# Supersonic mechanisms for charge and energy transfers in anharmonic molecular chains

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The dynamical theory of a quantum quasiparticle moving in a deformable anharmonic chain is extended into the supersonic region. Besides a supersonic self-trapping mode, which is a direct extension of the well-known subsonic Davydov-Scott mode, two additional dynamically stable transfer mechanisms have been discovered in this region: (i) the capture and transfer of the self-trapping state by a supersonic acoustic (lattice) soliton and (ii) the pairing of two lattice solitons via their interaction with a quasiparticle. [S0163-1829(96)01222-2]

## I. INTRODUCTION

The transports of vibrational energy and charge in molecular systems (e.g., in protein) are fundamental processes in physics, chemistry, and biology. One of the most promising actual transfer theories is the Davydov-Scott (DS) *self-trapping* mechanism, extensively described in Refs. 1 and 2, which originated from the classical works of Landau[3] and Pekar.[4] According to this mechanism, two-component solitons (moving polaronlike states), being stabilized by the counterbalance of the *intersite resonance interaction* and the *exciton-phonon coupling*, have been proved[5] to be *dynamically stable* carriers of vibrational energy. The latter is released by hydrolysis of adenosine triphosphate (ATP) at one end of an $\alpha$-helix protein molecule and transported to the other one. The amount of this vibrational energy is about 0.422 eV. It is partly stored in the high-frequency intramolecular C = O stretching mode (amide-I vibrations with frequency about 1665 $cm^{-1}$).

There are two approaches to the soliton modeling of the transport of vibrational energy in biological macromolecules. The original one is based on the exciton Hamiltonian scheme where, besides the usual electric dipole-dipole coupling between neighboring peptide groups, Davydov and Kyslukha[6] have introduced the short-range interaction of amide-I vibrations with low-frequency longitudinal *acoustic* phonons of the molecular chain. This interaction is caused by the dependence of the amide-I energy on the distances between neighboring peptide groups. As a result, the linear expansion term of this dependence gives rise to the *nonlinearity* of the self-interaction of excitons in the Davydov-Kyslukha model.[6] This model admits the *acoustic* self-trapping solitary wave solution called Davydov's soliton. The improved version of this model[7] is described by a pair of *coupled* difference-differential equations. The self-consistent soliton solution of these equations exists only for *subsonic* velocities.

The second approach to the soliton modeling of the energy transport in biological systems has been suggested and developed by Takeno[8] on the basis of his *classical* oscillator-lattice model. This two-sublattice model is a chain of harmonically coupled peptide groups and it describes the dynamical self-trapping of the high-frequency (intrapeptide) amide-I oscillations through their coupling with low-frequency vibrations of the peptide groups (as whole objects). The two-component solitary wave solution of the resulting equations of motion gives rise to a *subsonic moving breather (envelope soliton)* accompanied by a pulse of lattice compression. On the other hand, Davydov's wave function, which actually describes the adiabatic limit of the exciton-phonon picture, leads to the classical dynamical equations coinciding with the Schrödinger limit of the Klein-Gordon equation for the high-frequency component in the Takeno model. Therefore, both approaches are actually classical descriptions.

In the case of the dynamical self-trapping, the coupling of the amide-I mode to lattice vibrations in a polypeptide chain is usually modeled by some *harmonic* potential. Such an approximation is satisfactory in the standard polaron theory, when the dynamical self-trapping of excitons is due to their coupling to an *optical* mode of the lattice (e.g., as in crystalline acetanilide[9]). However, in the case of the dynamical *acoustic* self-trapping of a quantum of the amide-I mode or an excess electron,[10] the harmonic (linear) approximation of the acoustic phonon mode is valid only for sufficiently small values of the velocity of the self-trapped states, since with increasing velocities the amplitudes of the localized compressions of the chain rapidly increase up to infinity. As a result, adjacent chain molecules (peptide groups) would pass through each other, which, of course, is a completely unphysical situation. In order to avoid this difficulty in the DS theory a *hardening* (positive) anharmonicity must be added to the harmonic potential. Then, with decreasing distances between neighboring molecules, the intermolecular potential will increase faster than the usual *quadratic* behavior. As a result, the dynamical acoustic self-trapping theory can be extended to the whole interval of *subsonic* velocities, including the speed of longitudinal sound.[11]

On the other hand, any positive anharmonicity in a lattice results in the appearance of the well-known extremely stable *supersonic acoustic* (*lattice*) solitons[12] (e.g., the Toda solitons[13]) which can also be considered as effective carriers of energy in biological systems.[14] Their dynamical stability is due to the balance of the intermolecular anharmonicity and

 

the lattice dispersion. The mixture of *two* types of dispersion (the intersite resonance energy and the lattice discreteness) and of *two* types of nonlinearities (the exciton-phonon coupling and the lattice anharmonicity) gives rise to very complicated dynamics of such a system. So far only a few attempts are known to have tackled this problem analytically and numerically;[15–26] still its solution is far from being fully understood from the physical point of view. In this paper, on the basis of analytical and numerical studies, we show that the DS subsonic self-trapping mode *bifurcates* at the velocity of longitudinal sound, at least, into *three* dynamically stable supersonic soliton modes. One of them is still characterized by the self-trapping mechanism, however with supersonic velocities, while the appearance of the other two is due to the *coupling of the self-trapping states with the lattice solitons*.

The paper is organized as follows. Section II is to a large extent also an introductory part. There, we present the basic equations of motion to be studied in the next sections analytically and numerically. Then, the paper is divided into two parts. The first one is strictly analytical. The self-trapping (polaron) states and their interaction with the lattice solitons are investigated in Sec. III. In the next section, explicit soliton solutions for a cubic anharmonicity of the lattice are presented. There, the energies of the newly found soliton modes are discussed. After that first analytical part, in the second part of the paper numerical simulations are presented. The variational approach of Sec. V, together with the results of Sec. IV, is the basis for the subsequent numerical procedures. Detailed numerical results are shown in Sec. VI. The paper is concluded by a short summary and outlook.

## II. BASIC EQUATIONS

In what follows we call a quantum of the amide-I excitation or an excess electron a quantum quasiparticle. The main assumptions in the DS theory extended to many quasiparticles[1,2,27] are the following: (i) dealing with only *longitudinal* degrees of the one-dimensional (1D) lattice, (ii) the presence of nearest-neighbor interactions both for the lattice and for the quasiparticles, and (iii) the absence of interaction between quasiparticles. Under these assumptions, the basic equations of motion, which describe the coupling of a conserved number $\nu$ of noninteracting quantum quasiparticles to an anharmonic deformable molecular chain, can be obtained in the exciton formalism by using the *generalized* Davydov wave function.[21,27–29] As a result, they can be formulated in the dimensionless form[11,27]

$$i\frac{d\Phi_n}{d\tau}=-D(\Phi_{n+1}-2\Phi_n+\Phi_{n-1})-\frac{g}{2}(\rho_{n-1}+\rho_n)\Phi_n,$$

$$\frac{d^2\rho_n}{d\tau^2}=U'(\rho_{n+1})-2U'(\rho_n)+U'(\rho_{n-1})-\frac{g}{2}(|\Phi_{n+2}|^2-|\Phi_{n+1}|^2-|\Phi_n|^2+|\Phi_{n-1}|^2), \tag{1}$$

where the prime denotes a derivative with respect to the argument. The corresponding Hamiltonian is

$$\mathcal{H}=\sum_n\left\{\Phi_n^*\left[-D(\Phi_{n+1}-2\Phi_n+\Phi_{n-1})+\frac{g}{2}(u_{n+1}-u_{n-1})\Phi_n\right]+\frac{1}{2}\left(\frac{du_n}{d\tau}\right)^2+U(u_n-u_{n+1})\right\}. \tag{2}$$

Here $\Phi_n(\tau)$ is a discrete wave function of the quasiparticle while the relative displacement field $\rho_n(\tau)=u_n(\tau)-u_{n+1}(\tau)$ describes the lattice compression (if positive) or stretching (if negative). The dimensionless displacement $u_n$ of the $n$th chain molecule from its equilibrium position is scaled by the lattice constant $l$. The dimensionless time is given by $\tau=v_0t/l$ where $v_0$ is the velocity of longitudinal sound in the chain. Then the time unit corresponds to the duration of sound propagation over the distance $l$. For the quantum subsystem, the characteristic frequency $v_0/l$ is used to define an energy unit, so that the intersite energy $D$ and the coupling constant $g$ are given in units of $\hbar v_0/l$. The lattice energy [as well as the total chain energy given by Eq. (2)] is measured in units of $Mv_0^2$ with $M$ being the mass of a chain molecule. The intermolecular potential $U(\rho)=\rho^2/2+A(\rho)$ is supposed to be of a general form and its anharmonic part $A(\rho)$ is required to satisfy the following properties: (i) $\rho^{-2}A(\rho)$ is a monotonically increasing function on the half-axis $0<\rho<\infty$ and (ii) $\lim_{\rho\to0}\rho^{-2}A(\rho)=0$.

The wave function $\Phi_n(\tau)$ is normalized by

$$\sum_n|\Phi_n(\tau)|^2=\nu\sigma\equiv Q, \tag{3}$$

where $\sigma$ is a scaling parameter which measures the ratio of the characteristic energies of both the quantum and lattice subsystems: $\sigma=(\hbar v_0/l)/Mv_0^2=\hbar/Mv_0l$. This parameter may be interpreted as the ''charge'' of *one* quasiparticle. Therefore the (dimensionless) quantity $Q$ can be considered as the nontopological charge of the whole system with $\nu$ quasiparticles. The dimensionless form (1) of the equations of motion with the normalization condition (3) appears to be convenient because it does not depend explicitly on the number $\nu$. For all $\nu$ we have the same dynamical equations and the dependence on $\nu$ appears only in Eq. (3). The limiting case of a pure anharmonic lattice corresponds to zero charge ($Q=0$) in the constraint (3).

The pair of *coupled* difference-differential equations (1) with the constraint (3) is a starting system to be studied in this paper. The present form is convenient from the point of view of numerical simulations because the wave oscillations of the high-frequency part (carrier) of the complex field $\Phi_n(\tau)$ are reduced to a minimum level. In the *decoupling* limit ($g\to0$) the linear band of the small-amplitude waves $\Phi_n(\tau)=\exp[i(nk-\varepsilon_b\tau)]$ with the dimensionless wave number of the carrier $k\in[-\pi,\pi]$ is

$$\varepsilon_b=4D\sin^2\frac{k}{2}. \tag{4}$$

Then the (dimensionless) group velocity is given by

$$s\equiv\frac{v}{v_0}=\frac{d\varepsilon_b}{dk}=2D\sin k. \tag{5}$$

At the middle of the band ($k=\pi/2$), the group velocity has its maximum ($s_b=2D$). Therefore, in order to have a quasiparticle motion in the supersonic regime, the inequality $D>1/2$ must be imposed on the parameters of the chain.

To investigate analytically the set of equations (1) in a general case $g>0$, we separate the wave function $\Phi_n(\tau)$ into low- and high-frequency parts. In other words, we look for solutions of Eqs. (1) in the form of a modulated plane wave,

$$\Phi_n(\tau)=\phi_n(\tau)e^{\{i[nk-(\varepsilon_b+\varepsilon)\tau]\}}, \tag{6}$$

where the real functions $\phi_n(\tau)$ describe a wave envelope with weak variation from site to site. In this paper we are interested only in localized solutions with *zero* boundary conditions. This means that both the lattice fields $\phi_n(\tau)$ and $\rho_n(\tau)$ have to decrease to zero sufficiently fast when $n\to\pm\infty$. The free quasiparticle energy $\varepsilon_b$ in Eq. (6) is given by Eq. (4) while the perturbed (*bound*) energy $\varepsilon=\varepsilon(k)<0$ has to be determined.

Substituting the representation (6) into the equations of motion (1), we obtain the following equations for the envelope $\phi_n(\tau)$, the relative displacement field $\rho_n(\tau)$, and the spectral parameter $\varepsilon$:

$$\frac{d\phi_n}{d\tau}=D\sin k(\phi_{n-1}-\phi_{n+1}), \tag{7}$$

$$D\cos k(\phi_{n+1}-2\phi_n+\phi_{n-1})+\frac{g}{2}(\rho_{n-1}+\rho_n)\phi_n+\varepsilon\phi_n=0, \tag{8}$$

$$\frac{d^2\rho_n}{d\tau^2}=U'(\rho_{n+1})-2U'(\rho_n)+U'(\rho_{n-1})$$

$$-\frac{g}{2}(\phi_{n+2}^2-\phi_{n+1}^2-\phi_n^2+\phi_{n-1}^2). \tag{9}$$

According to the constraint (3), solutions for the envelope $\phi_n(\tau)$ have to be found on the multidimensional sphere

$$\sum_n \phi_n^2(\tau)=Q. \tag{10}$$

Next, we assume both the lattice fields $\phi_n$ and $\rho_n$ to be weakly varying from site to site. Then the continuum approximation can be adopted in calculating these fields. Note that when investigating only wide excitations, we may miss interesting effects due to strong localization.[30–34] Since in Eq. (6) the carrier wave is still considered as a discrete lattice field, more exactly, this approximation can be referred to as a quasicontinuum limit.[35] Hence, in Eqs. (7)–(10), we replace $n\to x, \phi_n(\tau)\to\phi(x,\tau)$, and $\rho_n(\tau)\to\rho(x,\tau)$. Thereby the differences in Eqs. (7)–(10) are replaced by spatial derivatives. As a result, Eq. (7) is transformed to $\phi_\tau+2D\sin k\phi_x=0$. In the case of a stationary envelope, it is simply reduced to the band spectrum (4). The other equations are transformed to

$$D\cos k\phi_{xx}+g\rho\phi+\varepsilon\phi=0, \tag{11}$$

$$\rho_{\tau\tau}-U'(\rho)_{xx}-\frac{1}{12}\rho_{xx\tau\tau}+g(\phi^2)_{xx}=0, \tag{12}$$

where the eigenfunction $\phi(x,\tau)$ is normalized by $\int\phi^2dx=Q$. Equation (11) represents a stationary Schrödinger equation. Its potential $\rho(x,\tau)$ has to be determined from Eq. (12). Note that the inhomogeneity of the deformation $\rho(x,\tau)$ depends on $\phi(x,\tau)$, i.e., the solution of Eq. (11). For bound (localized) states, the ground-state energy $\varepsilon$ has to be negative. This is only possible when the term cos*k* in Eq. (11) is positive. Therefore, for localized solutions, the interval of admissible values for the wave number $k$ is reduced to $|k|<\pi/2$. We take the interval $0\leqslant k<\pi/2$ and using Eq. (5) we can determine the number $k$ in terms of the velocity $s$ through the equation $D\cos k=(D^2-s^2/4)^{1/2}$.

Compared to the previous studies,[11] the lattice equation (12) contains an extra fourth-order derivative term. This dispersion term appears due to the discreteness of the lattice. Instead of Eq. (12), another form can be used,[18] namely,

$$\rho_{\tau\tau}-U'(\rho)_{xx}-\frac{1}{12}\rho_{xxxx}+g(\phi^2)_{xx}=0. \tag{13}$$

Both Eqs. (12) and (13) are of the Boussinesq type with the linear dispersion laws $\omega^2=k^2/(1+k^2/12)$ and $\omega^2=k^2(1-k^2/12)$, respectively. Compared to the latter, the dispersion law for Eq. (12) is well defined for all $k$. Therefore it is referred to as the *improved* Boussinesq equation.[36] Equation (13) is called the *ill-posed* Boussinesq equation. However, as was mentioned before, for the bound states we have $k<\pi/2$ and therefore the basic discrete equation (8) will also work in this region within the ill-posed approximation. Note that in both cases the dispersion is negative; i.e., the group velocity decreases with increasing wave numbers $k$.

For stationary profiles moving in the frame $\xi=x-s\tau$, Eqs. (11) and (12) [or (13)] become

$$a\phi''+g\rho\phi+\varepsilon\phi=0,\ b\rho''+(1-s^2)\rho+\frac{d}{d\rho}A(\rho)=g\phi^2. \tag{14}$$

Here the coefficients $a$ and $b$ are defined through $a=D\cos k$ and $b=s^2/12$. This value for $b$, which depends on the velocity $s$, occurs for the improved Boussinesq equation (12). In the other case, Eq. (13), the value is $b=1/12$. Notice also that for sufficiently large $D$ the long-wavelength approximation ($k\to0$) can be applied. Then it is allowed to set approximately $a=D$, even for supersonic velocities ($s>1$). In any case, we should emphasize that solutions of Eqs. (14) do not depend significantly on the explicit velocity dependences of $a$ and $b$. Thus, in the following we ignore in the analytical considerations the velocity dependences of $a$ and $b$. However, for numerical applications, to be given below, we shall, of course, keep the variations with velocity. The wave function $\phi(\xi)$ in Eqs. (14) is normalized by

$$\int\phi^2(\xi)d\xi=Q. \tag{15}$$

Finally, for analytical calculations of the total energy of the system when lattice dispersion is taken into account, we need a correct quasicontinuum approximation of the Hamiltonian function (2). Using Eq. (6), we find

$$\mathcal{H}=\mathcal{H}\{\phi;\beta,\rho\}=Q\varepsilon_b+\int dx\Big[D\cos k\,\phi_x^2-g\phi^2\rho + \frac{1}{2}\beta_x(1-\partial_x^2/12)^{-1}\beta_x+U(\rho)\Big], \quad (16)$$

which corresponds to Eqs. (11) and (12). Then the Schrödinger equation (11) follows from the variation

$$\frac{\delta}{\delta\phi}\Big(\mathcal{H}-\varepsilon\int\phi^2dx\Big)=0. \quad (17)$$

Obviously, Eq. (12) appears from the Hamiltonian equations

$$\beta_\tau=-\frac{\delta\mathcal{H}}{\delta\rho}=g\phi^2-U'(\rho), \quad (18)$$

$$\rho_\tau=\frac{\delta\mathcal{H}}{\delta\beta}=-(1-\partial_x^2/12)^{-1}\beta_{xx}. \quad (19)$$

Using the relation $\rho=-u_x$, we find from Eq. (19) $\beta_x=(1-\partial_x^2/12)u_\tau$. Substituting this relation into the Hamiltonian (16) and using Eq. (11), we can evaluate the following expression for calculating the total energy:

$$\mathcal{E}=Q(\varepsilon_b+\varepsilon)+\int dx\Big[\frac{1}{2}u_\tau^2+\frac{1}{24}u_{x\tau}^2+U(\rho)\Big]. \quad (20)$$

The first term on the right-hand side (RHS) is the band energy of $\nu$ free quasiparticles, the second one is their bound energy in the deformation potential $\rho(x,\tau)$, and the integral term represents the total energy of the pure lattice deformation. Note that the second term in the integral on the right-hand side of Eq. (20) takes into account the lattice dispersion originating from the fourth-order derivative term in Eq. (12). For traveling wave (TW) solutions with constant profiles the expression (20) is reduced to

$$\mathcal{E}=Q(\varepsilon_b+\varepsilon)+\int d\xi\Big[\frac{s^2}{2}\rho^2+\frac{b}{2}\rho'^2+U(\rho)\Big]. \quad (21)$$

The basic equations (1) with the integrals of motion (2) and (3) are used in this paper for numerical simulations. Equations (8) and (9) are useful in the numerical procedure developed in Sec. VI for seeking both the soliton components $\phi_n$ and $\rho_n$. Finally, the continuum equations (14) with the integrals (15) and (21) are starting objects for analytical studies. The thereby obtained soliton solutions are used as initial conditions in numerical simulations. Even when the discrete equations are used in numerical studies, we deal only with wide soliton profiles for both the lattice fields $\phi_n$ and $\rho_n$.

## III. SELF-TRAPPING (POLARON) STATES AND THEIR INTERACTION WITH LATTICE SOLITONS

In this section we show on the basis of an analysis of Eqs. (14) that in the supersonic region *two* transport mechanisms can exist. One of them is due to the nonlinearity induced by the interaction of quantum quasiparticles with classical lattice vibrations while the other one is caused by the anharmonicity in the lattice vibrations themselves. Starting with Eqs. (14), we notice that for any potential well $-\rho(\xi)$ there is, at least, one bound state $\varepsilon$. Therefore, one can conclude the existence of a symmetric bell-shaped wave function $\phi(\xi)$ if the function $\rho(\xi)$ is also assumed to be of a symmetric bell-shaped form. Then the one-to-one mappings $\xi\leftrightarrow\phi$ and $\xi\leftrightarrow\rho$ take place for $0\leqslant\xi<\infty$ and therefore the function $\phi(\rho)\equiv\phi[\xi(\rho)]$ can be defined within the domain $0\leqslant\rho\leqslant\rho_0$. Using zero boundary conditions, Eqs. (14) can be transformed to the following integral equation:

$$\xi=\pm\sqrt{b/2}\int_{\rho_0}^{\rho}Z(r)^{-1/2}\frac{dr}{r}, \quad (22)$$

where the function $Z$ is defined by

$$Z(\rho)=g\rho^{-2}\int_0^\rho\phi^2(r)dr+\frac{1}{2}(s^2-1)-\rho^{-2}A(\rho). \quad (23)$$

The amplitude $\rho_0>0$ of the soliton component $\rho(\xi)$ is a nontrivial solution of the equation $Z(\rho)=0$.

The necessary condition for the existence of a soliton solution is that $Z(\rho)$ be *convex* and *positive* on the interval $0<\rho<\rho_0$. Thus, in the case of a pure lattice ($g=0$), exactly the existence of the well-known supersonic ($s>1$) lattice solitons follows from the function (23). When a quasiparticle is present in the system ($g>0$), then the behavior of the function $\phi(\rho)$ in the limit $\rho\to0$ ($\xi\to\pm\infty$) determines what kind of two-component solitons can exist. Indeed, in the case of a *linear* behavior of the function $\phi^2(\rho)$ at $\rho\to0$, and *only* in this case, $\lim_{\rho\to0}\rho^{-2}\int_0^\rho\phi^2(r)dr$ is *finite* and therefore for $Z(\rho)>0$ (in some finite interval $0<\rho<\rho_0$), in general, the first (self-trapping) term on the RHS of Eq. (23) is important. This means that the *self-trapping* transfer mechanism is possible with both *subsonic* and *supersonic* velocities; it will be referred to as the $p$ (polaron) mode. The presence of a *positive* anharmonicity $A(\rho)$ leads to some spreading of the soliton profile, essentially improving at high velocities the conditions for the continuum approximation. Without $A(\rho)$, *only* the *subsonic self-trapping* mechanism works in the system.

Another possibility for the existence of soliton solutions is a sufficiently rapid (*nonlinear*) behavior of the function $\phi^2(\rho)$ in the limit $\rho\to0$, such that the inequality $g\int_0^\rho\phi^2(r)dr<A(\rho)$ is satisfied for some finite interval $0<\rho<\rho_0$. In this case, the contribution originating from $A(\rho)$ is responsible for the stabilization of soliton motion, while the first (integral) term on the RHS of Eq. (23) only changes the soliton profile and increases the amplitude $\rho_0$. A soliton of this type cannot be referred to as a polaron. A family of these solutions describes the *capture* and *transfer* of a quasiparticle (which always is self-trapped itself) by an acoustic soliton or, in other words, the *coupling* of the self-trapping state with a supersonic lattice soliton. Because of that, it may be called the *l-p* (lattice-polaron) mode.

To be more concrete, we now determine the lowest eigenvalues $\varepsilon$ of the nonlinear spectral problem given by Eqs. (14). Since we look for bell-shaped soliton profiles, the variable $\xi$ can be eliminated from these equations.[37,38] Then one gets for $\phi(\rho)\equiv\phi[\xi(\rho)]$

$$\frac{d^2\phi}{d\rho^2}W+\left[\left(\frac{d\phi}{d\rho}\right)^2-\phi\frac{d^2\phi}{d\rho^2}-\frac{b}{2a}\right](g\rho+\varepsilon)\phi$$
$$-\frac{d\phi}{d\rho}\left[\frac{a}{b}\left(\frac{d\phi}{d\rho}\right)^2-\frac{1}{2}\right]\left(\frac{dW}{d\rho}-g\phi^2\right)=0, \tag{24}$$

where $W=(1-s^2)\rho^2/2+A(\rho)$. Substituting the asymptotic relation

$$\phi^2(\rho)\cong C_{\alpha-1}\rho^{\alpha} \tag{25}$$

for $\rho\to 0$, with a positive constant $C_{\alpha-1}$, into Eq. (24), we find the whole spectrum of the lowest eigenvalues $\varepsilon$. This spectrum consists of *two* bands. The first one corresponds to $\alpha=1$ and describes the ground-state energy eigenvalues of the $p$ mode:

$$\varepsilon=-a\mu^2\equiv\varepsilon_p,\quad \mu^2=(C_0g-1+s^2)/4b. \tag{26}$$

This mode has both subsonic and supersonic velocities in the vicinity of the sound velocity $s=1$ . The second band corresponds to $\alpha>1$ and describes the eigenvalues of the $l$-$p$ mode:

$$\varepsilon=-a\alpha^2\eta^2\equiv\varepsilon_{l\text{-}p},\quad \eta^2=(s^2-1)/4b. \tag{27}$$

As follows from Eqs. (27), the bound states for the $l$-$p$ mode can exist only for $s>1$, so that only *supersonic* solitons of this kind can propagate. The constant $C_0$ and the power $\alpha$ are determined by the normalization condition (6). They can be calculated once the potential $U(\rho)$ is given explicitly.

## IV. EXPLICIT SOLITON SOLUTIONS FOR A CUBIC ANHARMONICITY

The general conclusions on the existence of *two* supersonic transport mechanisms by the two-component solitons with constant bell-shaped profiles in both the components, given in Sec. III, can be illustrated and further extended in the particular case of the intermolecular potential with a positive cubic anharmonicity:

$$A(\rho)=\frac{1}{3}\gamma\rho^3,\quad \gamma>0. \tag{28}$$

The essential point is that under the additional condition $a\gamma/bg\equiv\kappa=3$, *both bell-shaped* solutions of the set of Eqs. (14) and (15) can be given *explicitly*. The constraint $\kappa=3$ fixes some value of the velocity $s$ due to the dependence of the coefficients $a$ and $b$ in Eqs. (14) on this parameter. However, this dependence does not drastically change the dynamics of the system. Moreover, when we use the ill-posed Boussinesq equation (13), in the long-wavelength limit ($k\to 0$) we have[18] $a=D$ and $b=1/12$. Therefore, instead of fixing some value of the velocity $s$, we may approximately impose a constraint on the parameters of the system, namely, $4D\gamma/g\simeq 1$.

Assuming the ansatz (25) in the *whole* interval $0<\rho<\rho_0$, we can get from Eqs. (22) and (23) the explicit profiles of both the $p$ and $l$-$p$ modes. Thus, in the case $\alpha=1$, we find the *normalized* soliton profile

$$\phi_p(\xi)=\left(\frac{Q\mu}{2}\right)^{1/2}\cosh^{-1}(\mu\xi),\rho_p(\xi)=\frac{2a}{g}\mu^2\cosh^{-2}(\mu\xi), \tag{29}$$

where $\mu$ satisfies the cubic equation

$$4\mu(\mu^2-\eta^2)=3\mu_0^3. \tag{30}$$

Here the velocity parameter $\eta$ is defined in Eqs. (27) and $\mu_0=(Qg^2/12ab)^{1/3}$ can be referred to as the characteristic inverse width of a soliton. This equation has a positive unique root on the whole interval $0\leqslant s<\infty$. The limit $b\to 0$ and $\gamma\to 0$ under the condition $\kappa=3$ immediately leads to Davydov's subsonic solution,[1,2,5] and therefore it may be referred to as the Davydov limit. Note that the constraint $\kappa=3$ in the solution (29) and (30) appears as a result of imposing the linear behavior ($\alpha=1$) in the ansatz (25) on the whole interval $0<\rho<\rho_0$.

The $l$-$p$ soliton solution ($\alpha>1$) can also be presented explicitly in the case of a cubic anharmonicity, even without the constraint $\kappa=3$.[18,22] It corresponds to $\alpha=2$ in the ansatz (25). The (non-normalized) two-component soliton solution is

$$\phi_{l\text{-}p}(\xi)=\delta\left(\frac{\kappa-1}{2}\right)^{1/2}\eta^2\cosh^{-2}(\eta\xi),$$
$$\rho_{l\text{-}p}(\xi)=\frac{6a}{g}\eta^2\cosh^{-2}(\eta\xi), \tag{31}$$

where $\delta=6\sqrt{2ab}/g$ . Here the bound energy $\varepsilon$ and the parameter $\eta$ are given by Eqs. (27) with $\alpha=2$ . The explicit form of the $l$-$p$ solution (31) can be normalized [according to Eq. (29)] only at the fixed value of the velocity $s=s_1$ given by

$$\eta=\frac{1}{2}\left(\frac{2}{\kappa-1}\right)^{1/3}\mu_0\equiv\eta_1. \tag{32}$$

Similarly to the $p$ solution (29) and (30), the latter constraint is due to imposing the quadratic behavior of the function $\phi^2(\rho)$ [$\alpha=2$ in the ansatz (25)], again, on the whole interval $0<\rho<\rho_0$. For other values $s\neq s_1$, the wave function and deformation potential given by Eqs. (31) will slightly change their profiles, when, of course, the normalization condition (15) is taken into account. In this case, the asymptotic power $\alpha$ will also deviate from the value 2. In the particular case, when the constraint $\kappa=3$ is imposed, the ''projection'' of the profile (31) onto the sphere (15) can be given explicitly. The projected profile is still *bell-shaped* and its explicit form can be derived by using a two-soliton solution[24] of the Jacobi inversion problem for the Hénon-Heiles two-particle system. The value $\kappa=3$ is one of the integrable cases of the system of Eqs. (14) and in this particular case the $l$-$p$ (bell-shaped) profile takes the form

$$\phi_{l\text{-}p}(\xi)=\frac{\delta}{3}\alpha(\alpha^2-1)\eta^2\Theta^{-1}(\xi)\cosh^{-1}(\alpha\eta\xi),$$
$$\rho_{l\text{-}p}(\xi)=\frac{2a}{g}(\alpha^2-1)\eta^2\Theta^{-2}(\xi)[\alpha^2\cosh^{-2}(\alpha\eta\xi) \tag{33}$$

$$+\tanh^2(\alpha\eta\xi)\cosh^{-2}(\eta\xi)],$$

where $\Theta(\xi)=\alpha-\tanh(\alpha\eta\xi)\tanh(\eta\xi)$ and the parameter $\alpha$ is a root of the equation

$$\alpha(\alpha^2-1)^2\int_{-1}^{1}\left[\alpha-y\tanh\left(\frac{\tanh^{-1}y}{\alpha}\right)\right]^{-2}dy=\frac{3}{2}\left(\frac{\mu_0}{\eta}\right)^3. \tag{34}$$

This equation gives the function $\alpha=\alpha(s)$ and therefore the spectral parameter $\varepsilon=\varepsilon(s)$ can be determined according to Eqs. (27). In the particular case $\eta=\eta_1=\mu_0/2$, given by Eq. (32), the solution of Eq. (34) is $\alpha=2$ and the two-component profile (33) is reduced to Eqs. (31). For other values of the velocity $s$ (or the parameter $\eta$) Eq. (34) should be solved numerically.

The binding energy $\mathcal{E}_b=\mathcal{E}_p+\mathcal{E}_l-\mathcal{E}_{l-p}$ of the $l$-$p$ state can also be calculated numerically for any $s>1$. However, for $s=s_1$ and $\kappa=3$, when $\eta=\mu_0/2$ [see Eq. (32)], these calculations can easily be done analytically by using the solutions (26)–(31). In this case, Eq. (30) can be solved explicitly, and its positive root is $\mu=\mu_0$. Moreover, we find that the bound energy $\varepsilon$ is the same for both the $p$ and $l$-$p$ states: $\varepsilon_p=\varepsilon_{l-p}=-a\mu_0^2$. Next, the $\rho$ components in Eqs. (29) and (31) are reduced to

$$\rho_p(\xi)=\frac{2a}{g}\mu_0^2\cosh^{-2}(\mu_0\xi),$$

$$\rho_{l\text{-}p}(\xi)=\frac{3a}{2g}\mu_0^2\cosh^{-2}\left(\frac{\mu_0}{2}\xi\right), \tag{35}$$

and the Boussinesq limit ($a\to 0$, $g\to 0$, and $\kappa\to 1$) of the $l$-$p$ mode becomes

$$\rho_l(\xi)=\frac{a}{2g}\mu_0^2\cosh^{-2}\left(\frac{\mu_0}{2}\xi\right). \tag{36}$$

Substituting these profiles into the general expression (21) for the total energy, we find $\mathcal{E}_b=16a^2b\mu_0^5/5g^2>0$. This proves that a polaron and a lattice soliton do couple, creating a new *coupled lattice-polaron state*. It follows from Eqs. (35) and (36) that the amplitude of the chain deformation in the case of the lattice-polaron state exceeds that of a pure lattice soliton, as can also be seen from the function (23) for a general form of the anharmonicity $A(\rho)$.

Finally, one can observe that in the limit $s\to 1$ the profile (33) is transformed into the $p$ soliton solution given by Eqs. (29) and (30). Therefore, we can conclude that at $s=1$ the *subsonic* DS self-trapping mode *bifurcates*, or *splits*, into the two supersonic soliton modes $p$ and $l$-$p$ described by Eqs. (26), (29), (30) and Eqs. (27), (33), (34), respectively.

## V. VARIATIONAL APPROACH

In this section we develop a variational approach which can be applied to the case of a *general* intermolecular potential $U(\rho)$. To this end, we notice that the stationary equations (14) can be represented as the variational equations $\delta(\mathcal{L}+\varepsilon\int\phi^2dx)/\delta\phi=0$ and $\delta\mathcal{L}/\delta\rho=0$ with the Lagrangian function

$$\mathcal{L}=\int d\xi\left[-a\phi'^2+g\phi^2\rho+\frac{b}{2}\rho'^2+\frac{1}{2}s^2\rho^2-U(\rho)\right]. \tag{37}$$

The Lagrange multiplier $\varepsilon$ has to be determined from the first of Eqs. (14). Multiplying it by $\phi(\xi)$, integrating from $-\infty$ to $\infty$, and using the normalization condition (15), we obtain

$$\varepsilon=Q^{-1}\int(a\phi'^2-g\phi^2\rho)d\xi. \tag{38}$$

Since we are looking for bell-shaped soliton solutions, we choose the trial functions in the form

$$\phi(\xi)=(Q\mu/c_\alpha)^{1/2}\cosh^{-\alpha}(\mu\xi),\quad \rho(\xi)=\rho_0\cosh^{-2}(\mu\xi), \tag{39}$$

where $c_\alpha=\int\cosh^{-2\alpha}\zeta d\zeta$ and the *three* variational parameters $\alpha$, $\mu$, and $\rho_0$ are to be determined from the extremum conditions $\partial\mathcal{L}/\partial\alpha=0$, $\partial\mathcal{L}/\partial\mu=0$, and $\partial\mathcal{L}/\partial\rho_0=0$. The first of these conditions yields the relation

$$\rho_0=\alpha(\alpha+1)a\mu^2/g. \tag{40}$$

The two other conditions lead to equations which can be written in symmetric form, if we take into account Eq. (40):

$$\frac{F(\rho_0)}{\mu}=\frac{2}{3}\left(\frac{s^2}{\mu}-\frac{4}{5}b\mu\right)\rho_0+Qg\frac{2\alpha}{(\alpha+1)(2\alpha+1)},$$
$$\frac{G(\rho_0)}{\mu}=\frac{2}{3}\left(\frac{s^2}{\mu}+\frac{4}{5}b\mu\right)\rho_0+Qg\frac{\alpha}{2\alpha+1}, \tag{41}$$

where the functions $F$ and $G$ are defined by

$$F(\rho_0)=\frac{1}{\rho_0}\int_0^{\rho_0}\left(1-\frac{\rho}{\rho_0}\right)^{-1/2}U(\rho)\frac{d\rho}{\rho},$$

$$G(\rho_0)=\frac{1}{2}[F(\rho_0)+\rho_0F'(\rho_0)]. \tag{42}$$

Finally, substituting the trial functions (39) into Eq. (38), we obtain

$$\varepsilon=-\alpha^2a\mu^2. \tag{43}$$

In the particular case of the cubic anharmonicity (28), the general equations (41) become

$$(\mu^2-\eta^2)\mu=\frac{9(2-\alpha)}{(\alpha+1)^2(2\alpha+1)}\mu_0^3,$$
$$\left[\tfrac{1}{6}\alpha(\alpha+1)\kappa\mu^2-\eta^2\right]\mu=\frac{9(\alpha+3)}{4(\alpha+1)^2(2\alpha+1)}\mu_0^3. \tag{44}$$

It can easily be verified that, in all the particular cases treated above analytically, Eqs. (44) admit exact solutions, as should be expected. In particular, both the Davydov ($b\to 0$ and $\gamma\to 0$) and Boussinesq ($a\to 0$, $g\to 0$, and $\kappa\to 1$) limits can be drawn from these equations. They also contain the $p$ and $l$-$p$ solutions given by Eqs. (29) and (30) at $\kappa=3$. In a general case, when $\alpha\neq 1$ or 2, Eqs. (44) can be solved numerically.

Note that the soliton amplitude $\rho_0$ and the bound energy $\varepsilon$ are calculated according to Eqs. (40) and (43), respectively.

## VI. NUMERICAL INVESTIGATION OF THE SOLITON SOLUTIONS

In this section we develop a numerical approach for seeking wide soliton profiles of the envelope $\phi_n$ and the displacement field $\rho_n$. It will allow us to find all the soliton modes treated analytically in the previous sections and some more specific solutions. Then, taking the soliton solutions as *initial* conditions for numerical simulations of the equations of motion (1), we can gain some insight into their stability. In other words, the *final* profiles of both the lattice fields $\phi_n$ and $\rho_n(\tau)$ obtained by standard simulations at sufficiently large times $\tau$ allow us to decide whether or not the numerically obtained initial soliton is a *stable* solution of Eqs. (1).

The main idea of the numerical scheme is to accomplish in an appropriate way a *discretization* of *time* derivatives in the *difference-differential* equations of motion transforming them into *difference* equations. Then soliton solutions can be obtained under minimization of the corresponding Lagrangian or some other finite-dimensional function. For the present case, we need to discretize the derivative $d^2\rho_n/d\tau^2$ on the right-hand side of Eq. (9). For TW solutions, which are *weakly varying from site to site*, such a procedure can be carried out by requiring that $d^2\rho_n \simeq s^2\rho''$. The next step is to replace the continuum derivative $\rho''$ by an appropriate *spatial difference* derivative. The dispersion of the acoustic longitudinal waves in the continuum limit requires expansions in the relative displacements of the chain molecules up to the fourth order. We approximately substitute Eq. (9) by

$$\begin{aligned} s^2\Big[&\rho_{n+1}-2\rho_n+\rho_{n-1}-\frac{1}{12}(\rho_{n+2}-4\rho_{n+1} \\ &+6\rho_n-4\rho_{n-1}+\rho_{n-2})\Big] \\ &=U'(\rho_{n+1})-2U'(\rho_n)+U'(\rho_{n-1}) \\ &-\frac{g}{2}(\phi_{n+2}^2-\phi_{n+1}^2-\phi_n^2+\phi_{n-1}^2). \end{aligned} \tag{45}$$

The difference equation (45) can be ''integrated'' twice and, as a result, we get

$$\begin{aligned} &s^2\rho_n-\frac{s^2}{12}(\rho_{n+1}-2\rho_n+\rho_{n-1})+\frac{g}{2}(\phi_n^2+\phi_{n+1}^2)-U'(\rho_n) \\ &=0. \end{aligned} \tag{46}$$

Both Eqs. (8) and (46) can be represented in the Lagrangian form

$$\frac{\partial}{\partial\phi_n}\left(\mathcal{L}+\varepsilon\sum_n \phi_n^2\right)=0, \qquad \frac{\partial\mathcal{L}}{\partial\rho_n}=0, \tag{47}$$

where the Lagrangian is defined by

$$\begin{aligned} \mathcal{L}=\mathcal{L}\{\phi_n,\rho_n\}=\sum_n\Big[&-a(\phi_{n+1}-\phi_n)^2+\frac{g}{2}(\phi_n^2+\phi_{n+1}^2)\rho_n \\ &+\frac{1}{2}s^2\rho_n^2+\frac{b}{2}(\rho_{n+1}-\rho_n)^2-U(\rho_n)\Big], \end{aligned} \tag{48}$$

and the Lagrange multiplier $\varepsilon$ is calculated according to Eq. (8):

$$\begin{aligned} \varepsilon=-\frac{1}{2Q}\sum_n\frac{\partial\mathcal{L}}{\partial\phi_n}\phi_n=2a-\frac{1}{Q}\sum_n\Big[&2a\phi_n\phi_{n+1} \\ &+\frac{g}{2}(\phi_n^2+\phi_{n+1}^2)\rho_n\Big]. \end{aligned} \tag{49}$$

A soliton solution of Eqs. (8) and (46) follows from the conditional extremum of the Lagrangian (48):

$$\mathcal{L}\to\text{extr}:\sum_n \phi_n^2=Q. \tag{50}$$

For the chain of $N$ molecules we have chosen cyclic boundary conditions; i.e., we put $n-1=N$ if $n=1$, and $n+1=1$ if $n=N$. The number of lattice cells $N$ has been chosen in such a way that the cyclic boundary conditions do not affect the soliton profile. It is sufficient to take $N$ to be 10 times larger than the soliton width.

For all subsonic velocities, the function $-\mathcal{L}$ is obviously bounded from below, and therefore the self-trapping mode can be found as a conditional minimum of the minimization problem

$$-\mathcal{L}\to\min:\sum_n \phi_n^2=Q \tag{51}$$

by applying the steepest-descent method. In particular, the self-trapping soliton solution can be obtained by the descent, starting from the vector $\{\phi_n^0,\rho_n^0\}_{n=1}^N$, where $\phi_{N/2}^0=Q^{1/2}$, $\phi_n^0=0$ if $n\neq N/2$, and $\rho_n=0$ for all $n=1,\ldots,N$. The grid spacing for the first step of the descent is taken to be $h_0=1$. Let $\{\phi_n^k,\rho_n^k\}_{n=1}^N$ be a vector and $h_k$ be a grid spacing obtained at the $k$th step. Then, we define the next step by the iteration

$$\phi_n^{k+1}=c_1(\phi_n^k+c_2h_k\mathcal{L}_{\phi_n}), \quad \rho_n^{k+1}=\rho_n^k+c_2h_k\mathcal{L}_{\rho_n}, \tag{52}$$

where the constants $c_1$ and $c_2$ are defined by

$$\begin{aligned} c_1&=\left[Q\Big/\sum_n(\phi_n^k+c_2h_k\mathcal{L}_{\phi_n})^2\right]^{1/2}, \\ c_2&=\left[\sum_n(\mathcal{L}_{\phi_n}^2+\mathcal{L}_{\rho_n}^2)\right]^{-1/2}. \end{aligned} \tag{53}$$

Here $\mathcal{L}_{\phi_n}$ and $\mathcal{L}_{\rho_n}$ are the partial derivatives with respect to $\phi_n$ and $\rho_n$, respectively. The iteration is accepted if $\mathcal{L}\{\phi_n^{k+1},\rho_n^{k+1}\}<\mathcal{L}\{\phi_n^k,\rho_n^k\}$. In this case, $h_{k+1}=h_k$. Otherwise, we put $h_k=h_k/2$ and repeat the iteration process. The descent process is completed when the grid spacing $h_k$ becomes less than some $\epsilon$ which characterizes the required accuracy of minimization.

It should be noticed that in principle the lattice dispersion term (with $b>0$) in (48) is not needed to obtain the subsonic solutions. This mode can be obtained even if $b=0$. However, for $s>1$, there are neither minimum nor maximum points at the Lagrangian surface (48). The extremum points, which correspond to supersonic soliton solutions, are only of the saddle type, and therefore it is impossible to find any supersonic solution by minimization of the function (48). The most convenient way is to seek the vector $\{\phi_n\}_{n=1}^{N}$ as a conditional minimum of the problem

$$-\mathcal{L}_1 \equiv \sum_n \left[ a(\phi_{n+1}-\phi_n)^2 - \frac{g}{2}(\phi_n^2+\phi_{n+1}^2)\rho_n \right]$$

$$\rightarrow \min_{\phi_1,\ldots,\phi_N} : \sum_n \phi_n^2 = Q, \tag{54}$$

while the relative displacements $\rho_n$ should be found as unconditional minima of the problem

$$\mathcal{F}_2 = \frac{1}{2}\sum_n \mathcal{L}_{\rho_n}^2 \rightarrow \min_{\rho_1,\ldots,\rho_N}. \tag{55}$$

The special analytical solutions for the $p$ and $l$-$p$ soliton modes, found in the previous sections, have been chosen as starting points for the descent. The self-consistency process is considered to be completed if the discrete functional

$$\mathcal{F} = \frac{1}{2}\sum_n [\mathcal{L}_{\phi_n}^2 + \mathcal{L}_{\rho_n}^2] \tag{56}$$

reaches its minimum. The function (56) may be considered as a ''deformation'' of the Lagrangian surface (48), carried out in such a way that all the saddle points are transformed into minimum points at the deformed surface. Those minima which correspond to bell-shaped profiles are chosen as appropriate soliton solutions of our problem. Other minima describing, e.g., bell-shaped configurations accompanied by any ripples, etc., are excluded from further consideration.

The system of Eqs. (1) has been integrated by the standard fourth-order Runge-Kutta method with constant grid spacing $h$. The accuracy of the integration can be checked by the conserved integrals of motion given by Eqs. (2) and (3). The grid spacing $h=0.025$, which provides the conservation of the integrals of motion during total time of integration with an accuracy to five leading digits, has been used. Typical results of numerical simulations of the equations of motion (1) are as follows.

In Fig. 1, profiles of the DS self-trapping mode at the sound velocity ($s=1$) are shown. The profiles are plotted at the initial time ($\tau=0$) and the final time $\tau=1000.05$ after movement over 1000 chain sites. The initial profiles have been found by the numerical minimization scheme. As can clearly be seen from this figure, there is perfect coincidence of the initial and final profiles.

Profiles of the $l$-$p$ soliton at the initial time ($\tau=0$) and the final time ($\tau=996.05$) are depicted in Fig. 2. Note that at the final time we have a passage over 1000 chain sites. The initial profile has been found by the minimization scheme while the final profile has been obtained by the numerical simulations of the equations of motion (1). The initial and final profiles are plotted and they coincide perfectly. The velocity of the soliton is $s=1.004$.

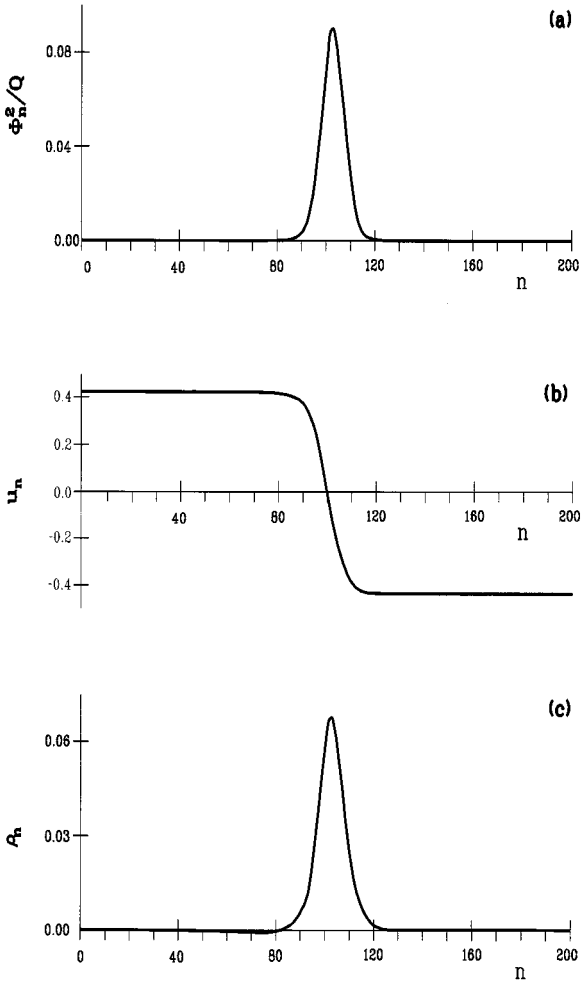


FIG. 1. Profiles of the Davydov-Scott self-trapping mode at the sound velocity ($s=1$) for the initial time ($\tau=0$) and the final time $\tau=1000.05$. They completely overlap when plotted at the same positions.

In Fig. 3, the profiles of the $l$-$p$ soliton at the initial time ($\tau=0$) and the final time ($\tau=956.05$) after the passage over 1000 chain sites are shown. Initially the soliton velocity is $s=1.05$ and its final value is $s=1.046$. The difference between the final and initial velocities is due to decreasing the accuracy of the minimization scheme for narrow soliton profiles.

The pairing of two lattice solitons by a quasiparticle at the velocity $s=1.004$ is demonstrated in Fig. 4. Both the initial ($\tau=0$) and the final ($\tau=996.82$) profiles are presented. During this time the soliton has passed 1000 chain sites. The initial profiles have been obtained by the numerical minimization scheme while the final profiles have been found as a result of the numerical simulations of the equations of motion (1). The initial and final profiles coincide perfectly. The *equilibrium* distance between the lattice solitons is not so large; the wave function $\phi_n$ is still one-humped and a weak two-humpness of the deformation field appears at this value of velocity $s$.

The pairing of two lattice solitons by a quasiparticle at the velocity $s=1.05$ is more clearly shown in Fig. 5. The initial

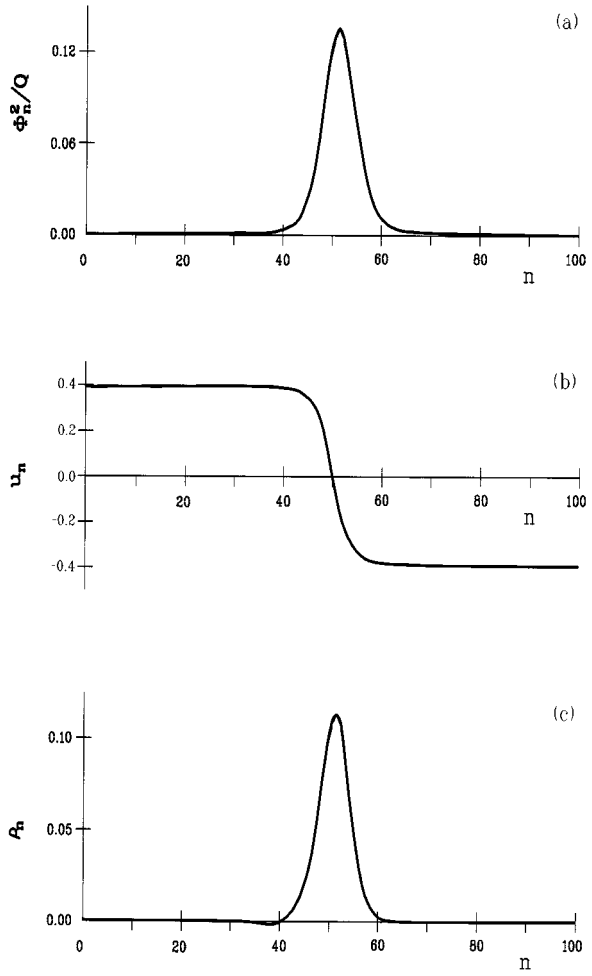


FIG. 2. The profiles of the *l-p* soliton at the initial time ($\tau=0$) and the final time ($\tau=996{,}05$). After backshift in space, they coincide perfectly. The velocity of the soliton is $s=1.004$.

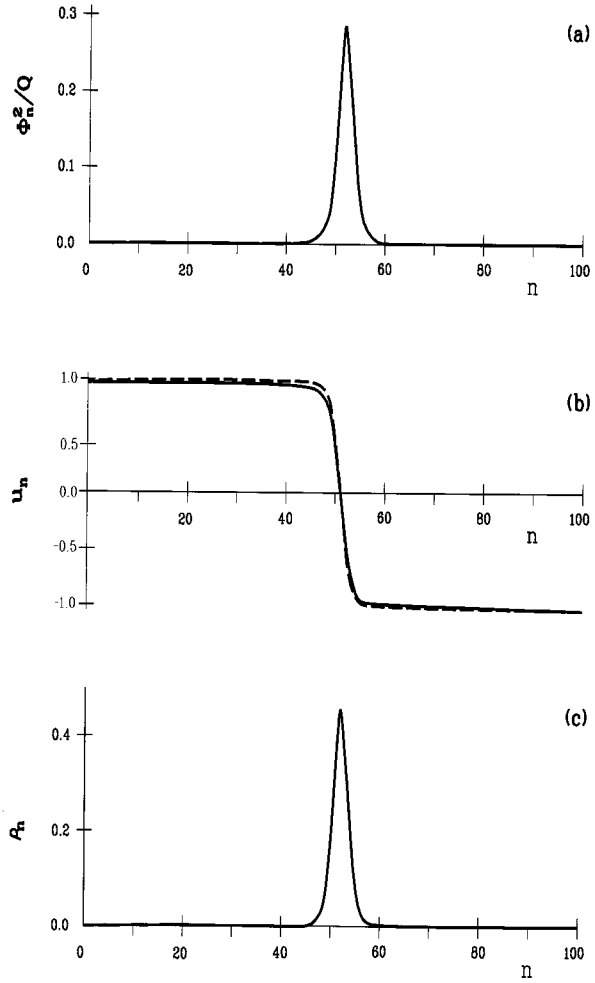


FIG. 3. Same as Fig. 2, but now initially the soliton velocity is $s=1.05$ and its final value is $s=1.046$. The solid line is for $\tau=0$ while the dashed line is for the backshifted profile at $\tau=956.05$.

profiles (curves 1, 2, 3) have been found by the minimization techniques while the final profiles (curves 4, 5, 6) have been obtained as a result of numerical simulations of Eqs. (1). The final coupled state has passed 1000 chain cells, the initial time is $\tau=0$, and the final time is $\tau=945.05$. The final velocity has the value $s=1.046$. The difference between the final and initial velocities is due to decreasing accuracy of the minimization scheme when the soliton profiles become narrow. Only initially this discrepancy happens; afterwards the soliton has a permanent profile and the constant velocity $s=1.046$. The equilibrium distance between the lattice solitons has been increased, so that both the wave function and the relative displacement field have two humps.

Thus, from the numerical simulations carried out in this paper we can draw two important conclusions. First, they confirm our analytical predictions on the existence of *two* supersonic transport mechanisms: (i) *supersonic self-trapping* and (ii) *capture of the self-trapping solitons by the lattice solitons*. Second, and more important in view of additional new results, they demonstrate the *stability* of the predicted coherent structures. Therefore, stable supersonic mechanisms for transport by solitons exist.

To conclude the numerical part of this paper, one should mention the *spectral* method developed recently[34] for numerically seeking stationary soliton profiles in discrete systems. This method could also be applied to studies of the equations of motion (1), and some problems concerning the interaction of a quasiparticle with a nonlinear lattice seem to be of future interest. First, the bifurcation of the self-trapping mode could be proved in a more straightforward way and the *complete* set of supersonic soliton modes could be derived, e.g., a 3*l-p* mode, etc. New bifurcation points in the supersonic region might exist. Second, the minimization scheme allows us to treat only *continuum* solutions while the spectral method is a useful tool for seeking stationary intrinsically *discrete* solutions.[34]

## VII. SUMMARY AND OUTLOOK

In this paper, we have investigated the dynamics of a finite and conserved number of noninteracting quasiparticles (quanta of an intramolecular excitation or excess electrons) coupled to longitudinal phonons of a 1D anharmonic lattice (molecular chain). The interatomic (intermolecular) potential has been considered to be of a general form with *hardening* anharmonicity satisfying all the physical requirements. As a result, in such a chain we have discovered the bifurcation of the DS self-trapping (polaron) mode at the sound velocity

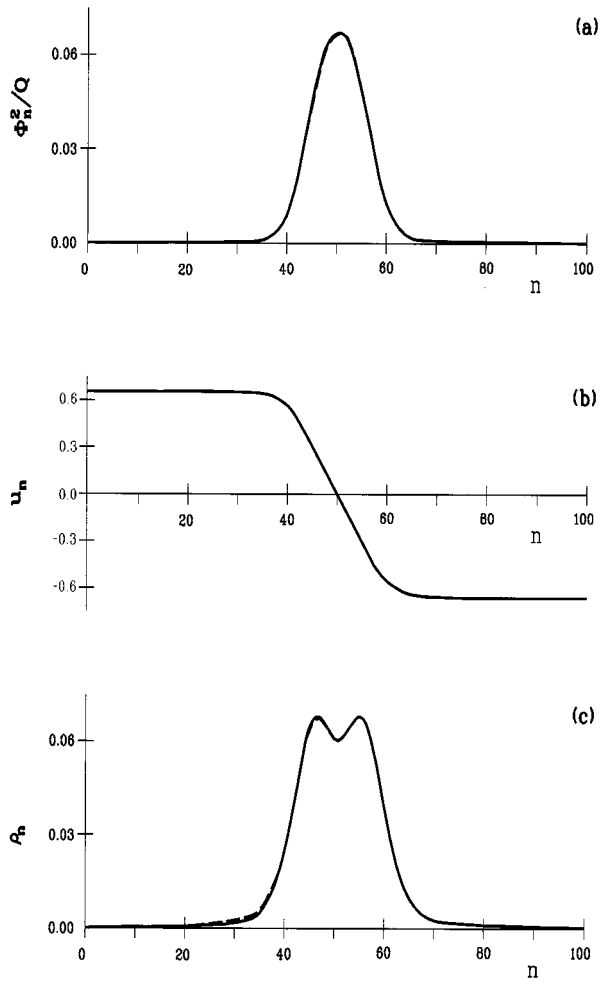


FIG. 4. The pairing of two lattice solitons by a quasiparticle at the velocity $s=1.004$. Both the initial ($\tau=0$) and final ($\tau=996.82$) profiles are presented. The initial and final profiles coincide perfectly, even after a passage of 1000 chain cells.

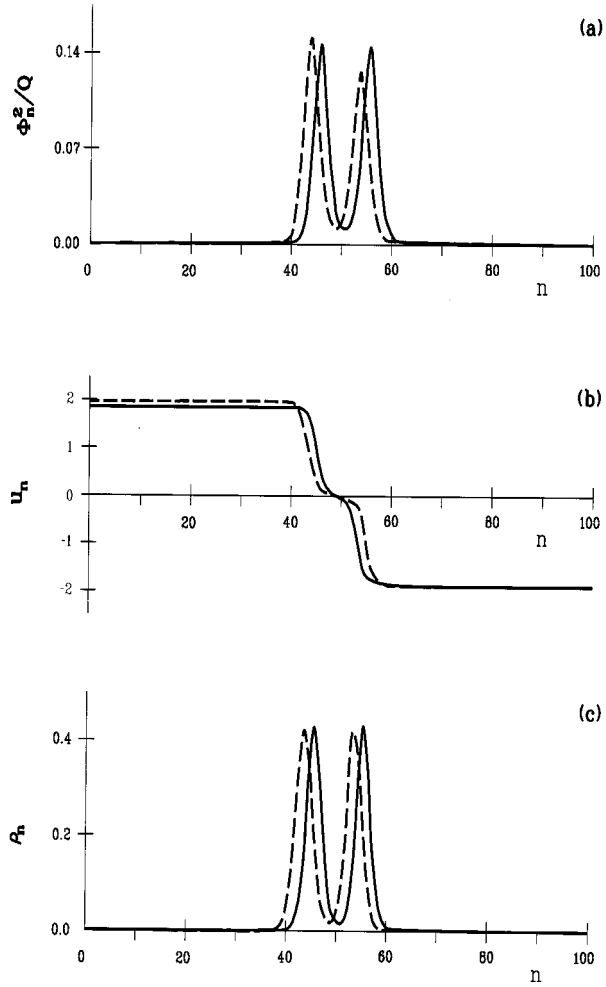


FIG. 5. Same as Fig. 4, but at the velocity $s=1.05$. The initial profiles (solid lines) have been found by the minimization techniques while the final (backshifted) profiles (dashed lines) have been obtained as a result of numerical simulations of the equations of motion (1) at $\tau=945.05$. The final velocity is $s=1.046$.

into *three* supersonic, dynamically stable modes: (i) the *pure self-trapping p* mode which exists with both subsonic and supersonic velocities; (ii) the *capture and transfer* of the self-trapping state by *one* acoustic (lattice) soliton, i.e., an *l-p* mode; and (iii) the *pairing of two lattice solitons at some fixed distance* via their interaction with a quasiparticle, i.e., a 2*l-p* mode. The *l-p* as well as the 2*l-p* modes only exist in two-component *supersonic* soliton forms. In other words, the self-trapping mode exists with both subsonic and supersonic velocities. When it overcomes the sound velocity, then, at least, one or two lattice solitons can attach the polaron, creating together with it a *coupled* state. The total energy of this coupled two-component soliton state increases. However, the energy is less than the sum of the energies of the (two-component) polaron state and of the (one-component) lattice soliton when they are moving with the same velocity but displaced at sufficiently large distance, considered as noninteracting objects. In the particular case of a cubic anharmonicity with a fixed value of the soliton velocity, this result has been proved analytically.

While studying the existence of *supersonic* soliton modes and their dynamical stability, we have developed a numerical method which may be also useful in other studies. More exactly, both the *p* and *l-p* soliton modes have been treated analytically and, although there are some difficulties with different constraints, it was possible to come to important conclusions concerning the physical mechanisms of the supersonic transport of quantum quasiparticles (intramolecular excitations or extra electrons). So far, the pairing of two lattice solitons has been discovered only numerically. Therefore, the numerical studies in this paper are important for two reasons: (i) They prove the dynamical stability of the *p* and *l-p* soliton solutions (obtained analytically) which have bell-shaped profiles for both the wave function and the deformation field. (ii) In addition, we expect that a *pairing* of more than two lattice solitons may also occur and the present method could be applied and adapted to such studies.

The essential point of this paper is that we have thoroughly taken into account *dispersion effects due to the lattice discreteness*. Previous studies of the 1D acoustic polaron problem in anharmonic lattices could only treat self-trapping states with subsonic velocities, $0\leqslant s\leqslant 1$. When the dispersion term with $b>0$ is involved in the dynamical process of soliton stabilization, then a hardening lattice anharmonicity (with, e.g., a cubic coefficient $\gamma>0$) will play a crucial role,

resulting in the appearance of supersonic states. In this case, due to the dispersion $b$ and the nonlinearity $\gamma$, the supersonic ''continuation'' of the DS self-trapping mode takes place. On the other hand, the well-known lattice (acoustic) solitons can appear and couple to the self-trapping mode (to be ''attached'' to it). The four parameters—two dispersions $a$ (in the quantum subsystem) and $b$ (in the lattice subsystem), and two nonlinearities $g$ (coupling of both the subsystems) and $\gamma$ (anharmonicity in the lattice subsystem)—are involved in the process of stabilized soliton motion. The interplay parameter $\kappa = a\gamma/bg$ appears in the theory. It can be considered as the ratio of the ''reduced'' nonlinearity in the lattice subsystem $(\gamma/b)$ to the reduced nonlinearity in the quantum subsystem $(g/a)$. The value $\kappa = 1$ is critical; in this paper it was defined as the Boussinesq limit. In the region $\kappa > 1$, the coupling of the self-trapping soliton with the lattice soliton happens, while for $\kappa < 1$ a quasiparticle only with higher-energy levels (when the soliton envelope $\phi_n$ has, e.g., one node) can be coupled. However, the latter states have been shown numerically to be dynamically unstable.

Finally, it should be emphasized that the present paper is devoted only to those two-component soliton solutions of the equations of motion (1) which have a stationary profile (one-phase or one-speed soliton solutions). One of these components represents a moving wave function of a quasiparticle. The latter is described by the envelope $\phi_n(\tau)$ of a permanent profile with the carrier frequency given by the eigenvalue $\varepsilon$. The motion of this envelope soliton is accompanied by the lattice deformation field $\rho_n(\tau)$, which also has a permanent profile. If the time evolution (in the framework of a numerical scheme) of such profiles is stationary, we call them dynamically stable soliton solutions. In this paper, the physical mechanism for each soliton mode is discussed. However, in the case when the Davydov and Boussinesq (lattice) solitons are initially displaced at some finite distance, some attractive interaction between them appears, and, as a result, the solitons start to *oscillate when passing through each other*. Such an oscillating motion has been observed numerically in a recent paper[25] which appeared just when this work was already completed. This motion describes the *collision* process of the Davydov and Boussinesq solitons when their centers are initially displaced at some finite distance. However, if the centers of these solitons are placed at the same position, a *stationary bell-shaped* (in both the components $\phi$ and $\rho$), two-component profile, describing the coupled *l-p* state, exists. The latter (stationary) state has been treated in this paper exactly. In the case of a cubic anharmonicity (28), the *l-p* coupling has been shown to occur if $\kappa > 1$.

Two aspects are also important to emphasize: (i) The existence of supersonic solitons means that the solitonic transport mechanism in, e.g., biophysical systems will be much more effective than thought before. (ii) Since the lattice solitons participate in the *mixed* transfer mechanism, the supersonic transport is expected to be *thermally* more stable than the *pure* self-trapping. The dynamics of nonstationary strongly localized states in anharmonic chains[26,39] and the thermal stability[40–42] of supersonic nonlinear excitations are other topics of future interest.

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