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# STABILITY OF ACOUSTIC AND OPTICAL SOLITONS IN A DIATOMIC CHAIN

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In this paper we will be concerned with the propagation of solitons of the compressive and rarefactive type in nonlinear atomic chains, i.e. we look for permanent profile solutions that preserve their form under collisions (except for a possible phase shift) or they are long lived. For interatomic potentials that can be expanded in a Taylor series in the relative atomic displacements (keep the first few terms) approximate analytic results can be combined with computer experiments if we consider smoothly varying waves.

A related discrete problem is the propagation of pulses in distributed transmission lines{1}. An LC-circuit with two nonlinear capacitors interchanged can serve as an analog computer for the diatomic chain but with a modified interatomic potential. With some modifications and the inclusion of electronic polarizability the nonlinear diatomic chain could be a reasonable model to describe ferroelectrics{2} and go beyond the self consistent phonon approximation.

The continuous limit in monatomic chains leads to equations for which the soliton solutions are known. For diatomic chains, however, little work has been done and this only in the case where two smooth functions can describe the displacements of the two different masses $M_1$ and $M_2$ {3-6}. For a diatomic chain there are both kink excitations of the acoustic type and modulated waves. Here the case $M_1 \neq M_2$ will be considered ($M_1 = M_2$ being a limiting case)except for the envelope type solutions where we present the monatomic case but also give some results for $M_1 \neq M_2$.

In the model the nearest neighbor atoms (NN), with relative displacement R, feel a potential

$$\Phi(R)= G(\frac{1}{2} R^2+ \frac{1}{3} AR^3+ \frac{1}{4} BR^4) \qquad (1)$$

where G,A and B are force constants (A=0 unless stated otherwise) The equations of motion for the displacements $Z_n(W_n)$ of the odd (even) particles with mass $M_1(M_2)$ in the nth cell (two atoms per cell of length 2D) are given by

$$M_1\ddot{Z}_n= G(W_n - 2Z_n + W_{n-1}) +GA \{(W_n-Z_n)^2- (Z_n-W_{n-1})^2\}$$
$$+ GB \{(W_n-Z_n)^3 - (Z_n-W_{n-1})^3\} \qquad (2a)$$

$$M_2\ddot{W}_n= G(Z_{n+1} - 2W_n + Z_n) +GA \{(Z_{n+1} - W_n)^2-(W_n-Z_n)^2\}$$
$$+ GB \{(Z_{n+1}-W_n)^3 - (W_n-Z_n)^3\} \qquad (2b)$$

We can decouple the two equations to $0(\varepsilon^m)$ (m=4 for acoustic, m=3 for optical) with $\varepsilon$ a small dimensionless parameter by choosing $Z\sim 0(\varepsilon^1)$, $Z_x\sim 0(\varepsilon^{1+j})$, $Z_t\sim 0(\varepsilon^{1+k})$ and similarly for w. The 1,j,k could be different for acoustic or optical excitations. We go to the continuum limit (with x=2nD) and use an ansatz {3,6}that relates W(x,t) with Z(x,t) and its derivatives.

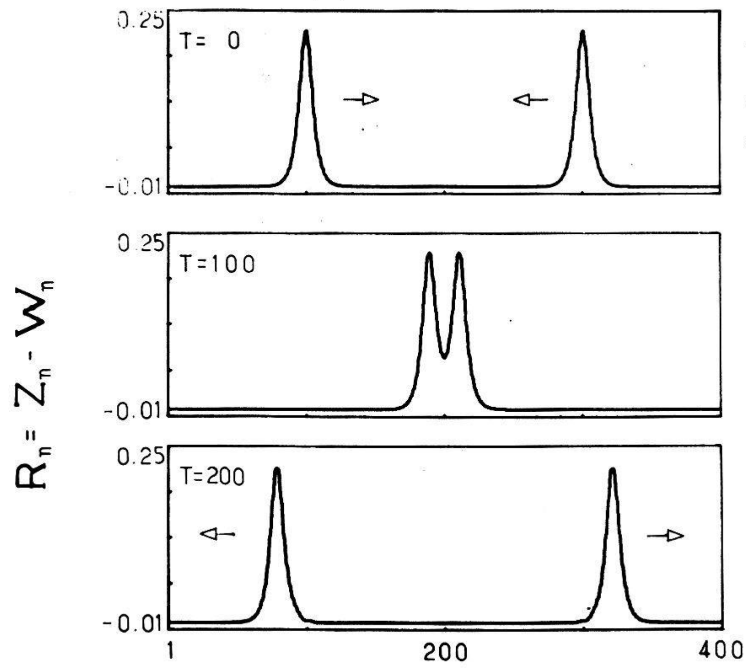
$$W(x,t)=\lambda(Z+b_1DZ_x+b_2\frac{D^2}{2} Z_{xx}+b_3\frac{D^3}{6} Z_{xxx}+b_4\frac{D^4}{24}Z_{xxxx}) \qquad (3)$$

The constants $\lambda,b_1,b_2,b_3,b_4$ are determined so that the two equations of motion are compatible to $0(\varepsilon^m)$, and $\lambda$ can take two values $\lambda_{1,2}=1,-M_1/M_2$. The equation for Z(x,t) is easily solved and analytical details are given in previous work {3,6}.

<u>i. $\lambda_1=1$(acoustic mode):</u> we obtain a Boussinesq type equation for $u=Z_x$

$$u_{tt}=c_o^2u_{xx}+p(u^2)_{xx}+q(u^3)_{xx}+hu_{xxxx} \qquad (4)$$

with p,q and h depending on G,A,B,$M_1$ and $M_2$. For (NN) interactions the solution is a supersonic kink for Z(compressive or rarefactive depending on the values of the parameters p,q,h). If we include second nearest neighbors (SNN) the dispersive term can become negative (h< 0) so that we have subsonic kinks. This has been found for $M_1=M_2${7} . For $M_1\neq M_2$ and (SNN) we can easily apply the previous procedure for a quartic potential (A=0 in (1))if we include a nonlinear term in the ansatz of equation (3), and obtain eqn(4) with different constants. Computer simulations have shown these kinks (pulses in $Z_x$) to propagate with no lattice pinning or discreteness effects for any mass ratio if the soliton width L is much larger than D. Since $L\sim 1/\sqrt{V-c_o}$ the solitons must be moving near the speed of sound $c_o$.




In Fig. 1 we show a quasi-elastic head on collision between two acoustic excitations for a diatomic chain of 400 atoms and additive SNN interactions

Figure 1

ii. $\lambda=-M_1/M_2$ (optical mode): For the quartic potential (A=0) and small but finite Z,W of $O(\varepsilon)$ we obtain keeping terms to $O(\varepsilon^3)$in (2) an envelope soliton for the odd atoms:

$$Z(x,t)= A_m \text{sech}\left(\frac{x-v_e t}{L_e}\right)\cos\left(\frac{x-v_o t}{L_o}\right) \qquad (5)$$

The amplitude $A_m$, the width determining parameters for the envelope $L_e$ and the carrier wave $L_o$ and their corresponding speeds $v_e$ and $v_o$ are given in terms of two small arbitrary parameters plus a wavenumber k and a frequency $\omega$ which are related through the the linear dispersion relation for the optical branch near $k\approx 0$ { 6 }. The displacement of the even atoms can be obtained from the ansatz in (3). Computer simulations show that the solution keeps its permanent profile even for mass ratios up to $M_1/M_2\approx 5$, where pinning phenomena start appearing. This is probably due to the omission of terms of $O(\varepsilon^5)$ whose coefficients become significant for very different masses. Collision experiments of optical with acoustic excitations show their stability { 6 } while in Fig.2 we present two optical excitations in a head-on collision which is quasielastic. We plot the displacements $Z_n$ of the odd (full line) and $W_n$ of the even (dashed line) atoms for different times

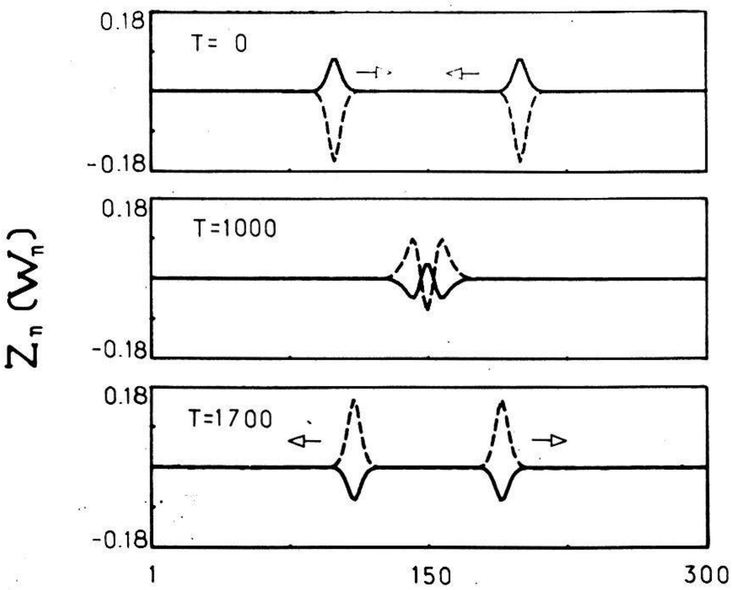



Fig. 2 Optical-Optical soliton collision for a diatomic chain of 300atoms. $Z_n$ (solid line), $W_n$ (dashed lined) of the evolution (the two curves are $180^0$ out of phace). For the parameters used the width of the oscillations of the odd (or even) atoms is of the order of $L_e$ and since $v_e << v_o$ the pattern appears to be breathing.

The optical solution in (5) valid near $k \approx 0$ can be extended to cover the whole dispersion curve by looking for fast oscillating solutions with a smoothly varying envelope. To do this we must separate the oscillations by writing for the monatomic chain displacement

$$Y_n(t) = F_n(t) e^{i(knD - \omega t)} + c.c. \qquad (6)$$

and then take the continuum limit of the envelope function $F_n(t)$. For simplicity here we consider $M_1 = M_2$ with a quartic potential (A=0) while the addition of a cubic term ($A \neq 0$ for $M_1 = M_2$) will be discussed. The calculations for $M_1 \neq M_2$ are quite lengthy and are presented elsewhere ( 9 ). The solution is easy for $F \approx O(\varepsilon)$ with $F_x \approx O(\varepsilon^2)$, $F_t \approx O(\varepsilon^2)$ while k and $\omega$ to $O(\varepsilon)$ are related by the linear dispersion relation

$$\omega^2 = 4 \frac{C_o^2}{D} \sin^2 \frac{kD}{2} \qquad (7)$$

By writing the complex amplitude in the continuum limit as:

$$F(x,t) = \Phi(x - v_e t) e^{i\vartheta_x (x - v_c t)} \qquad (8)$$

with $\Phi$ real, and keeping terms to $O(\varepsilon^3)$ we obtain for $\Phi$

$$\lambda \Phi_{xx} = p\Phi - q\Phi^3 \qquad (9)$$

with

$$\lambda = v_e^2 - C_o^2 \cos kD \qquad (10a)$$

$$q = 48\frac{C_o^2}{D^2} B \sin^4 \frac{kD}{2} \qquad (10b)$$

p is given by a complicated expession including $v_c$ and is of $O(\varepsilon^2)$ and $v_e$ is the group velocity $d\omega/dk$ to $O(\varepsilon)$. By multiplying (9) with $\Phi_x$ and integrating we get:

$$\frac{1}{2}\Phi_x^2 - \frac{1}{2}\frac{p}{\lambda}\Phi^2 + \frac{1}{4}\frac{q}{\lambda}\Phi^4 = \text{const.} \qquad (11)$$

If $p/\lambda < 0$ and $q/\lambda < 0$ $\Phi$ is a pulse

$$\Phi = \sqrt{p/\lambda}\ \text{sech}\ \{ \sqrt{p/q}\ (x - v_e t) \} \qquad (12)$$

while for $p/\lambda < 0$ and $q/\lambda < 0$ the envelope is a kink. Since $\lambda > 0$ over the k-range, except a region near $k \approx 0$, and for $B > 0$ i.e. if the quadratic and quartic terms in the potential are additive, we have envelope solitons, while for competitive terms ($B < 0$) we get dark envelope solitons. If we look at the modulational stability of plane waves we find they are unstable for $B > 0$ but stable for $B < 0$ for any k. If we include, however a cubic part {8} there is a critical frequency above which plane waves are modulationally unstable depending on the competition between the cubic and quartic coefficients A and B. The critical frequency is $\omega_c^2 = 4a(3/2 - a)$ with $a = A^2/B$. The inclusion of the cubic term makes the derivation tedious and will not be presented. If we include (SNN) even for $A=0$ the stability depends on whether the force constants for (NN) and (SNN) have the same or opposite sign, and on the k value {9}. To check the conclusions on modulational stability we must take into account long range interactions.

In Fig. 3 we present an envelope soliton with a wavevector $k \approx 1/D$, which is quite stable while propagating even after a collision with the fixed end of the chain. Computer experiments are going on to check their stability under head on collisions, and look at other k-values.

The nonlinear excitations considered here should also appear in the structure factor calculations of molecular dynamics . The statistical mechanics of these systems have not been

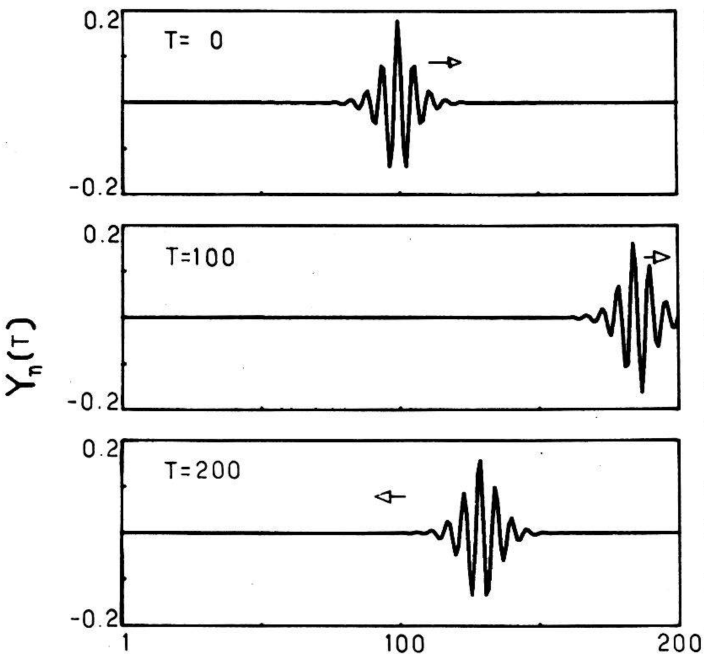



Fig. 3 Envelope soliton with k=1 for a monatomic chain of 200 particles.

worked out (as in the $\Phi^4$ problem in the displacive limit) so it is not obvious whether the nonlinear excitations would give distinct features, and is left for future work. We must check the modulational stability of plane waves for a cubic and quartic potential including long range interactions. In regions where dispersion is negative there are possibilities of nonelastic collisions between acoustic excitations subject to resonance conditions. Finally the interaction of these solitons with mass or force constant impurities and their stability to disorder should be of physical interest.

Concluding we see that in 1-d monatomic and diatomic chains there are stable and long-lived kink excitations of the acoustic type and envelope solitons which include optical solitons The modulational stability of plane waves depends strongly on the quadratic part of the potential.

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