AL}}[(n+1)-x_0]\}\cosh\{\beta_{\mathrm{AL}}[(n-1)-x_0]\}}\times\mathrm{Im}\{f(c_n^s)\exp[-i\alpha(n-x_0)-i\sigma]\},\tag{18}$$

$$\dot{\beta}_{\mathrm{AL}}=\sinh\beta_{\mathrm{AL}}\sum_{n=-\infty}^{\infty}\frac{\cosh[\beta_{\mathrm{AL}}(n-x_0)]}{\cosh\{\beta_{\mathrm{AL}}[(n+1)-x_0]\}\cosh\{\beta_{\mathrm{AL}}[(n-1)-x_0]\}}\times\mathrm{Im}\{f(c_n^s)\exp[-i\alpha(n-x_0)-i\sigma]\},\tag{19}$$

with the perturbational term

$$f(c_n^s)=(|c_n^s|^2-|c_{n+1}^s|^2)c_{n+1}^s\,.\tag{20}$$

Evaluation of the sums with the help of the Poisson formula yields

$$\dot{\alpha}=-[F_\alpha^c(\beta_{\mathrm{AL}})\cos(2\pi x_0)+F_\alpha^s\sin(2\pi x_0)]\cos\alpha,\tag{21}$$

$$\dot{x}_0=\frac{2\sinh\beta_{\mathrm{AL}}}{\beta}\sin\alpha+[F_{x_0}^c(\beta_{\mathrm{AL}})\cos(2\pi x_0)+F_{x_0}^s\sin(2\pi x_0)]\sin\alpha,\tag{22}$$

$$\dot{\beta}_{\mathrm{AL}}=[F_{\beta_{\mathrm{AL}}}^c(\beta_{\mathrm{AL}})\cos(2\pi x_0)+F_{\beta_{\mathrm{AL}}}^s(\beta_{\mathrm{AL}})\sin(2\pi x_0)]\sin\alpha,\tag{23}$$

with coefficients

$$F_\alpha^c(\beta_{\mathrm{AL}})=\frac{\pi}{\beta_{\mathrm{AL}}}\sum_{s=1}^{\infty}\sinh^{-1}\left(\frac{\pi^2 s}{\beta_{\mathrm{AL}}}\right)\left\{\frac{\pi s}{\beta_{\mathrm{AL}}}[\mathrm{sech}\,\beta_{\mathrm{AL}}\sinh(2\beta_{\mathrm{AL}})+\sinh\beta_{\mathrm{AL}}]-\frac{1}{48}\mathrm{sech}^3\beta_{\mathrm{AL}}\left[\frac{3\pi s}{\beta_{\mathrm{AL}}}\left(2+\frac{\pi s}{\beta_{\mathrm{AL}}}\right)\sinh(2\beta_{\mathrm{AL}})+\frac{6\pi s}{\beta_{\mathrm{AL}}}\sinh(4\beta_{\mathrm{AL}})-\frac{\pi s}{\beta_{\mathrm{AL}}}\left(2+\frac{\pi s}{\beta_{\mathrm{AL}}}\right)\sinh(6\beta_{\mathrm{AL}})\right]\right\},\tag{24}$$

$$F_\alpha^s(\beta_{\mathrm{AL}})=\frac{\pi}{\beta_{\mathrm{AL}}}\sum_{s=1}^{\infty}\sinh^{-1}\left(\frac{\pi^2 s}{\beta_{\mathrm{AL}}}\right)\left\{[1+2\cosh(2\beta_{\mathrm{AL}})]\mathrm{sech}\,\beta_{\mathrm{AL}}-2\cosh\beta_{\mathrm{AL}}-\frac{1}{8}\mathrm{sech}^3\beta_{\mathrm{AL}}\left[1+\left(\frac{\pi s}{\beta_{\mathrm{AL}}}\right)^2[1+\cosh(4\beta_{\mathrm{AL}})]\right]\right\},\tag{25}$$

$$F_{x_0}^c(\beta_{\mathrm{AL}})=2\sinh^5\beta_{\mathrm{AL}}\sum_{s=1}^{\infty}\sinh^{-1}\left(\frac{\pi^2 s}{\beta_{\mathrm{AL}}}\right)\left[\frac{1}{48}\left\{\left[3-18\left(\frac{\pi s}{\beta_{\mathrm{AL}}}\right)^2\right]\frac{\pi}{\beta_{\mathrm{AL}}}\sinh(2\beta_{\mathrm{AL}})+\frac{6\pi}{\beta_{\mathrm{AL}}}\sinh(4\beta_{\mathrm{AL}})+\left[1+8\left(\frac{\pi s}{\beta_{\mathrm{AL}}}\right)^2\right]\frac{\pi}{\beta_{\mathrm{AL}}}\sinh(6\beta_{\mathrm{AL}})\right\}\mathrm{sech}^4(2\beta_{\mathrm{AL}})-\frac{\pi}{\beta_{\mathrm{AL}}}\mathrm{sech}^2\beta_{\mathrm{AL}}\sinh(2\beta_{\mathrm{AL}})-\sinh^{-1}\left(\frac{\pi^2 s}{\beta_{\mathrm{AL}}}\right)\frac{\pi^2}{\beta_{\mathrm{AL}}}\cosh\left(\frac{\pi^2 s}{\beta_{\mathrm{AL}}}\right)\times\left(\frac{1}{192}\left\{\left[3-4\left(\frac{\pi s}{\beta_{\mathrm{AL}}}\right)^2\right]\frac{\pi s}{\beta_{\mathrm{AL}}}\sinh(2\beta_{\mathrm{AL}})+\frac{24\pi}{\beta_{\mathrm{AL}}}\sinh(4\beta_{\mathrm{AL}})+\left[1+\left(\frac{\pi s}{\beta_{\mathrm{AL}}}\right)^2\right]\frac{\pi s}{\beta_{\mathrm{AL}}}\sinh(6\beta_{\mathrm{AL}})\right\}\mathrm{sech}^4\beta_{\mathrm{AL}}-\frac{\pi s}{\beta_{\mathrm{AL}}}\mathrm{sech}^2\beta\sinh(2\beta)\right)\right],\tag{26}$$

$$F^{s}_{x_0}(\beta_{\rm AL}) = -2\sinh^5\beta_{\rm AL}\sum_{s=1}^{\infty}\sinh^{-1}\left(\frac{\pi^2 s}{\beta_{\rm AL}}\right)\left\{\frac{\pi s}{8\beta_{\rm AL}}\operatorname{sech}^4\beta_{\rm AL}[1+\cosh(4\beta_{\rm AL})] + \sinh^{-1}\left(\frac{\pi^2 s}{2\beta_{\rm AL}}\right)\frac{\pi^2}{\beta_{\rm AL}}\cosh\left(\frac{\pi^2 s}{\beta_{\rm AL}}\right)\left[4-[1 + \cosh(2\beta_{\rm AL})]\operatorname{sech}^2\beta_{\rm AL} - \sinh^2\beta_{\rm AL}\operatorname{cosech}^2(2\beta) - \frac{1}{4}\left[1+\left(\frac{\pi s}{\beta_{\rm AL}}\right)^2[1+\cosh(4\beta_{\rm AL})]\right] + 4\sinh^4\beta_{\rm AL}[1+\cosh(4\beta_{\rm AL})]\right]\right\}, \tag{27}$$

$$F^{c}_{\beta_{\rm AL}}(\beta_{\rm AL}) = \frac{\pi}{\beta_{\rm AL}}\sinh\beta_{\rm AL}\sum_{s=1}^{\infty}\sinh^{-1}\left(\frac{\pi^2 s}{\beta_{\rm AL}}\right)\left\{\frac{1}{16}\left[1-6\left(\frac{\pi s}{\beta_{\rm AL}}\right)^2\right]\frac{\pi}{\beta_{\rm AL}}\sinh(2\beta_{\rm AL}) + \frac{24\pi}{\beta_{\rm AL}}\sinh(4\beta_{\rm AL}) + \left[1+8\left(\frac{\pi s}{\beta_{\rm AL}}\right)^2\right]\frac{4\pi}{\beta_{\rm AL}}\sinh(6\beta_{\rm AL})\operatorname{sech}^4(2\beta_{\rm AL}) - \frac{\pi}{\beta_{\rm AL}}\operatorname{sech}^2\beta_{\rm AL}\sinh(2\beta_{\rm AL})\right\}, \tag{28}$$

$$F^{s}_{\beta_{\rm AL}}(\beta_{\rm AL}) = \frac{\pi}{2\beta_{\rm AL}}\sinh\beta_{\rm AL}\sum_{s=1}^{\infty}\sinh^{-1}\left(\frac{\pi^2 s}{\beta_{\rm AL}}\right)\left\{4-[1+\cosh(2\beta_{\rm AL})]\operatorname{sech}^2\beta_{\rm AL} - \sinh^2\beta_{\rm AL}\operatorname{cosech}^2(2\beta) - \frac{1}{4}\left[1+\left(\frac{\pi s}{\beta_{\rm AL}}\right)^2[1+\cosh(4\beta_{\rm AL})]\right] + 4\sinh^4\beta_{\rm AL}[1+\cosh(4\beta_{\rm AL})]\right\}. \tag{29}$$

The nonlinear dynamics of the system (17)–(19) is conveniently analyzed on the x_0-α phase plane for fixed $\beta_{\rm AL}$. Taking into account the influence of $\beta_{\rm AL}$ leads merely to a breathing of the phase plane trajectories. A plot of these trajectories reveals straight horizontal lines (not shown here) so that the dynamics is characterized by moving solitons. Hence the perturbational term (20) imposes no restrictions to the free movement of the soliton center x_0.

For an illustration of the solitonic exciton movement induced by a vibronic Toda soliton we numerically integrated the system (5) and (6) for a lattice consisting of 500 sites. At the central site $n=250$ a vibronic Toda soliton is launched and the excitonic subsystem is excited with the initial condition $c_n(0)=\sinh\beta_{\rm AL}\operatorname{sech}[\beta_{\rm AL}(n-250)]\exp(i\alpha n)$ corresponding to the AL soliton.

Before discussing the nonlinear coupled exciton vibron dynamics we consider briefly the linear evolution of the decoupled excitonic lattice, that is when $\gamma=0$ in Eq. (5). The solution of the linear lattice is then given by

$$c_n(t) = \sinh\kappa\sum_m i^{n-m} \times\exp(i\alpha m)\operatorname{sech}[\kappa m-\beta_T t]\mathcal{J}_{n-m}(2V_0 t), \tag{30}$$

from which we deduce an asymptotic decay according $|c_n(t)|^2 \sim \exp(-2\beta_T t)/t$, a behavior which is seen in Fig. 1. For a better illustration only the evolution of the lattice sites $160\leqslant n\leqslant 320$ are shown. Evidentially, exciton localization is excluded. However, for the coupled nonlinear exciton vibron system ($\gamma>0$) localized exciton solutions may be found. We depict in Figs. 2(a) and 2(b) the excitonic occupation amplitude $|c_n(t)|^2$ and the vibronic soliton state $\exp[-b(q_n - q_{n-1})-1]$, respectively. Apparently, similar to the vibrational amplitudes the exciton remains localized and is coherently transferred along the lattice in a solitonlike fashion too.

Finally we remark that we found very good agreement between the exciton solutions obtained from the dynamics of the coupled system (5) and (6) and those gained from the reduced nonlinear Schrödinger equation (15).

IV. ENERGY EXCHANGE BETWEEN THE EXCITONIC AND VIBRONIC SYSTEMS

In this section we investigate the energy exchange between the excitonic and vibrational subsystems. The findings of the last section indicate that for proper initial configurations the two subsystems evolve in a solitonic manner maintaining their initially allocated energy localization. The change of energy of the vibron subsystem is determined by

$$\frac{dH_{\rm vib}}{dt} = \{H_{\rm vib}, H\}, \tag{31}$$

giving with Eqs. (2), (3), and (4)

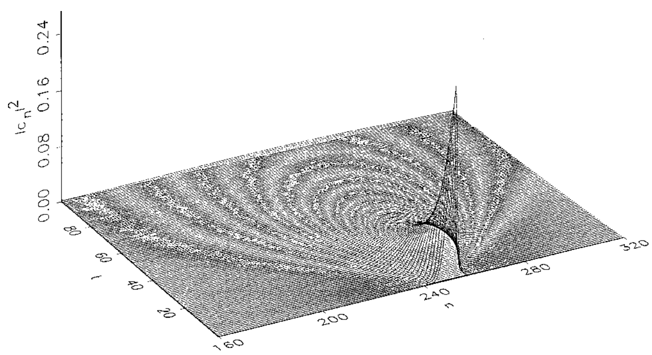

FIG. 1. The linear evolution of the decoupled excitonic subsystem (7). The initially localized excitonic state $c_n(t) = \sinh\beta_{\rm AL}\operatorname{sech}[\beta_{\rm AL}n]\exp(i\alpha n)$ corresponding to the AL soliton depletes all over the lattice in the course of time. Parameters: $\beta_{\rm AL} = 0.5$ and $\alpha = 0.2$.

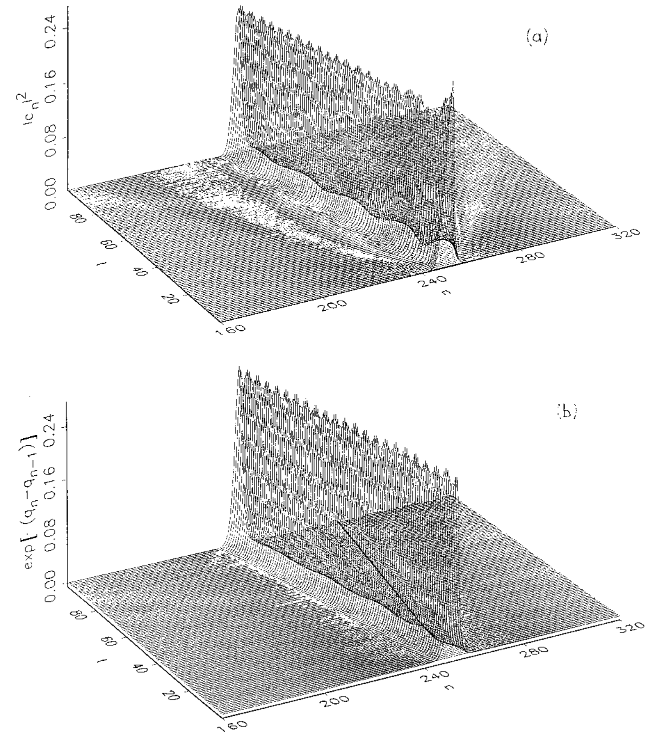

FIG. 2. The nonlinear evolution of the coupled exciton vibron system (5) and (6). The parameters for the vibronic Toda soliton are $\kappa=0.5$, $a=1$, and $b=0.05$. Concerning the excitonic system the parameters are the same as in Fig. 1.

$$\frac{dH_{\text{vib}}}{dt}=-bV_0\sum_{n=-\infty}^{\infty}(p_n-p_{n-1})\exp[-b(q_n-q_{n-1})]\times(c_n^*c_{n-1}+c_nc_{n-1}^*). \tag{32}$$

An equivalent expression is derived for the change of the energy of the excitonic subsystem. Actually, the change in energy of the excitonic system follows directly from the one of the vibronic system due to energy conservation.

Using the soliton solutions for the excitonic and vibronic system, respectively, the energy exchange rate per time unit T is given by

$$\begin{aligned}\Delta E=&\left|\frac{1}{T}\int_T dt\{H_{\text{vib}},H\}\right|\\=&2\beta_{\text{AL}}V_0\sinh\beta_{\text{AL}}\tanh^2\kappa\left|\cos\alpha\frac{1}{T}\int_T dt\right.\\&\times\sum_n\frac{\tanh[\kappa n-\beta_T t]}{1-\tanh^2\kappa\tanh^2[\kappa n-\beta_T t]}\\&\times(1-2\tanh^2[\kappa n-\beta_T t])(1+\text{sech}^2\kappa\,\text{sech}^2[\kappa n\\&-\beta_T t])\text{sech}[\beta_{\text{AL}}(n-ut)-y_0]\\&\left.\times\text{sech}\{\beta_{\text{AL}}[(n-1)-ut]-y_0\}\right|.\end{aligned} \tag{33}$$

The variable y_0 determines the relative distance between the vibronic and the excitonic soliton centers.

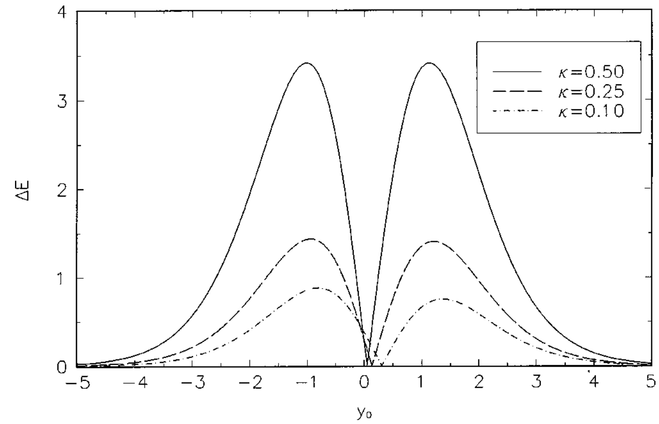

FIG. 3. The energy exchange rate ΔE in dependence on the soliton distance y_0. We plot the expression for ΔE given in Eq. (34) divided by $2\beta_{\text{AL}}V_0\sinh\beta_{\text{AL}}\tanh^2\cos\alpha$. Curve parameter is κ as indicated.

In computing the sums in Eq. (33) we note that the arguments of the n-dependent terms are of the form $(\kappa n-\beta_T t)$ and $[\beta_{\text{AL}}(n-ut)-y_0]$. Consequently, the sums in Eq. (33) are invariant under t translations, and thus actually t independent. We get then

$$\begin{aligned}\Delta E=&2\beta_{\text{AL}}V_0\sinh\beta_{\text{AL}}\tanh^2\kappa\\&\times\left|\cos\alpha\sum_n\frac{\tanh(\kappa n)}{1-\tanh^2\kappa\tanh^2(\kappa n)}\right.\\&\times(1-2\tanh^2[\kappa n])[1+\text{sech}^2\kappa\,\text{sech}^2(\kappa n)]\\&\left.\times\text{sech}[\beta_{\text{AL}}n-y_0]\text{sech}[\beta_{\text{AL}}(n-1)-y_0]\right|.\end{aligned} \tag{34}$$

In Fig. 3 we show the energy exchange rate given by expression (34) as a function of the relative soliton position y_0 for various κ. From these graphs we conclude that the smaller κ the more is the energy exchange suppressed. For each graph there exists a value $y_0\simeq 0$ for which the energy exchange rate vanishes. With increased κ the position of the minimum gets even closer to $y_0=0$. It is this particular regime of no energy exchange between the exciton and vibron system which enabled us to derive the reduced nonlinear Schrödinger equation (15) in the preceding section. Furthermore, the graphs exhibit two extrema of maximal energy exchange

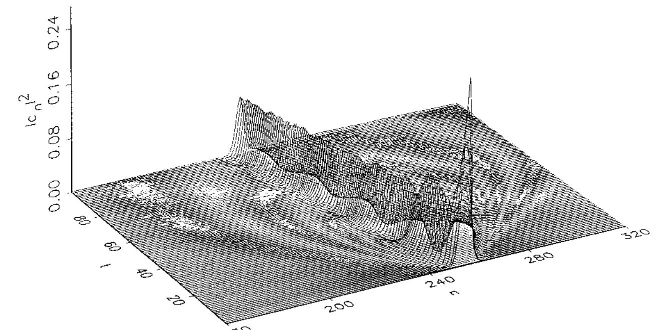

FIG. 4. Amplitudes of the excitonic system when the relative position of the Toda and AL soliton, respectively, is taken to be $y_0=2$.

rate for $y_0 \sim \pm 1$ and beyond them the monotone curves decay with growing $|y_0|$. Enhancing κ has the effect that the curves decay more rapidly with growing distance $|y_0|$. The latter fact becomes plausible by noting that the larger κ the smaller is the width of a soliton (determined by $1/\kappa$) and hence, their mutual influence diminishes with larger distances $|y_0|$. Finally, for soliton distances $|y_0| \geqslant 5$ there takes no energy exchange place between the excitonic and vibronic subsystems. In Fig. 4 we illustrate the energy transfer from the excitonic into the vibronic system by plotting the evolution of the excitonic occupation amplitudes $|c_n(t)|^2$ for a relative soliton distance $y_0 = 2$. According to the considerations above (compare Fig. 3) for such a distance the coupled system is in the regime of moderate energy transfer. As the Fig. 4 reveals the excitonic amplitudes diminishes during an initial transient phase of energy transfer from the excitonic into the vibronic system. Nevertheless, at the end of this transfer transient the reduced exciton amplitudes get stabilized and evolve in the following as a soliton.

V. SUMMARY

In the present paper we investigated the transfer dynamics of the coupled exciton vibron system of a one-dimensional molecular chain model. In the realm of a Holstein-type Hamiltonian the longitudinal intersite vibrations of the lattice were described by the nonlinear dynamics of a Toda lattice. The exciton motion across the molecular units was presented by a tight-binding system which, if decoupled from any molecular vibrational degrees of freedom, would evolve linearly making exciton localization impossible. However, as a striking feature of the coupled exciton vibron dynamics we demonstrated that not only the vibrational Toda solitons are preserved but also render their localization *and* mobility properties to the excitonic system. We stress the mutual appearance of exciton localization and mobility for mere exciton localization happens already in the Holstein system in the form of immobile localized modes pinned by the lattice. The mobility of the localized exciton in the present situation allows for stable and loss-free excitonic energy transfer along the molecular chain.

ACKNOWLEDGMENTS

This work was supported by the Deutsche Forschungsgemeinschaft through the Heisenberg program (Grant No. He 3049/1-1).

[1] L.D. Faddeev and L.A. Takhtajan, *Hamiltonian Methods in the Theory of Solitons* (Springer-Verlag, Berlin, 1987).
[2] M. J. Ablowitz and P. A. Clarkson, *Solitons, Nonlinear Evolulution Equations and Inverse Scattering* (Cambridge University Press, New York, 1991).
[3] M. Remoissenet, *Waves Called Solitons* (Springer-Verlag, Berlin, 1978).
[4] A.S. Davydov and N.I. Kislukha, Phys. Status Solidi B **59**, 465 (1973); A.S. Davydov, J. Theor. Biol. **38**, 559 (1973); A.S. Davydov and N.I. Kislukha, Sov. Phys. JETP **44**, 571 (1976); A. S. Davydov, Phys. Rev. B **25**, 898 (1982).
[5] A.S. Davydov, *Solitons in Molecular Systems* (Reidel, Dordrecht, 1985).
[6] J.C. Eilbeck, P.S. Lomdahl, and A.C. Scott, Phys. Rev. B **30**, 4703 (1984).
[7] A.C. Scott, P.S. Lomdahl, and J.C. Eilbeck, Chem. Phys. Lett. **113**, 29 (1985).
[8] A.C. Scott and J.C. Eilbeck, Chem. Phys. Lett. **132**, 23 (1986).
[9] *Davydov's Soliton Revisited*, edited by P.L. Christiansen and A.C. Scott (Plenum, New York, 1991).
[10] T.D. Holstein, Ann. Phys. (N.Y.) **8**, 325 (1959); **8**, 343 (1959).
[11] M. Toda, *Theory of Nonlinear Lattices* (Springer-Verlag, Berlin, 1981).
[12] M. J. Ablowitz and J. F. Ladik, J. Math. Phys. **17**, 1011 (1976).
[13] A.J. Sievers and S. Takeno, Phys. Rev. Lett. **61**, 970 (1988); S. Takeno, J. Phys. Soc. Jpn. **58**, 759 (1989); J.B. Page, Phys. Rev. B **41**, 7835 (1990); K. Hori and S. Takeno, J. Phys. Soc. Jpn. **61**, 2186 (1992); S. Takeno and S. Homma, *ibid.* **60**, 731 (1991); **62**, 835 (1993); S. Takeno, *ibid.* **61**, 2821 (1992); S.R. Bickham, S.A. Kiselev, and A.J. Sievers, Phys. Rev. B **47**, 14 206 (1993); K.W. Sandudsky, J.B. Page, and K.E. Schmidt, *ibid.* **46**, 6161 (1992).
[14] Yu.S. Kivshar and D.K. Campbell, Phys. Rev. E **48**, 3077 (1993).
[15] Yu.S. Kivshar, Phys. Rev. E **48**, 4132 (1993).
[16] R.S. MacKay and S. Aubry, Nonlinearity **7**, 1623 (1994).
[17] S. Flach and C.R. Willis, Phys. Rep. **295**, 181 (1998).
[18] D. Hennig and G.P. Tsironis, Phys. Rep. **307**, 333 (1999).
[19] Ch. Claude, Yu.S. Kivshar, K.H. Spatschek, and O. Kluth, Phys. Rev. B **47**, 14 228 (1992).
[20] Yu.S. Kivshar and M. Salerno, Phys. Rev. E **49**, 3543 (1994).
[21] S. Flach and C.R. Willis, Phys. Rev. Lett. **72**, 1777 (1994).
[22] D. Chen, S. Aubry, and G.P. Tsironis, Phys. Rev. Lett. **77**, 4776 (1996).
[23] D. Hennig, G.P. Tsironis, and H. Gabriel, Phys. Rev. E **49**, 3653 (1994).
[24] P.L. Christiansen, J.C. Eilbeck, V.Z. Enol'skii, and Yu.B. Gaididei, Phys. Lett. A **166**, 129 (1992).
[25] A.A. Vakhnenko and Yu.B. Gaididei, Theor. Math. Phys. **68**, 873 (1986).
[26] D. Cai, A.R. Bishop, and N. Grønbech Jensen, Phys. Rev. E **53**, 1202 (1996).
[27] R. Scharf and A.R. Bishop, Phys. Rev. A **43**, 6535 (1991); M. Salerno, *ibid.* **46**, 6856 (1992); Phys. Rev. B **47**, 14 228 (1993); Yu.S. Kivshar and M. Peyrard, Phys. Rev. A **46**, 3198 (1992); Yu.S. Kivshar and M. Salerno, Phys. Rev. E **49**, 3543 (1994); M.H. Hays, C.D. Levermore, and P.D. Miller, Physica D **79**, 1 (1994); V.V. Konotop, O.A. Chubykalo, and L. Vázquez, Phys. Rev. E **48**, 563 (1993); D. Cai, A.R. Bishop, N. Grønbech-Jensen and M. Salerno, Phys. Rev. Lett. **74**, 1186 (1995); D. Cai, A.R. Bishop, and N. Grønbech Jensen, *ibid.* **72**, 591 (1994); D. Cai, A.R. Bishop, N. Grønbech-Jensen, and M. Salerno, *ibid.* **74**, 1186 (1995); D. Cai, A.R. Bishop, and N. Grønbech Jensen, Phys. Rev. E **52**, 5784 (1995); D. Hennig, K.Ø. Rasmussen, H. Gabriel, and A. Bülow, *ibid.* **54**, 5788 (1996).