Perturbative study of classical Ablowitz-Ladik type soliton dynamics in relation to energy transport in α-helical proteins

K. Kundu
Institute of Physics, Bhubaneswar 751 005, India
(Received 27 July 1999; revised manuscript received 3 December 1999)

Classical Ablowitz-Ladik type soliton dynamics from three closely related classical nonlinear equations is studied using a perturbative method. Model nonintegrable equations are derived by assuming nearest neighbor hopping of an exciton(vibron) in the presence of a full exciton(vibron)-phonon interaction in soft molecular chains in general and spines of α-helices in particular. In all cases, both trapped and moving solitons are found implying activation energy barrier for propagating solitons. Analysis further shows that staggered and nearly staggered trapped solitons will have a negative effective mass. In some models the exciton(vibron)-phonon coupling affects the hopping. For these models, when the conservation of probability is taken into account, only propagating solitons with a broad profile are found to be acceptable solutions. Of course, for the soliton to be a physically meaningful entity, total nonlinear coupling strength should exceed a critical value. On the basis of the result, a plausible modification in the mechanism for biological energy transport involving conformational change in α-helix is proposed. Future directions of the work are also mentioned.

PACS number(s): 05.45.Yv, 05.60.Cd, 82.30.Nr, 87.15.By

I. INTRODUCTION

Integrable nonlinear equations with single soliton and multisolitons solutions constitute a very rich facet, albeit not the only one, of nonlinear dynamics. These integrable equations can either be continuous or discrete. In the first category, we have the famous Korteweg-de Vries (KdV) equation. Another important example is continuous nonlinear Schrödinger equation (CNLSE). In the other category, famous examples include Toda equation and Ablowitz-Ladik equation [1–9]. There is again a class of nonlinear equations that is as such not integrable, but in some way similar to one of the known integrable equations. A good example is Salerno equation [1,10,11]. In such a situation, soliton dynamics can be studied by one or the other prescribed perturbation methods [1,12–16]. Here in this paper, we plan to study soliton dynamics of nonlinear equations that can arise in soft molecular chains due to interaction of excitation with acoustic phonon. Soliton in soft molecular chains arising from above mechanism is generally refered to as Davydov's soliton, which is also an example of envelop soliton [1,17–22]. Other examples of envelop solitons are Zakharov solitons in plasma physics [23] and vibron solitons in nonlinear lattices [24]. Soliton mechanisms have been proposed also in a number of biomolecular and molecular processes [22,25]. One good example in the biological area is the attempt to explain the structural and dynamical flexibility of DNA by a soliton mechanism [22,26–29]. However, most well studied of all is the problem of storage and transport of biological energy by Davydov's soliton in α-helical proteins. The α-helix is a stable structure of proteins. It is a major constituent of structural proteins in hair and skin. It also plays a functional role in the transmembrane proteins that pump ions across the active membrane of nerve cells. We plan to use the problem of biological energy transport as paradigm in our analysis. So, we delineate next the present level of theoretical understanding of the problem [1,17–22,30–36], which is relevant for our purpose.

To understand the significance of Davydov's solitons vis-a-vis the relevant biochemical problem, we note the following. (i) Biological energy is released in units of 0.42 eV [22,30] by the hydrolysis of adenosine triphosphate (ATP) to diphosphate (ADP) and (ii) a basic biological resonance unit is ''C=O'' (or amide-I bond) which has a quantum of energy of 0.205 eV (1610 cm^{-1}) [18,22,31]. Most importantly, amide-I bond is found in every peptide group of every protein. This universality of amide-I bonds in proteins led to the idea that these bonds might be pivotal in the storage as well as in the transport of the biological energy released from the hydrolysis of ATP. However, for this to happen, the lifetime of the excitation in amide-I bonds should be enhanced to the level of biologically important time scale [32]. According to Davydov, such a scenerio is possible on an α-helix protein due to the trapping of vibrational energy in amide-I bonds by interaction with acoustic phonons moving along spines [18,22,31,33].

In an α-helical protein the basic sequence of C and N has a pitch of 5.4 Å [34]. Three spines that are almost longitudinal are superimposed on this basic structure. A spine in an α-helical protein is basically a hydrogen bonded chain. In this chain carbonyl oxygen is hydrgen-bonded to amide hydrogen and it is repeated. An α-helical protein can, therefore, be viewed as an one-dimensional array of unit cells comprised primarily of amide group (H—N—C═O). These unit cells are connected by three soft springs of H-bonds as shown below [1,22,35].

$$\cdots O{=}C{-}N{-}H\cdots O{=}C{-}N{-}H\cdots O{=}C{-}N{-}H\cdots O{=}C{-}N{-}H\cdots O{=}C{-}.$$

So, spines in α-helix are good examples of soft molecular chain as required in Davydov's model. Davydov's model further assumes that excitations are moved along the chain by dipole-dople interaction (J) among amide-I bonds. Davydov's original calculation considers only a single channel or spine. Continuous approximation is used to transform relevant equations of motion to CNLSE. It is further known that CNLSE can sustain both single soliton and multisoliton solutions [5]. An order of magnitude analysis later indicated that the hydrogen bond anharmonicity in a real α-helix is about the right magnitude to support the soliton formation [34,36]. As an alternative to original Davydov's solitons, Takeno proposed the concept of vibron solitons [24]. It is also contended that vibron solitons are possibly better candidates than Davydov's solitons for soliton-like entities in molecular hydrogen-bonded and biological systems.

The influence of the discrete nature of the chain on the soliton dynamics was later studied numerically [31,34,36]. Some analytical information was also obtained by variational method [37]. In another work, the effect of the discrete nature of the chain on the soliton dynamics was studied by a perturbative method [14]. In this work also, as in the original Davydov's model, the acoustic phonon only affects the site energy of the exciton. Authors found both trapped and moving solitons. This result shows that discretization leads to a finite activation energy for enabling the soliton motion and the soliton steering across the chain may be achieved by means of an appropriate external field. We would like to point out that discrete nonlinear equation considered by these authors is nonintegrable. So, the system will have more propensity towards forming trapped solitons than the moving ones. In the context of standard discrete nonlinear Schrödinger equation, this aspect has also been extensively studied [38–48].

It should again be pointed out that acoustic phonon can also affect the the hopping between sites by altering the separation between them [49,50]. This aspect is considered in the numerical analysis, but in conjunction with diagonal coupling. Since, both couplings are considered, this model will be refered to as full model. In our calculations that follow, only nearest neighbor hopping will be allowed. In the numerical work by Scott on the full model, coupling of the acoustic phonon to the dipole-dipole coupling (J) of amide-I vibration is assumed to be nominal. In another numerical work , however, magnitude of these two coupling strengths is considered to be same [34,36]. We further note in this context that in trans-polyacetylene soliton is found by considering only electron-phonon coupling in the hopping term [49,50]. In biological systems, wide-ranging conformational changes are encountered. Given the commonness of the phenomenon in biology, it is indeed possible for the α-helix to undergo a conformational change by which the coupling of the dipole-dipole term (J) to the acoustic phonon might be enhanced to an important degree. So, in this paper along with the full model with the above mentioned restriction on hopping, we consider a model in which acoustic phonon is coupled only to the hopping process (J). The model with sole off-diagonal coupling leads to a nonlinear equation, which is very similar to Ablowitz-Ladik equation, (AL) [9]. As it will be shown later, a solution of this equation can be approximated to a good degree by a broad profile envelope soliton of AL type. On the other hand, the full model as we shall see also, contains a genuine AL part, which is the nonlinearity responsible for the soliton solution. Another interesting nonlinear equation that will be considered here as an offshoot of the full model is modified Salerno equation. Its one of the limiting forms is AL equation. So, the soliton dynamics of these three equations is studied by perturbative method using the soliton of AL equation as the zeroth-order solution [14–16].

The organization of the paper is as follows. In the next section, called formalism, we derive above mentioned nonlinear equations of motion using semiclassical approximation. In this section, we also analyze the structure of the solution of the model with sole off-diagonal coupling. In the following section, we discuss the perturbative calculation and include the pertinent results from three models. We first present the analysis of modified Salerno model. Then, we consider the model with only off-diagonal coupling. We end the section by considering the full model. We discuss then, which comes as a natural consequence of our calculations, a plausible modification in the mechanism for the transport of energy in α-helical proteins. We summarize next major results of the paper. Future scopes emanating from this work are also delineated in this section. In addition, four appendices are included to discuss important points of the perturbative calculation.

II. FORMALISM

A. Derivation of equations of motion

For the purpose of clarity, we focus on the propagation of a vibration, presumably amide-I, along a single spine in an α-helical protein. To model this problem, we use the Hamiltonian, H_{SSH} which is the standard SSH Hamiltonian [49,50] together with the Holstein part, H_{h} [51]. So, we have

$$H_{\mathrm{SSH}}=H^0_{\mathrm{SSH}}+H_{\mathrm{h}}, \tag{1}$$

where

$$H^0_{\mathrm{SSH}}=\frac{1}{2M}\sum_n p_n^2+\frac{K}{2}\sum_n (\beta_n-\beta_{n+1})^2 + \sum_n [J-\alpha(\beta_n-\beta_{n+1})](a^\dagger_{n+1}a_n+a^\dagger_n a_{n+1}) \tag{2}$$

and

$$H_{\mathrm{h}}=-\chi\sum_n (\beta_{n+1}-\beta_{n-1})a^\dagger_n a_n . \tag{3}$$

β_n in these expressions represents the displacement of the nth H-N-C=O unit from its equilibrium position and a_n ($a^\dagger_n$) annihilates (creates) a spinless vibron (a quantum of excitation in the amide-I bond) in a Wannier-type orbital localized at site n. p_n in Eq. (2) is the momentum conjugate to the coordinate β_n and in fact satiesfies $p_n=M\dot{\beta}_n$. The terms involving only the lattice coordinates represent the kinetic energy $[(1/2M)\Sigma p_n^2]$ and the potential energy, $[\frac{1}{2}K\Sigma(\beta_n-\beta_{n+1})^2]$ due to the extension or the compression of H bonds. The vibron hopping term in Eq. (2), which describes

the transfer of a vibron from the carbonyl site to an adjacent one, contains a constant piece (J) plus a term (α), which describes the change in the hopping due to the change in the relative displacement of two adjacent H-N-C=O units. The H_h part of the full Hamiltonian is derived by assuming that the on-site interaction of the amide-I vibration with the lattice acoustic phonon (expansion and contraction of H bonds) changes the self-energy of the vibron [14,52]. Modeling these changes in hopping as well as in site energy by a linear coupling of the lattice coordinates, $(\beta_n-\beta_{n+1})$, $n\in Z$ to the vibrons is clearly an approximation valid only for small deviations from equilibrium. The independence of the diagonal coupling constant, χ on the site indices $\{n\}$ is yet another simplifying approximation in this Hamiltonian. The same thing can also be said about α, the off-diagonal coupling constant. We note that for α-helical proteins, a choice set of parameters for the amide- I mode is $J=9.67\times10^{-4}$ eV, K $=1.21$ eV/Å^2, $\chi=38.7\times10^{-3}$ eV/Å, $\alpha=6.2\times10^{-4}$ eV/Å and $M=114.47$ amu [35]. An *ab initio* SCF-MO calculation gives $\alpha=1.22\times10^{-3}$ eV/Å [53]. Another similar calculation yields $\alpha=4.15\times10^{-4}$ eV/Å [54].

For energy transport in proteins, other modes might also be important for the formation and the propagation of Davydov's solitons [53]. One such good candidate is ν(NH) mode. The same *ab initio* SCF-MO calculation shows that for the ν(NH) mode, magnitudes of J(NH) and α(NH) are quite sensitive to changes in the H-bond length [53]. So, for a more comprehensive study other modes should also be included in the full Hamiltonian. Since, we are primarily interested in the perturbative analysis of soliton formation in Ablowitz-Ladik type equations, for simplicity, we restrict ourselves to one mode only.

To develop the classical description of a single mode and a single quantum vibron dynamics from Eq. (1), we treat $\{p_n\}$ and $\{\beta_n\}$ as classical variables. Furthermore, we consider a normalized state vector, $|\Psi\rangle$ where

$$|\Psi\rangle=\sum_{n\in Z} c_n(t)|n\rangle. \tag{4}$$

$|n\rangle$ is the Wannier state associated with the nth site and due to the normalization condition, we have $\Sigma|c_n|^2=1$. Now taking the expectation value of $H_{\rm SSH}$ over the state vector, $|\Psi\rangle$ we get,

$$\begin{aligned}\mathcal{E}(\{p_n,\beta_n,c_n,c_n^\star\})&=\langle\Psi|H_{SSH}|\Psi\rangle\\&=\sum_n\left[\frac{p_n^2}{2M}+\frac{K}{2}(\beta_n-\beta_{n+1})^2\right]\\&\quad+\sum_n\left[J-\alpha(\beta_n-\beta_{n+1})\right]\\&\quad\times(c_{n+1}^\star c_n+c_n^\star c_{n+1})\\&\quad-\chi\sum_n(\beta_{n+1}-\beta_{n-1})|c_n|^2.\end{aligned} \tag{5}$$

$\mathcal{E}$ in Eq. (5) can be shown to be a constant of motion. So, using this quantity as the relevant classical Hamiltonian, we derive our equations of motion.

$$\begin{aligned}i\hbar\dot{c}_n&=\frac{\partial\mathcal{E}}{\partial c_n^\star}=J(c_{n+1}+c_{n-1})+\alpha(\beta_{n+1}-\beta_n)c_{n+1}\\&\quad+\alpha(\beta_n-\beta_{n-1})c_{n-1}-\chi(\beta_{n+1}-\beta_{n-1})c_n\end{aligned} \tag{6}$$

$$\begin{aligned}M\ddot{\beta}_n&=K(\beta_{n+1}+\beta_{n-1}-2\beta_n)+\alpha(c_{n+1}^\star c_n+c_n^\star c_{n+1})\\&\quad-\alpha(c_{n-1}^\star c_n+c_n^\star c_{n-1})-\chi(|c_{n+1}|^2-|c_{n-1}|^2).\end{aligned} \tag{7}$$

In the general case, the dynamics of the coupled system described by Eqs. (6) and (7) is rather complicated. However, the situation simplifies appreciably, if the inertia of the elastic subsystem can be ignored. Consider two quantities, namely $\mathcal{V}_{ex\ max}$, the maximal velocity of the exciton and $\mathcal{V}_{ac}$, the velocity of sound. If

$$\mathcal{R}=\left(\frac{\mathcal{V}_{ex\ max}}{\mathcal{V}_{ac}}\right)^2\equiv\frac{4MJ^2}{K\hbar^2}\ll1, \tag{8}$$

we then have the desired situation [14]. Since, in the problem of energy transport in proteins, $\mathcal{R}\sim0.08$, the condition (8) is evidently satisfied. Ignoring the inertia term we solve Eq. (7) to obtain

$$(\beta_n-\beta_{n-1})=\frac{\chi}{K}(|c_n|^2+|c_{n-1}|^2)-\frac{\alpha}{K}(c_{n-1}^\star c_n+c_n^\star c_{n-1}). \tag{9}$$

Finally the insertion of Eq. (9) in Eq. (6) yields

$$\begin{aligned}i\hbar\dot{c}_n&=-\frac{\chi^2}{K}(|c_{n+1}|^2+|c_{n-1}|^2+2|c_n|^2)c_n\\&\quad+\frac{\chi\alpha}{K}(c_{n+1}^\star c_n+c_n^\star c_{n+1}+c_{n-1}^\star c_n+c_n^\star c_{n-1})c_n\\&\quad+J(c_{n+1}+c_{n-1})-\frac{\alpha^2}{K}(c_{n+1}^\star c_n+c_n^\star c_{n+1})c_{n+1}\\&\quad-\frac{\alpha^2}{K}(c_{n-1}^\star c_n+c_n^\star c_{n-1})c_{n-1}\\&\quad+\frac{\chi\alpha}{K}(|c_{n+1}|^2+|c_n|^2)c_{n+1}\\&\quad+\frac{\chi\alpha}{K}(|c_n|^2+|c_{n-1}|^2)c_{n-1}.\end{aligned} \tag{10}$$

We next define

$$g=\frac{\alpha^2}{KJ},\quad\gamma=-\frac{\chi^2}{KJ},\quad\delta=\frac{\chi\alpha}{KJ},\quad\lambda=g+2\delta-\gamma,$$

$$\epsilon=\frac{\gamma}{\lambda},\quad\epsilon_1=\frac{\delta}{\lambda},\quad\epsilon_2=\frac{g}{\lambda},\quad\tau=\frac{Jt}{\hbar},$$

$$c_n=\exp(in\pi)\frac{\Phi_n}{\sqrt{\lambda}}\exp(2i\tau),\ \text{and}\ \rho_{nm}=\Phi_n^\star\Phi_m.$$

Introduction of these definitions in Eq. (10) and some simple algebra gives

$$i\dot{\Phi}_n - 2\Phi_n + (1+\rho_{n,n})(\Phi_{n+1}+\Phi_{n-1}) = \mathcal{F}_p(\Phi_n), \quad (11)$$

where

$$\begin{aligned}\mathcal{F}_p(\Phi_n) = {} & \epsilon(\rho_{n+1,n+1}+\rho_{n-1,n-1}+2\rho_{nn})\Phi_n \\ & - \epsilon_1(\rho_{n,n+1}+\rho_{n+1,n}+\rho_{n,n-1}+\rho_{n-1,n})\Phi_n \\ & - \epsilon\rho_{nn}(\Phi_{n+1}+\Phi_{n-1}) \\ & - \epsilon_1[(\rho_{n+1,n+1}-\rho_{nn})\Phi_{n+1} \\ & + (\rho_{n-1,n-1}-\rho_{nn})\Phi_{n-1}] \\ & - \epsilon_2[(\rho_{n,n+1}+\rho_{n+1,n}-\rho_{nn})\Phi_{n+1} \\ & + (\rho_{n,n-1}+\rho_{n-1,n}-\rho_{nn})\Phi_{n-1}]. \end{aligned} \quad (12)$$

When $\alpha=0$, we get from Eq. (11) a variant of discrete nonlinear Schrödinger equation (ADNLSE) where acoustic phonon is considered instead of the usual optical phonon [14]. This equation is studied perturbatively for soliton solutions. When we formally consider the first term of $\mathcal{F}_p(\Phi_n)$, $n \in Z$, we have

$$\begin{aligned} & i\dot{\Phi}_n - 2\Phi_n + (1+\rho_{n,n})(\Phi_{n+1}+\Phi_{n-1}) \\ & \quad = \epsilon(\rho_{n+1n+1}+\rho_{n-1,n-1}+2\rho_{nn})\Phi_n . \end{aligned} \quad (13)$$

We refer to Eq. (13) as modified Salerno equation (MSE). We further note that the quantity, $\mathcal{N}=\Sigma_{n\in Z}\ln[1+|\Phi_n|^2]$ is conserved for MSE. When $\epsilon=0$, we have Ablowitz-Ladik equation [1,9]. This is known to have a single soliton solution. So, for $|\epsilon| \ll 1$, we have an instructive example where the soliton dynamics can be studied by a standard perturbative method [14–16]. Finally when $\chi=0$, we get

$$\begin{aligned} & i\dot{\Phi}_n - 2\Phi_n + (1+\rho_{n,n+1}+\rho_{n+1,n})\Phi_{n+1} \\ & \quad + (1+\rho_{n,n-1}+\rho_{n-1,n})\Phi_{n-1} = 0. \end{aligned} \quad (14)$$

We next analyze Eq. (14) for possible soliton-like solutions.

B. Analysis of Eq. (14) for solitons

In order to gain an understanding of the nature of the solution of Eq. (14) we consider the integrable Ablowitz-Ladik discrete nonlinear Schrödinger equation (ALDNLS). The integrable ALDNLS system of equations reads [1,9,15]

$$i\dot{Q}_n - 2Q_n + (Q_{n+1}+Q_{n-1})(1+|Q_n|^2) = 0, \quad n \in Z. \quad (15)$$

The exact one-soliton solution of the ALDNLS is

$$Q_n(\tau) = \frac{\sinh\mu}{\cosh[\mu(n-x)]}\exp[ik(n-x)-i\aleph] \quad (16)$$

with the following equations for the soliton parameters:

$$\dot{\mu}=0, \ \ \dot{k}=0, \ \ \dot{\aleph}=\omega, \quad (17)$$

$$\omega = 2[1-\cosh\mu\cos k] \quad (18)$$

$$\dot{x} = \frac{2}{\mu}\sinh\mu\sin k. \quad (19)$$

So, for each μ there exists a band of velocities [see Eq. (19)] at which the localized state or the one-soliton state can travel without experiencing any Peierls-Nabarro (PN) pinning due to the lattice discreteness [11,55].

A careful inspection of Eq. (14) reveals that if $|\Phi_{n+1}| \sim |\Phi_n|$, $n \in Z$, it is then a perturbed ALDNLS. To investigate this further we write

$$f(\mu,k) = 2\cosh\mu\cos k \ \text{ and } \ \Phi_n = \frac{1}{\sqrt{2f}}\Psi_n\exp(ikn - i\omega\tau) \quad (20)$$

and both μ and k satisfy Eq. (17). We further define

$$\begin{aligned} F^{(1)}(\Psi_n) = {} & \dot{\Psi}_n + \sin k\left[1+\frac{\Psi_n(\Psi_{n+1}+\Psi_{n-1})}{2\cosh\mu}\right] \\ & \times(\Psi_{n+1}-\Psi_{n-1}) \end{aligned} \quad (21)$$

$$\begin{aligned} F^{(2)}(\Psi_n) = {} & (\omega-2)\Psi_n + \cos k(\Psi_{n+1}+\Psi_{n-1}) \\ & + \frac{\cos k}{2\cosh\mu}\Psi_n(\Psi_{n+1}^2+\Psi_{n-1}^2). \end{aligned} \quad (22)$$

Introducing Eq. (20) in Eq. (14) we obtain $F^{(j)}(\Psi_n)=0$, $j=1,2$ and $n \in Z$. We now assume that

$$\Psi_n = Q_n\exp[-ik(n-x)+i\aleph] \quad (23)$$

and also make use of Eqs. (18) and (19). This, in turn yields

$$F^{(1)}(\Psi_n) = 2\sinh\mu\sin k\tanh[\mu(n-x)]\frac{\Psi_n^5}{(1+\Psi_n^2)^2}$$

$$F^{(2)}(\Psi_n) = -\frac{\cos k}{\cosh\mu}\frac{\Psi_n^3}{(1+\Psi_n^2)} - 2\cosh\mu\cos k\frac{\Psi_n^5}{(1+\Psi_n^2)^2}.$$

If $k \sim (2m+1)\pi/2$, $m \in Z$, $|\sinh(\mu)| \ll 1$ but $|\sinh\mu/\sqrt{\cos k}|$ is finite, Eq. (20) along with Eq. (23) then constitutes a reasonably good approximation to the exact solution of Eq. (14). We next apply a standard perturbative method [14–16] to study sequentially soliton solutions of Eqs. (13), (14), and (11).

III. RESULTS AND DISCUSSION

A. Solitons in the perturbative regime of MSE, Eq. (13)

To apply the perturbation scheme to MSE, Eq. (13), Eq. (16) is used as the zeroth order solution, $\Phi_n^0 = Q_n$, $n \in Z$. In this perturbative scheme, it is further assumed that parameters, k, x, μ, and $\aleph$ depend on time. By means of these dependences the zeroth order approximation, Eq. (16) makes it possible to take into account the main effect of the perturbation, $\epsilon\mathcal{F}_p(\Phi_n)$—the adiabatic adjustment to it of the soliton. The procedure is well laid out in Ref. [14]. This method transforms the evolution of the discrete soliton of Eq. (13) to the analysis of a system of coupled ODE's involving x, k,

TABLE I. Nature of fixed points.

$x_s=\frac{l}{2}$	$k_s=n\pi$	Nature	Stability	$x_s=\frac{l}{2}$	$k_s=n\pi$	Nature	Stability
l	n			l	n		
even	even	hyperbolic	unstable	even	odd	limit cycle	Stable
odd	odd	hyperbolic	unstable	odd	even	limit cycle	Stable

and μ. However, the equation for $\dot{\aleph}$, albeit it can be obtained, is not needed for the analysis [14–16].

Using the standard procedure we derive equations for $\dot{k}$, $\dot{\mu}$, and $\dot{x}$. Inasmuch as $Q_n \exp[-ik(n-x)-i\aleph]$ is real, the perturbation term in MSE does not contribute to $\dot{\mu}$ and $\dot{x}$ [14]. Equations for these three variables are given below.

$$\dot{\mu}=0 \tag{24}$$

$$\dot{x}=2\frac{\sinh\mu}{\mu}\sin k=-2\frac{\sinh\mu}{\mu}\frac{\partial\cos k}{\partial k} \tag{25}$$

$$\dot{k}=\frac{\epsilon}{2}\left(\frac{2\pi}{\mu}\right)^3\sinh^2\mu\ G(\mu,x) \tag{26}$$

where

$$S(\mu,x)=\sum_{s=1}^{\infty}\frac{\frac{\pi^2 s}{\mu}}{\sinh\left(\frac{\pi^2 s}{\mu}\right)}\cos(2\pi s x) \tag{27}$$

$$G(\mu,x)=-\frac{\mu}{2\pi^3}\frac{\partial S(\mu,x)}{\partial x}. \tag{28}$$

We note that μ is a constant. When $\sinh^2\mu<1$ and $\mu\leqslant\pi$ it can be shown that

$$\mathcal{N}\approx\frac{\sqrt{\pi}}{\mu}\sum_{n=1}^{\infty}\frac{(-1)^{n+1}}{n}\frac{\Gamma(n)}{\Gamma\left(\frac{1}{2}+n\right)}\sinh^{2n}\mu. \tag{29}$$

So, μ can be approximately related to the constant of motion, $\mathcal{N}$.

For the fixed point analysis, we note that $\dot{x}_s=0$ yields $k_s=n\pi$, $n=0,\pm1,\pm2\ldots$. Similarly, $\dot{k}_s=0$ yields $x_s=l/2$, $l=0,\pm1,\pm2\ldots$. In the subsequent analysis, we approximate $S(\mu,x)$ by the first term in the sum. For $\mu\leqslant\pi$, this is a reasonable approximation. We define $z_1=x-x_s$ and $z_2=k-k_s$. We further define

$$A(\mu)=2\frac{\sinh\mu}{\mu} \tag{30}$$

$$B(\mu,\epsilon)=2\epsilon\frac{\sinh^2\mu}{\mu^2}\frac{\frac{\pi^2}{\mu}}{\sinh\frac{\pi^2}{\mu}}. \tag{31}$$

In the vicinity of fixed points, we have

$$\dot{z}_1=(-1)^n A(\mu)z_2 \tag{32}$$

$$\dot{z}_2=(-1)^l 4\pi^2 B(\mu,\epsilon)z_1. \tag{33}$$

After some trivial algebra, we get frm Eqs. (32) and (33)

$$\frac{z_1^2}{A(\mu)}-(-1)^{(n+l)}\frac{z_2^2}{4\pi^2 B(\mu,\epsilon)}=\text{Constant}. \tag{34}$$

From Eq. (34), we then get for the fixed points the following results shown in Table I.

We consider now Eqs. (30) and (31). We note that when $\mu\to0$, $A(\mu)\to2$, and $B(\mu,\epsilon)\to0$. On the other hand, when $\mu\to\infty$, $A(\mu)\to2e^{\mu}/\mu$ while $B(\mu,\epsilon)\to2\epsilon e^{2\mu}/\mu^2$. So, for $\epsilon>0$, there exists a μ_c such that $A(\mu_c)-B(\mu_c,\epsilon)=0$. The magnitude of μ_c, of course varies with ϵ. This is shown in Fig. 1. Relevance of this section will be transparent as we proceed further.

From Eqs. (25) and (26) we get

$$\frac{dH_{\text{eff}}}{d\tau}=-2\frac{\sinh\mu}{\mu}\frac{\partial\cos k}{\partial k}\dot{k}-\frac{\epsilon}{2}\left(\frac{2\pi}{\mu}\right)^3\sinh^2\mu\ G(\mu,x)\dot{x}=0. \tag{35}$$

So, within a possible addition of a μ dependent constant, we have

$$H_{\text{eff}}(\mu,\epsilon,k,x)\approx-A(\mu)\cos k+B(\mu,\epsilon)\cos2\pi x. \tag{36}$$

Since, we are considering $\mu\leqslant\pi$, $S(\mu,x)$ in Eq. (35) is again approximated by the first term of the sum in Eq. (27). We further note that H_{eff} is periodic both in k and x. It is easily seen from Eq. (36) that

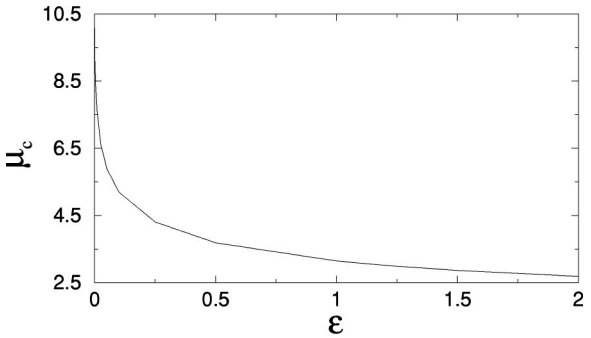

FIG. 1. This figure pertains to modified Salerno equation (MSE), Eq. (13) in the text. It shows the dependence of the critical value of μ, μ_c on the parameter, ϵ for $H_{\text{eff}}(\mu,\epsilon,k,x)$, Eq. (36) derived from MSE. Both μ_c and ϵ are dimensionless. Further details are given in the text.

$$\dot{x}=\frac{\partial H_{\rm eff}}{\partial k} \quad \text{and} \quad \dot{k}=-\frac{\partial H_{\rm eff}}{\partial x}. \tag{37}$$

We should also note that $H_{\rm eff}(\mu,\epsilon,k,x)$ is a constant of motion and it defines approximately the total energy in the soliton. It is to be noted that a potential energy ensues due to imparting of nonintegrability in Eq. (13) by the perturbation term. Denoting this potential by $\Delta U(\mu,\epsilon)$ we find that

$$\Delta U(\mu,\epsilon)=H_{\rm eff}(\mu,\epsilon,0,0)-H_{\rm eff}\left(\mu,\epsilon,0,\frac{1}{2}\right)=2B(\mu,\epsilon). \tag{38}$$

So, the effect of nonintegrability disappears if $\epsilon=0$ or becomes negligible if $\pi^2/\mu \gg 1$.

From Eq. (36) we find that $E_{\rm min}=-[A(\mu)+B(\mu,\epsilon)]$ and $E_{\rm max}=[A(\mu)+B(\mu,\epsilon)]$. We further define $U_0(\mu,\epsilon,x)=B(\mu,\epsilon)\cos 2\pi x$ and $U_{\pm}(\mu,\epsilon,x)=U_0(\mu,\epsilon,x)\pm A(\mu)$, because this will not change equations of motion. We then get $E_{\rm min}\leqslant U_{-}\leqslant(B-A)$ and $(A-B)\leqslant U_{+}\leqslant E_{\rm max}$. We now consider different cases for the dynamics. These are also shown in Figs. 2(a) and 2(b) respectively. Figure 2(a) describes the situation for $\mu<\mu_c$ while Fig. 2(b) is for $\mu>\mu_c$. Furthermore, in Fig. 2(b) we define $k=2\pi\Phi$ to make the figure symmetric. We consider now the dynamics in the spatial or x direction.

Case I : $\mu<\mu_c$. So, $A(\mu)>B(\mu,\epsilon)$.

(i) $-(A+B)=E_{\rm min}<E<(B-A)<0$. In this limit, the soliton is in the potential well defined by U_{-}. So, the dynamics in x is finite and oscillatory. (ii) $(B-A)<E<(A-B)$. Since, $U_{-}<E<U_{+}$, the motion in x is infinite. In other words, we get propagating solitons. (iii) $(A-B)<E<(A+B)=E_{\rm max}$. In this case, the soliton is in the potential well defined by U_{+}. So, the motion in x is again finite and oscillatory.

Case II : $\mu>\mu_c$. So, $A(\mu)<B(\mu,\epsilon)$.

In this case, since $(B-A)>0$, there is no region in the energy domain where the soliton will not experience any potential energy for its motion in the x direction. So, the motion in x is always finite and oscillatory.

We consider next the other scenerio of the dynamics in the k direction. We define $u_0(\mu,k)=-A(\mu)\cos k$ and $u_{\pm}(\mu,\epsilon,k)=u_0\pm B(\mu,\epsilon)$. We then have the following situations.

(i) $-(A+B)<E<(A-B)<0$. In this case, the soliton is inside the potential, u_{-}. So, the motion in the k space finite and oscillatory. (ii) $0<(A-B)<E<(B-A)>0$. The motion in the k direction is infinite due to the absence of a confining potential in this energy range. This is shown in Fig. 2(b) by two broken curves lying on respective separatices. (iii) $(B-A)<E<(B+A)$. The soliton experiences the potential u_{+} in the k direction. So, the corresponding motion is finite and oscillatory. (iv) For $\mu<\mu_c$, $A(\mu)>B(\mu,\epsilon)$. So, it is clear from the analysis of the motion in the x direction that the motion in k will always be finite and oscillatory.

For further understanding of the dynamics, we consider $H_{\rm eff}$ given by Eq. (36) around $k=0$ and $k=\pm\pi$. We find around $k=0$ that

$$H_{\rm eff}\approx\frac{1}{2}A(\mu)k^2+U_{-}(\mu,\epsilon,x). \tag{39}$$

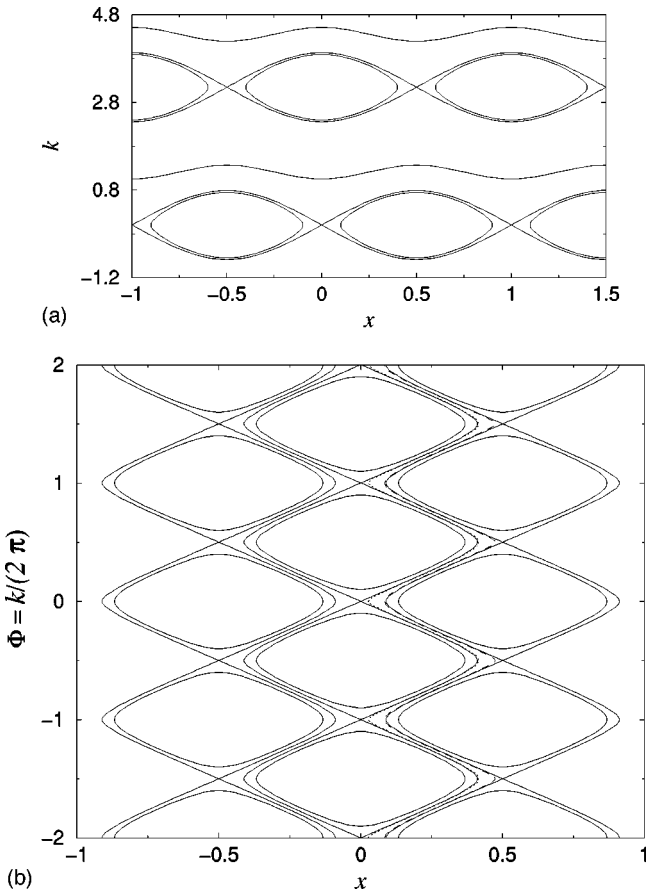

FIG. 2. (a) This figure pertains to MSE, Eq. (13) in the text. This figure shows the phase diagram of the dynamics of solitons in the (x,k) plane, which is derived from $H_{\rm eff}(\mu,\epsilon,k,x)$ given by Eq. (36) in the text. For this case, $\epsilon=1.0$. So, $\mu_{\rm c}=\pi$. Since, $k_{\rm cr}$ is taken to be $\pi/4$ as a choice, this in turn gives $\mu=2.052$ from Eq. (41) in the text. So, this is the phase diagram for $\mu<\mu_{\rm c}$. All quantities are dimensionless. (b) This figure pertains to MSE, Eq. (13). $\mu=3.2$. Since, all other parameters and details are same as in Figure 2(a), it is the figure for $\mu>\mu_{\rm c}$. However, here $k=2\pi\Phi$. So, this is the phase diagram in the (x,Φ) plane instead of usual (x,k) plane. This is done to make the figure symmetric. Two propagating modes in the Φ-direction are shown by broken curves. Again, all quantities are dimensionless.

So, the effective mass of the soliton, $m_{\rm eff}$ is $A(\mu)^{-1}$. For $\mu\ll 1$ we get $m_{\rm eff}\approx\ m_0(1-\mu^2/6)$ where the rest mass, m_0 is taken to be $\frac{1}{2}$. This implies that the presence of integrablity reduces the effective mass of the soliton. Again from Eqs. (32) and (33), we find that the frequency, ω of the small vibrations of the soliton center of mass near the bottom of the potential well is

$$\omega=2\pi\sqrt{A(\mu)B(\mu,\epsilon)}. \tag{40}$$

It is also clear from the discussion that there is a critical value of k, $k_{\rm cr}$ such that for $k>k_{\rm cr}$, we shall get spatially propagating soliton. For $\mu<\mu_{\rm c}$, $k_{\rm cr}$ is given by the following equation

$$k_{\rm cr}=\arccos\left[1-\frac{2\ B(\mu,\epsilon)}{A(\mu)}\right]. \tag{41}$$

We also note that, inasmuch as $B(\mu,\epsilon)\to 0$ for $\pi^2/\mu \gg 1$, $k_{cr}\to 0$. On the other hand, when $\mu=\mu_c$, $k_{cr}=(2n+1)\pi$, $n=0,\pm 1,\pm 2\ldots$. For $\mu>\mu_c$, Eq. (41) shows that no k_{cr} exists.

Around $k=\pm\pi$, we write $k=\pm\pi-\theta$. Then, from Eq. (36) we get

$$H_{\text{eff}}=-\frac{1}{2}A(\mu)\theta^2+U_+(\mu,\epsilon,x). \tag{42}$$

When $k=0$, we have an unstaggered localized state, while for $k=\pm\pi$, we have a staggered localized state. We note that for these values of k, the velocity of the Ablowitz-Ladik soliton is zero. We find that for staggered as well as nearly staggered localized states, m_{eff} of the localized soliton is negative. Obviously, a localized state of a negative effective mass is mechanically unstable at a minimum of $U_+(\mu,\epsilon,x)$. So, the staggered as well as nearly staggered localized states will either be pinned or oscillate at the top of the potential. This is precisely found because at the top of U_+, k is $\pm\pi$. So, the kinetic energy is zero. This is consistent with the numerical result in Ref. [11].

Finally, we note that the analysis in this section is done within the leading order approximation by assuming that $\epsilon>0$. When $\epsilon<0$, we set $x=y\pm\frac{1}{2}$. Then, within the same leading order analysis and in variables y and k, result will remain the same. We consider now the addition of the second term of $\mathcal{F}_p(\Phi_n)$ [Eqs. (11) and (12)] to Eq. (13). A careful inspection of formulas given in Refs. [14] and [15] will show that this term will not contribute to equations for $\dot{x}$ and $\dot{\mu}$. Again, it can be simply shown that this term also does not contribute to the equation for $\dot{k}$. In other words, in this perturbation scheme, the term is innocuous.

B. Perturbed Ablowitz-Ladik soliton dynamics of Eq. (14)

To apply the perturbation scheme to Eq. (14), we note that for this case Eqs. (11) and (12) take the following form

$$i\dot{\Phi}_n-2\Phi_n+(1+\rho_{n,n})(\Phi_{n+1}+\Phi_{n-1})=\epsilon_2\mathcal{F}_p(\Phi_n), \tag{43}$$

where

$$\epsilon_2\mathcal{F}_p(\Phi_n)=-(\rho_{n,n+1}+\rho_{n+1,n}-\rho_{nn})\Phi_{n+1}-(\rho_{n,n-1}+\rho_{n-1,n}-\rho_{n,n})\Phi_{n-1}. \tag{44}$$

Again, the standard method transforms the evolution of the discrete soliton of Eq. (14) to the analysis of a system of coupled ODE's involving x, k, and μ [14–16]. Equations for first two variables read

$$\dot{k}=\left(\frac{2\pi}{\mu}\right)^3[\sinh\mu\cos k]^2\ G(\mu,x) \tag{45}$$

$$\dot{\mu}=\tanh\mu\tan k\ \dot{k}, \tag{46}$$

where $G(\mu,x)$ is is given by Eqs. (27) and (28). From Eqs. (45) and (46) we find that

$$\sinh\mu\cos k=c=\text{Constant}. \tag{47}$$

To understand the physical origin of Eq. (47) we examine our ansatz, Eq. (16). We note that x has the dimension of length while both μ and k have the dimension of inverse length or momentum. So, both of these cannot be simultaneously conjugate variables to x. Consequently, these two variables must be related by a functional relationship as in Eq. (47). For the full problem where phonons alter both site energies and hopping, μ and k are also found to be related. However, the relationship is not as trivial as Eq. (47) and it will be discussed later. The equation for the remaining variable, x reads

$$\dot{x}=F(\mu,x)\sinh\mu\tanh\mu\sin k, \tag{48}$$

where $F(\mu,x)$ is defined as follows.

$$S_1(\mu,x)=\sum_{s=1}^{\infty}\left\{\left[\frac{\frac{\pi^2 s}{\mu}}{\sinh\left(\frac{\pi^2 s}{\mu}\right)}\right]^2\cosh\left(\frac{\pi^2 s}{\mu}\right)\cos(2\pi s x)\right\}$$

$$f_1(c,\mu)=\frac{2\left[1+2c\coth(2\mu)-\frac{2c}{\mu}\right]}{\mu^2}$$

$$F(\mu,x)=f_1(c,\mu)[1+2S(\mu,x)]+\frac{2c}{\mu^3}[1+2S_1(\mu,x)] \tag{49}$$

and $S(\mu,x)$ has already been defined by Eq. (27). To derive these formulas [Eqs. (26), (29), (45), (46), and (49)], we have made use of the famous Poisson's sum formula [14,56], which reads

$$\sum_{n=-\infty}^{\infty}f(n\mu)=\frac{1}{\mu}\int_{-\infty}^{\infty}dy\left[1+2\sum_{s=1}^{\infty}\cos\left(\frac{2\pi s y}{\mu}\right)\right]f(y). \tag{50}$$

Other relevant integrals are given in Appendix A.

To obtain fixed points for this of set ODE's we set $\dot{x}_s=0$ and $\dot{k}_s=0$. We further note that $\dot{k}_s=0$ also implies that $\dot{\mu}_s=0$ [Eq. (46)]. By comparing Eqs. (45) and (48) with Eqs. (26) and (25) respectively, we find that this system also has two sets of fixed points. Two sets together gives $\{x_s,k_s\}=\{l/2,(n\ \pi)\}$, $l\&n\in Z$. Dependence of fixed points on l and n for this case is also similar to the case of MSE. Hence, here too Table I holds good. The structure of fixed points then tells that below a threshhold energy, only oscillatory localized states will exist. It is again easy to see from Eqs. (45) to (49) that if $\sinh\mu\tanh\mu\sin k\neq 0$, we then have

$$F(\mu,x)\frac{d\mu}{d\tau}+\left(\frac{\partial\tilde{H}_{eff}}{\partial x}\right)\frac{dx}{d\tau}=0, \tag{51}$$

where

$$\tilde{H}_{eff}(\mu,x,c)=\frac{4c}{\mu^2}S(\mu,x). \tag{52}$$

$S(\mu,x)$ is given by Eq. (27). We further define

$$\frac{dh(\mu,c)}{d\mu}=f_1(c,\mu)+\frac{2c}{\mu^3} \tag{53}$$

and

$$H_{\rm eff}(\mu,x,c)=h(\mu,c)+\tilde{H}_{eff}(\mu,x,c). \tag{54}$$

The evaluation of $h(\mu,c)$ is given in Appendix B. After some trite algebra it can be shown that

$$\frac{dH_{\rm eff}(\mu,x,c)}{d\tau}=-\frac{4\left[1+2c\coth(2\ \ \mu)+\frac{c}{\mu}\right]}{\mu^2}S(\mu,x)\frac{d\mu}{d\tau}. \tag{55}$$

Equations (45) and (46) define $d\mu/d\tau$. So, if $|\mu|$ is suitably bounded ($|\mu|\leqslant\pi$), we have an approximate constant of motion. This can be called an approximate effective Hamiltonian (see also Appendix C). Equations for $\dot{x}$, $\dot{\mu}$, and $\dot{k}$ are derived in Appendix D using the Poisson bracket formalism and the effective Hamiltonian given by Eq. (54). The phase diagram of the motion of the soliton in the (x,k) plane derived from Eqs. (47) and (54) for $c=2.0$ is shown in Figs. 3(a) and 3(b). While Fig. 3(a) shows the periodicity of the motion in the x direction, Fig. 3(b) gives us the picture in the k direction. This is a typical phase diagram showing both oscillatory localized solitons as well as propagating solitons. Again Fig. 4 shows the motion in the x direction for $c=1.2$. By comparing Figs. 3(a) and 4, we see that as $c\rightarrow 0$, the motion of the soliton tends to become free.

What happens if we use the ansatz (20) instead of (16)? Of course, $(\omega\tau)$ is replaced by $\aleph$. No significant change occurs. Since, we have to assume that both k and μ depend on time, an extra term will be added to the perturbation term [Eq. (44)]. However, its contribution to the evolution equations [Eqs. (45), (46), and (48)] can be shown to be zero. Furthermore, in these equations one factor of c is replaced by $\tanh\mu/4$. Again, the same procedure can be used to find the corresponding effective Hamiltonian.

C. The effect of normalization on the perturbative solution of Eq. (14)

We use here ansatz (20) instead of (16). The reason will be self evident. We note that $\Sigma|c_n|^2=1$, $n\in Z$ implies that $\Sigma_n|\Phi_n|^2=\lambda=g$. Now introducing Eqs. (20) and (23) and applying Eq. (50) we obtain

$$2g\cos k\ =\frac{\sinh\mu\tanh\mu}{\mu}[1+2S(\mu,x)]. \tag{56}$$

We now note that when $|\mu|\ll 1$, both $S(\mu,x)$ and $G(\mu,x)$ go to zero as $\exp[-(\pi^2/\mu)]$. So, in this limit the second term of Eq. (56) can be ignored. We also note that $\dot{\mu}\approx 0$ and $\dot{k}\approx 0$ in this limit. In other words both μ and k become practically time invariant. Another consequence is that Eq. (47) in practical terms becomes redundant also. Equation (56) then gives $\mu\approx 2g\cos k$ or $\mu_{max}\approx 2g$. The minimum soliton size (σ_m) is approximately $2\mu_{max}^{-1}$. We again note that in this limit

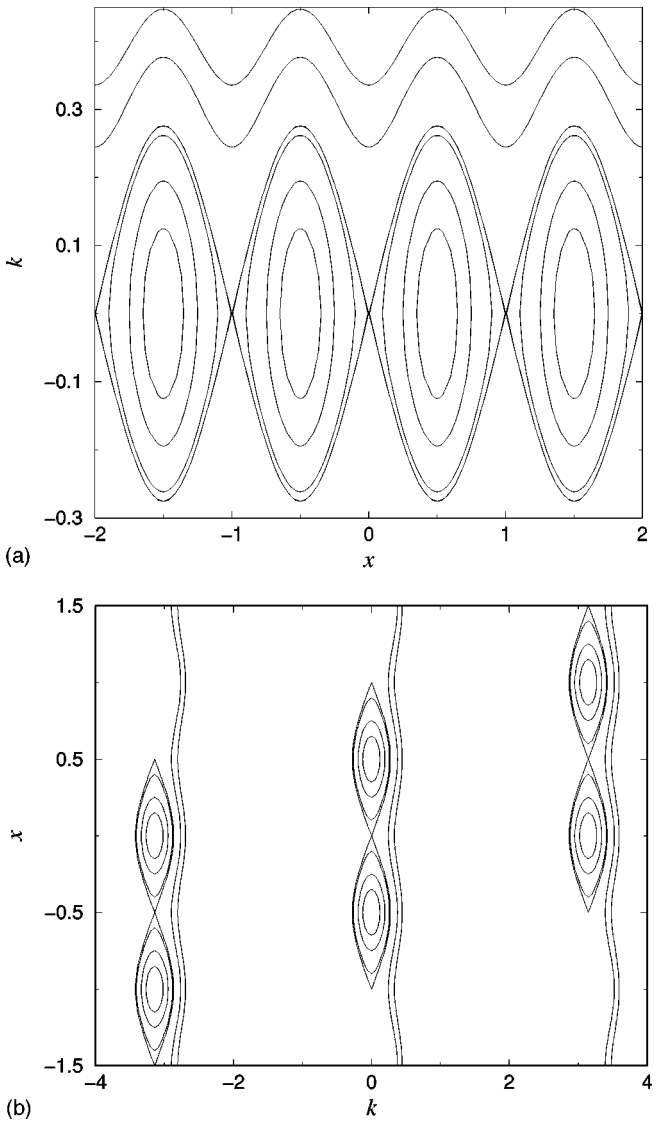

FIG. 3. (a). This figure pertains to the model with sole off-diagonal coupling. It is obtained from the corresponding, $H_{\rm eff}(\mu,x,c)$ given by Eq. (54) in the text. It shows the phase diagram of the dynamics of solitons in the x direction in the (x,k) plane for $c=2.0$. $\mu_s=\sinh^{-1}(c)=1.44$. All quantities are dimensionless. Further details can be found in the text. (b). It is again for the same model as in Fig. 3(a). It shows the dynamics of solitons in the k direction. $|c|=2.0$. Again all quantities are dimensionless. For two figures in the flanks, $k_{\pm}=k\pm\pi$. Also, $x_{k_{\pm}}=x\pm 0.5$.

$$\langle n\rangle=\sum_{n=-\infty}^{\infty}n|c_n|^2=x. \tag{57}$$

So, x becomes the center of mass of the distribution of the soliton packet. A striaght forward asymptotic analysis of Eq. (49) gives from Eq. (48)

$$\frac{dx}{d\tau}=2\left[\frac{\sinh\mu\tanh\mu}{\mu^2}\right]\sin k \tag{58}$$

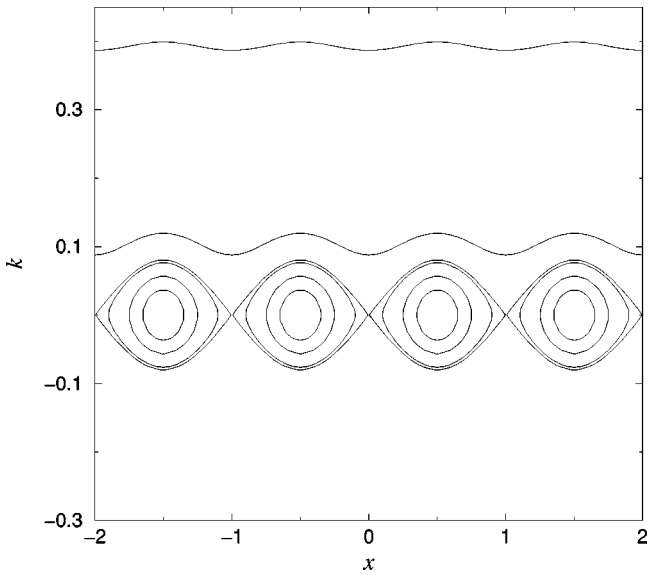

FIG. 4. It shows the phase diagram of the dynamics of solitons for the same model in the x direction but for $c=1.2$. $\mu_s=\sinh^{-1}(c)=1.016$. All quantities are dimensionless.

which is practically the velocity of AL solitons. Inasmuch as $\tau=|J/\hbar|t$, from Eq. (58) we get that the maximum velocity of the soliton, $\mathcal{V}_{ms}\approx 2\ |J/\hbar|$. For the amide-I, our calculation gives $\mathcal{V}_{ms}\sim\ 1.32\times\ 10^3$ m/s. For the calculation, the distance between two carbonyl groups is taken 4.5 Å [31]. $\mathcal{V}_{ms}$ is approximately 0.29 of the sound velocity in the spine [34,36]. Another interesting quantity is the extent of contraction or expansion of the chain due to the soliton formation. It is calculated below along with its definition [14].

$$\lim_{N\to\infty}(\beta_{N,s}-\beta_{-N,s})=-\frac{2\alpha}{K}\sum_{n=-\infty}^{\infty}\Re[c_n c_{n-1}^{\star}]$$
$$=\frac{2J}{\alpha}\sum_{n=-\infty}^{\infty}\Re[\Phi_n\Phi_{n-1}^{\star}]$$
$$=\frac{J}{\alpha}\tanh\mu. \tag{59}$$

So, for $\mu>0$ and J and α having the same sign, the chain will expand due to soliton formation. To understand its physical origin, we note that Eq. (14) is nonintegrable. So, moving solitons in this model should eventually be pinned [14,55]. This can be achieved here only by reducing the intersite transfer rate or equivalently by increasing bond lengths.

Finally, for the amide-I vibration, $\alpha(I)$ under normal physiological condition does not appear to exceed 2 pN [1 pN$\approx 6.24\times 10^{-4}$ eV/ Å]. For ν(NH), α(NH)$\sim$3 pN [53]. So, the magnitude of α for either of these two modes is not large enough to give a physically relevant value of σ_m. If $\alpha\sim 10$ pN, we get $\sigma_m\sim 30$ units. So, this can be taken as a crude critical value of α. We note in this context that in the numerical simulation in Ref. [36], the magnitude of α is allowed to vary from 20 to 60 pN. We further note that in α-helix under physiological conditions, $R(\mathrm{N}\cdots\mathrm{O})$, where R stands for the bond-length, is 2.79 ± 0.12 Å [22]. For the amide-I mode, it is also found theoretically that $\alpha(I)$ changes fron 2 to 3 pN if R(N---O) is changed from 2.916 to 2.722 Å [53]. For a similar change in $R(\mathrm{N}\cdots\mathrm{O})$, α(NH) for the ν(NH) mode changes from 3 to 8 pN [53]. Noteworthy sensitivity of α(NH) towards the change in $R(\mathrm{N}\cdots\mathrm{O})$ might have an important bearing on the mechanism of energy transport in proteins. This will be discussed later.

D. Perturbed Ablowitz-Ladik soliton in the full problem, Eq. (11)

We first note that Eq. (11) has a genuine Ablowitz-Ladik term, which is needed for a stable soliton. This arises due to coupling of diagonal and off-diagonal exciton(vibron)-phonon interactions. Using the perturbation scheme equations for $\dot{k}$ and $\dot{\mu}$ for the full problem are derived. To write equations for these two variables in compact form, we first define

$$G_1(\mu,x)=\frac{2}{\lambda}\left(\frac{\pi}{\mu}\right)^3\sinh^2\mu\ G(\mu,x) \tag{60}$$

$$M(k,\mu)=\left(\delta\frac{\sin k}{\cosh\mu}+2g\sin 2k\right)\tanh\mu \tag{61}$$

$$N(k,\mu)=2\gamma-\delta\frac{\cos k}{\cosh\mu}+4g\cos^2 k. \tag{62}$$

$G(\mu,x)$ is defined by Eq. (28). With these definitions we then have

$$\dot{k}=N(k,\mu)G_1(\mu,x)\quad\text{and}\quad\dot{\mu}=M(k,\mu)G_1(\mu,x). \tag{63}$$

So, the differential equation that defines a functional relationship between μ and k is $Mdk/dt-Nd\mu/dt=0$. The corresponding Pfaffian differential equation is $Mdk-Nd\mu=0$. We next consider two special cases. Case I : $\delta=0$. In this limit we have $\sinh^2\mu(\gamma+2g\cos^2 k)=$Constant. When $\gamma=0$, we get back Eq. (47). Case II : $\delta\neq 0$ but $g=0$. Physically this means that the off-diagonal coupling is sufficiently weak so that α^2 can be neglected. In this limit, we find that

$$\phi(k,\mu)=2\gamma\mu+\coth\mu(\delta\cos k/\cosh\mu-2\gamma)=\text{Constant}.$$

When $\delta=0$, it gives $\mu=$Constant, which agrees with the literature result [14].

In the general case, we have a Pfaffian differential equation of two variables, k and μ. According to the theorem [57], it will always possess an integrating factor, $\beta(k,\mu)$ [Appendix C]. So, there will always be a function, $\phi(k,\mu)$ such that

$$d\phi\ =\beta(Mdk-Nd\mu)=0.$$

Once, β is found from the appropiate ODE, the relation between k and μ can be found [57]. But, the problem does not appear to have any closed form analytical solution defying in turn a closed form analytical expression of H_{eff} for the full model. But, we note that the general case in spite of its structural complication, is similar in one important aspect at least to the case of purely off-diagonal coupling model. Both

μ and k vary with time in the general case also. So, the normalization condition will impose adiabatic variation of both variables in time as found in the previous case. This in turn needs $\pi^2/\mu \gg 1$, which is very easily deducable from Eq. (63). Consequently, the constraint relating μ and k can be treated as redundant in this limit of $\pi^2/\mu \gg 1$. Again, it is deducable from the previous model that without the normalization condition, the full model will also give both trapped and moving solitons. So, from known results and our calculations we see that due to off-diagonal coupling, however small, together with normalization condition full model will also prefer a moving soliton.

Since, for this model $\Sigma|c_n|^2=1$, $n \in Z$ implies $\Sigma_n|\Phi_n|^2 = \lambda$, we obtain in the limit of $\pi^2/\mu \gg 1$, $\lambda \approx 2\sinh^2 \mu/\mu$. Of course, to obtain this result, Eqs. (16) and (50) are made use of. Again, when $\pi^2/\mu \gg 1$, we see from Eq. (57) that x approximately determines the center of mass of the soliton. So, $\dot{x}$ is the velocity of the profile. In this limiting situation, the full model then gives

$$\dot{x} \approx 2\frac{\sinh\mu\tanh\mu}{\mu^2}\sin k + \frac{\delta}{\lambda}2\frac{\sinh\mu}{\mu}\left[1-\frac{\tanh\mu}{\mu}\right]\sin k. \tag{64}$$

We first note that in Eq. (64), there is a component in the velocity that is the velocity of Ablowitz-Ladik soliton. It is due to the genuine Ablowitz-Ladik term in Eq. (11). When all parameters have same sign, we have both $\delta > 0$ and $\lambda > 0$. Then a comparison with with Eq. (58) shows that the presence of both diagonal and off-diagonal couplings increases the velocity of the soliton. Now, in the numerical front, when we take $\chi = 40$ pN and $\alpha = 1$ pN as in Ref. [31], we get $\lambda \approx 0.56$ which, in turn gives $\mu = 0.273$. We then get $c\pi^2/\mu \approx 36$. So, the condition to use Eq. (64) is satisfied. We get from these data $\delta/\lambda \approx 0.024$. Consequently, the full model gives that the maximum velocity of soliton, $\mathcal{V}_{ms} \approx 1.3\times 10^3$ m/s. Corresponding result from numerical simulation is $\mathcal{V}_{ms} \approx 1.7\times 10^3$ m/s [31]. The intersite distance (d) in both cases is 4.5 Å [31]. We further get that the minimum soliton size, $\sigma_m \approx 7$. Next quantity to calculate is the extent of contraction or expansion of the chain due to soliton formation. To obtain this we introduce ansatz (16) to the definition [14]. This then gives

$$\lim_{N\to\infty}(\beta_{N,s}-\beta_{-N,s}) = 2\left[\frac{\chi}{K}+\frac{\alpha\mu}{K}\frac{\cos k}{\sinh\mu}\right]. \tag{65}$$

We next discuss the problem of soliton pinning and its effects on biological energy transport.

E. Soliton pinning and biological energy transport

There are two facets in the energy propagation, (1) an effective trapping of energy and (2) its effective release followed by its dissipation-free propagation to the desired location. Energy can be effectively trapped by diagonal coupling of the vibron to the phonon. In this context, a possibility that natural proteins may absorb radiation into a state that is optically self trapped and then relax to a state that is acoustically self trapped with a longer lifetime, is also proposed [1,58]. However, the moving soliton formed by diagonal coupling cannot be a very effective mechanism for the transport of energy. The system is inherently discrete. This discreteness will cause PN retardation to the moving soliton. Eventually, the soliton will be pinned due to the PN potential arising from the discreteness [11,55]. In mathematical language, nonintegrable character of the model equation will have a dominant effect. So, the relevance of the calculation involving only off-diagonal coupling of vibron with phonon in the spine is paramount. We first note that the model shows, just like in the diagonal case, both trapped and propagating solitons. However, when the conservation of the probability is taken into account, Ablowitz-Ladik type soliton is found in the propagating mode. This is definitely an important result. Albeit the calculation is done in the perturbative scheme, it is clear beyond doubt that an element of off-diagonal coupling, however small, is needed for the effective propagation of a soliton or a soliton-like moiety. This is further substantiated by the full model where both couplings are considered. Of course, the present formalism also shows that off-diagonal coupling cannot altogether remove PN pinning problem. Since, our model equation, Eq. (14) is comparable to AL equation, we expect that PN pinning will be suppressed considerably. Definitely, the propensity for the formation of self-localized states due to PN pinning should be investigated in detail. Regarding other two calculations, we note that the problem of pinning of solitons by PN potential in Salerno model is studied extensively by numerical integration [11]. It is found that solitons get pinned faster and faster as the strength of the nonintegrable term increases. This problem of pinning of solitons will not be any different for MSE, Eq. (13). In the full model we have the requisite AL nonlinear term which arises due to coupling of diagonal and off-diagonal interactions. Although AL term makes solitons transparent to PN potential, the relevant equation [Eq. (11)] also has extensive nonintegrable terms. So, the soliton in this model will also be pinned. We, however, expect that by increasing the off-diagonal coupling and concomitantly reducing the diagonal coupling, this pinning problem can be significantly reduced. This aspect needs thorough investigation.

We note in continuation that $\alpha(I)$ for the amide-I vibration in α-helix is very insensitive to the change in $R(\mathrm{N}\cdots\mathrm{O})$, where R stands for the bond-length. On the other hand, $\alpha(\mathrm{NH})$ for $\nu(\mathrm{NH})$ is very sensitive to any alternation in $R(\mathrm{N}\cdots\mathrm{O})$. Relevant theoretical data are quoted in the text. In view of the discussion above, we propose the following modification to the existing mechanism. In our scheme, to facilitate the transport, α-helix undergoes a conformational change which changes $R(\mathrm{N}\cdots\mathrm{O})$. In this conformationally changed system, energy is transferred from the amide-I mode to the neighboring $\nu(\mathrm{NH})$ mode or modes where the off-diagonal vibron-phonon coupling is sufficiently strong. This will aid the propagation of energy by a soliton like entity. At the concluding stage the system undergoes another conformational change either locally or globally to trap the soliton at the point of capture by enhancing or introducing anew diagonal vibron-phonon coupling. To the best of my knowledge, this mechanism of energy transfer has not been studied so far, at least in details.

IV. SUMMARY

The formation of moving soliton due to full exciton (vibron)-phonon coupling in a soft molecular chain in gen-

eral and in a spine of an α-helix in particular is studied here. This study is done within the framework of a Hamiltonian which contains the standard SSH part and a Holstein part. Relevant nonlinear equations are obtained using antiadiabatic approximation. An interesting nonlinear equation that is derived here for the first time as an offshoot of the full model is modified Salerno equation. This equation can be considered to describe a truncated model for biological energy transport. Again, this equation is studied by perturbative method for soliton dynamics. Analysis shows that nonintegrability in the equation introduces finite activation energy for enabling solitonic motion. This model also shows staggered and unstaggered localized states. Furthermore, staggered and nearly staggered localized states are shown to have negative effective mass. Perturbative analysis of the model with sole off-diagonal coupling also confirms that nonintegrability introduces finite activation energy for solitonic motion. It is further found from this model that an element of off-diagonal coupling, however small, and the conservation of the probability together give a propagating soliton. This in my opinion is a very important result. In the full model, the AL nonlinear term that stabilizes solitons is found. This term arises due to coupling of diagonal and off-diagonal exciton-phonon interactions. It is also suggested that the magnitude of off-diagonal coupling should be enhanced in the full model to reduce PN pinning problem that may be experienced by moving solitons. So, a full analytical calculation involving both diagonal and off-diagonal couplings, if possible, is desirable to discern the importance of both couplings. Again, models involving more than one mode should be considered. Other refinement in the theory will need the consideration of mechanical interaction between oscillators with more complex structure. Finally, these calculations might also be useful in understanding proton transport in biological systems and exciton transport in nonbiological hydrogen-bonded systems.

APPENDIX A: RELEVANT INTEGRALS

Following integrals are required for the perturbative calculation.

$$I(a,\beta)=\int_0^\infty \frac{\cos(ax)}{[\cosh(\beta x)]^2}dx=\frac{a\pi}{2\beta^2\sinh\left(\frac{a\pi}{2\beta}\right)} \tag{A1}$$

and $\beta>0$. This integral can be found in Ref. [59].

$$J(a,\mu)=\int_{-\infty}^{\infty}\frac{\cos(ax)}{[\cosh(x)\cosh(x-\mu)]^2}dx$$
$$=\frac{2\pi a\left[\sin\left(\frac{a\mu}{2}\right)\right]^2}{\left[(\sinh(\mu))^2\sinh\left(\frac{a\pi}{2}\right)\right]}$$
$$-\frac{2\pi a}{\left[(\sinh(\mu))^2\sinh\left(\frac{a\pi}{2}\right)\right]}\left[1-\coth(\mu)\frac{\sin(a\mu)}{a}\right]. \tag{A2}$$

Other two integrals that we need are $J(0,\mu)$ and $\partial J(a,\mu)/\partial a$. Furthermore, for all integrals involving the parameter a, we set $a=2\pi s/\mu,\ s\in Z$.

APPENDIX B: CALCULATION OF $h(\mu,c)$

For $\mu^2<\pi^2$, we have [59]

$$\coth\mu=\frac{1}{\mu}\left[1+\sum_{k=1}^{\infty}\frac{2^{2k}B_{2k}}{(2k)!}\mu^{2k}\right] \tag{B1}$$

where B_{2k} is the Bernoulli number of order $(2k)$ with the following expression [59].

$$B_{2k}=(-1)^{k-1}\frac{2(2k)!}{(2\pi)^{2k}}\zeta(2k) \tag{B2}$$

and ζ defines Riemann Zeta function. Now the insertion of B2 in B1 gives [59]

$$\frac{[\mu\coth\mu-1]}{\mu^3}=\frac{1}{3\mu}-\frac{2}{(\pi\mu)^3}\sum_{k=2}^{\infty}(-1)^k\zeta(2k)\left(\frac{\mu}{\pi}\right)^{2k}$$
$$=\frac{d\Gamma(\mu)}{d\mu} \tag{B3}$$

where the function $\Gamma(\mu)$ is defined by

$$a_j=\frac{\{\zeta[2(j+1)]-1\}}{j},\quad j\neq 0;$$

$$\Gamma(\mu)=\frac{1}{3}\ln\mu-\frac{1}{\pi^2}\ln\left[1+\left(\frac{\mu}{\pi}\right)^2\right]+\frac{1}{\pi^2}\sum_{j=1}^{\infty}(-1)^j a_j\left(\frac{\mu}{\pi}\right)^{2j}. \tag{B4}$$

As $n\to\infty$, $\zeta(n)\to 1$. So, $a_n\to 0$ as $n\to\infty$. The alternating infinite series in Eq. (B4) is convergent by the Leibnitz criterion [59]. It is also easy to show that the series is absolutely convergent with the radius of convergence of (2π). The numerical convergence of the sum in Eq. (B4) is also greatly improved [59]. Equation (53) can be rearranged to obtain

$$\frac{dh(\mu,c)}{d\mu}=\frac{2}{\mu^2}+16\,c\frac{[2\mu\coth(2\mu)-1]}{(2\mu)^3} \tag{B5}$$

and the constant c is defined by Eq. (47). The function, $h(\mu,c)$ can be obtained by using Eq. (B4).

APPENDIX C: PFAFFIAN DIFFERENTIAL EQUATIONS IN TWO VARIABLES AND THE EFFECTIVE HAMILTONIAN

Consider the following Pfaffian differential equation in two variables, say μ and x.

$$F(\mu,x)dx+G(\mu,x)d\mu=0. \tag{C1}$$

This is the Pfaffian differential form of Eq. (51). Another instructive example of a Pfaffian differential equation of two variables comes from Eq. (63). There is a fundamental difference between Pfaffian differential equations in two vari-

ables and those in a higher number of variables. If $F(\mu,x)$ and $G(\mu,x)$ satisfy the exact differentiality condition in a certain domain $\mathcal{D}$, there exists in $\mathcal{D}$ then exactly one function, $H(\mu,x)$ such that $H(\mu,x)=$constant. Again, a Pfaffian differential equation in two variables always possesses an integrating factor. So, if F and G do not satisfy the exact differentiality condition as such, it is always possible to find an integrating factor, $\kappa(\mu,x)$ such that (κF) and (κG) satisfy the exact differentiality condition [57]. For some special cases, $\kappa(\mu,x)$ can be easily found [57]. However, in the more general case it is a solution of a partial differential equation. This PDE arises from the exact differentiality condition.

It is then clear from this deliberation that the right hand side of Eq. (55) can be absorbed in the definition of $H_{\rm eff}$ by using an appropriate integrating factor. The extra term in Eq. (55) is a second order term. In the range of μ, considred in our calculation, its inclusion in $H_{\rm eff}$ will not add anything qualitatively different in the physics. With this consideration, this is ignored in the numerical calculation.

APPENDIX D: DERIVATION OF EQUATIONS OF MOTION

To derive the equations of motion, we first multiply both sides of Eqs. (45), (46), and (48) by c^{-1} and define a new time, $\tau'=c\tau$. So, all derivatives with respect to time here will imply derivatives with respect to τ'. c is, of course, defined by Eq. (47). We make a coordinate transformation, where $x\rightarrow x$ and $k\rightarrow\mu$. The latter transformation is defined by Eq. (47). It can be easily shown that the Jacobian matrix of the transformation is symplectic [2,60]. So, the transformation is canonical. Our fundamental Poisson brackets are

$$\{x,x\}=0=\{\mu,\mu\} \tag{D1}$$

$$\{x,\mu\}_{x,k}=\frac{\sinh\mu\tanh\mu\sin k}{c}. \tag{D2}$$

Of course, Eq. (D2) can be derived from Eq. (47). We now use basic properties of Poisson bracket to obtain equations of motion [60].

$$\dot{k}=\{k,H_{\rm eff}\}_{x,k}=-\frac{\partial H_{\rm eff}}{\partial x}; \tag{D3}$$

$$\begin{aligned}\dot{x}=\{x,H_{\rm eff}\}_{x,k}&=\frac{\partial H_{\rm eff}}{\partial x}\{x,x\}+\frac{\partial H_{\rm eff}}{\partial\mu}\{x,\mu\}_{x,k}\\&=\frac{\sinh\mu\tanh\mu\sin k}{c}\frac{\partial H_{\rm eff}}{\partial\mu};\end{aligned} \tag{D4}$$

$$\begin{aligned}\dot{\mu}=\{\mu,H_{\rm eff}\}_{x,k}&=\frac{\partial H_{\rm eff}}{\partial\mu}\{\mu,\mu\}-\frac{\partial H_{\rm eff}}{\partial x}\{\ x,\mu\}_{x,k}\\&=-\frac{\sinh\mu\tanh\mu\sin k}{c}\frac{\partial H_{\rm eff}}{\partial x}.\end{aligned} \tag{D5}$$

Albeit Eq. (48) is slightly modified due to the approximation in $H_{\rm eff}$, other two equations, namely Eqs. (45) and (46) are fully obtained.

[1] A. Scott, *Nonlinear Science: Emergence & Dynamics of Coherent Structures* (Oxford University Press, U.K., 1999).

[2] A. Das, *Integrable Models* (World Scientific, Singapore, 1989).

[3] P.L. Bhatnagar, *Nonlinear Waves In One-dimensional Dispersive Systems* (Clarendon Press, Oxford, U. K., 1979).

[4] D.B. Duncan, J.C. Eilbeck, H. Feddersen, and J.A.D. Wattis, Physica D **68**, 1 (1993).

[5] V.E. Zakharov and A.B. Shabat, Zh. Eksp. Teor. Fiz. **61**, 118 (1971) [Sov. Phys. JETP **34**, 62 (1972)].

[6] M. Toda, in *Topics in Current Physics: Solitons*, edited by R. K. Bullough and P. J. Caudrey (Springer-Verlag, Berlin,1980), pp. 143–155.

[7] M. Toda, *Theory of Nonlinear Lattices, Springer Series in Solid-State Sciences 20* (Springer-Verlag, Berlin, 1981).

[8] M. Wadati, in *Topics in Current Physics: Solitons*, edited by R.K. Bullough and P.J. Caudrey (Springer-Verlag, Berlin, 1980), pp. 287–299.

[9] M.J. Ablowitz and J.L. Ladik, Stud. Appl. Math. **55**, 213 (1976), J. Math. Phys. **17**, 1011 (1976), Stud. Appl. Math. **58**, 17 (1978).

[10] M. Salerno, Phys. Rev. A **46**, 6856 (1992).

[11] D. Cai, A.R. Bishop, and N. Grønbech-Jensen, Phys. Rev. Lett. **72**, 591 (1994).

[12] D.I. Kaup, SIAM (Soc. Ind. Appl. Math.) J. Appl. Math. **31**, 121 (1976).

[13] V.I. Karpman and E.M. Maslov, Zh. Eksp. Teor. Fiz. **73**, 537 (1977) [Sov. Phys. JETP **46**, 281 (1977)]; **48**, 252 (1978); **50**, 58 (1979); Phys. Lett. A **60**, 307 (1977); **61**, 355 (1977); V.I. Karpman, Pis'ma Zh. Eksp. Fiz. **25**, 296 (1977) [JETP Lett. **25**, 271 (1977)].

[14] A.A. Vakhnenko and Yu.B. Gaididei, [Teor. Mat. Fiz. **68**, 350 (1986) [Theor. Math. Phys. **68**, 873 (1987)].

[15] A.B. Aceves, C. De Angelis, T. Peschel, R. Muschall, F. Lederer, S. Trillo, and S. Wabnitz, Phys. Rev. E **53**, 1172 (1996).

[16] Ch. Claude, Y.S. Kivshar, O. Kluth, and K.H. Spatchek, Phys. Rev. B **47**, 14 228 (1993).

[17] A.S. Davydov, J. Theor. Biol. **38**, 559 (1973).

[18] A.S. Davydov and N.I. Kislukha, Zh. Eksp. Teor. Fiz. **71**, 1090 (1976) [Sov. Phys. JETP **44**, 571 (1976)].

[19] A.S. Davydov, A.A. Ermeko, and A.I. Sergienko, Ukr. Fiz. Zh. (Russ. Ed.) **23**, 983 (1978).

[20] A.S. Davydov, Zh. Eksp. Teor. Fiz. **78**, 789 (1980) [Sov. Phys. JETP **51**, 397 (1980)].

[21] A.S. Davydov and V.Z. Énol'skiĭ, Zh. Eksp. Teor. Fiz. **79**, 1888 (1980) [Sov. Phys. JETP **52**, 954 (1980)].

[22] A. Scott, *Davydov's Soliton*, Phys. Rep. **217**, 3 (1992).

[23] V.E. Zakharov, Zh. Éksp. Teor. Fiz. **62**, 1745 (1972) [Sov. Phys. JETP **35**, 908 (1972)].

[24] S. Takeno, in *Davydov's Soliton Revisited, Self-Trapping of Vibrational Energy in Protein*, Vol. 234 of NATO ASI Series, edited by P.L. Christeinsen and A.C. Scott (Plenum, New York, 1990), p. 31.

[25] S. Yomosa, J. Phys. Soc. Jpn. **52**, 1866 (1983).
[26] S.W. Englander, N.R. Kallenbach, A.J. Heeger, J.A. Krumhansal, and S. Litwin, Proc. Natl. Acad. Sci. USA **77**, 7222 (1980).
[27] A.C. Scott, Phys. Rev. A **31**, 3518 (1980).
[28] V. Muto, P.S. Lomdahl, and P.L. Christiansen, Phys. Rev. A **42**, 7452 (1990).
[29] W. Hai, Phys. Lett. A **186**, 309 (1994).
[30] R. F. Fox, *Biological Energy Transduction* (Wiley, New York, 1982).
[31] A.C. Scott, Phys. Rev. A **26**, 578 (1982).
[32] D.E. Green, Science **181**, 583 (1973), Ann. (N.Y.) Acad. Sci. **227**, 6 (1974).
[33] A.C. Scott, Phys. Lett. A **86**, 60 (1981).
[34] A.C. Scott, *Nonlinear Phenomena in Physics and Biology*, edited by R.H. Enns, B.L. Jones, R.M. Miura and S.S. Rangnekar (Plenum Press, New York 1981), Vol. 75, p. 7.
[35] *Davydov's Soliton Revisited, Self- Trapping of Vibrational Energy in Protein* (Ref. [24]), p. 3.
[36] J.M. Hyman, D.W. McLaughlin, and A.C. Scott, Physica D **3**, 23 (1981).
[37] V.A. Kuprievich, Physica (Utrecht) **14**, 395 (1985).
[38] M.I. Molina and G.P. Tsironis, Phys. Rev. B **47**, 15 330 (1993).
[39] M.I. Molina, G.P. Tsironis, and D. Hennig, Phys. Rev. E **50**, 2365 (1994).
[40] P.K. Datta and K. Kundu, Phys. Rev. B **53**, 14 929 (1996).
[41] B. Melomed and M.I. Weinstein, Phys. Lett. A **220**, 91 (1996).
[42] B.C. Gupta and K. Kundu, Phys. Lett. A **235**, 176 (1997).
[43] B.C. Gupta and K. Kundu, Phys. Rev. B **55**, 11 033 (1997).
[44] B.C. Gupta and K. Kundu, Phys. Rev. B **55**, 894 (1997).
[45] A. Ghosh, B.C. Gupta, and K. Kundu, J. Phys.: Condens. Matter **10**, 2701 (1998).
[46] K. Kundu and B.C. Gupta, Eur. Phys. J. B **3**, 23 (1998).
[47] S. Darmanyan, A. Kobyakov, and F. Lederer, Zh. Éksp. Teor. Fiz. **113**, 1253 (1998) [JETP **86**, 682 (1998)].
[48] B.C. Gupta, Phys. Rev. B **60**, 6194 (1999).
[49] A.J. Heeger, S. Kivelson, J.R. Schrieffer, and W.P. Su, Rev. Mod. Phys. **60**, 781 (1988).
[50] D.K. Campbell and A.R. Bishop, *Handbook of Conducting Polymers*, edited by Terje A. Skotheim (Marcel Dekker, New York, 1986), Vol. 2, pp. 937–966.
[51] A. S. Alexandrov and Sir Nevill Mott, *Polarons & Bipolarons* (World Scientific, Singapore, 1996), pp. 16–25.
[52] K. Kundu and D. Giri, J. Chem. Phys. **105**, 11 075 (1996); D. Giri and K. Kundu, Phys. Rev. B **53**, 4340 (1996).
[53] B. M. Pierce, in *Davydov's Soliton Revisited, Self-Trapping of Vibrational Energy in Protein* (Ref. [24]), p. 209.
[54] N. Østergård, in *Davydov's Soliton Revisited, Self-Trapping of Vibrational Energy in Protein* (Ref. [24]), p. 229.
[55] Y.S. Kivshar and D.K. Campbell, Phys. Rev. E **48**, 3077 (1993).
[56] J.M. Ziman, *Principles of The Theory of Solids*, 2nd ed. (Cambridge University Press, Cambridge, England, 1972), p. 319.
[57] I. Sneddon, *Elements of Partial Differential Equations*, International Student Edition (McGraw-Hill), p. 19; F.B. Hildebrand, *Advanced Calculus For Applications*, 2nd ed. (Prentice-Hall, New Jersey, 1976); W.E. Boyce and R.C. DiPrima, *Elementary Differential Equations*, 2nd ed. (John Wiley & Sons, Inc., 1969).
[58] A.R. Vasconcellos, M.V. Mesquita, and R. Luzzi, Phys. Rev. Lett. **80**, 2008 (1998).
[59] I.S. Gradsteyn and I.M. Ryzhik, *Table of Integrals, Series and Products*, 4th ed. (Academic Press, New York, 1980); M. Abramowitz and I.A. Stegun, *Handbook of Mathematical Functions*, 9th ed. (Dover, New York, 1970); G. Arfken, *Mathematical Methods For Physics*, 3rd ed. (Academic Press, New York, 1959), pp. 277–351.
[60] D.T. Greenwood, *Classical Dynamics* (Dover, New York, 1997), pp. 256–258; H. Goldstein, *Classical Mechanics* (Addison-Wesley, Reading, MA, 1950).