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The effect of soft modes on solitons in a linear lattice

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Abstract. Solitons are simulated in an anharmonic linear lattice that is susceptible to a soft mode instability. The soft mode characteristic is introduced in the system by the addition of a term $(-Au_n^2)$ in the potential between the neighbouring atoms and the evolution of the system is studied as the soft mode parameter A varies from zero to the square of the limiting optical frequency. It is shown that the displacement pattern of the system shows three regions. First there is a region in which the relative displacements of the atoms show large amplitude oscillations. This is followed successively by a domain in which the relative displacements of the atoms are negligible and then by the soliton itself. In the soft mode region, the displacements of the atoms preceding the soliton decrease drastically in a linear fashion first, parabolically next and later become steady. It further exhibits a kind of devil's stair cases.

Keywords. Solitons; linear lattice; soft modes; devil's stair case; phase transitions.

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1. Introduction

A linear lattice bound by anharmonic forces had been studied by Fermi *et al* (1955), Toda (1970), Zabusky and Kruskal (1965) and many others. Hardy and Karo (1977) had made theoretical and numerical studies of soliton-like behaviour in one-dimensional systems. Rolfe *et al* (1979) investigated the solitary wave motion on linear chains of equal masses which interact either in accordance with Morse or Lennard-Jones potentials with their nearest neighbours. The applications of solitons in solid state physics have been reviewed by Bishop and Schneider (1978).

In an earlier paper (Narasimha Iyer and Viswanathan 1983) we have described the results of the numerical experiments on the propagation of solitons in one-dimensional lattices and the effect of defects or density discontinuities on the propagation of these finite amplitude waves. Solitons can be generated in a linear lattice, in which neighbouring atoms interact through a strong anharmonic Morse potential, by imparting a strong initial impulse or a large displacement to one of the boundary atoms. It was shown that a localised mode appears at the site of a defect when a soliton crosses the site and further a defect or a density discontinuity in the lattice are sources of additional solitons that could propagate either forwards or backwards. When two solitons collide at a defect region, they reemerge without much distortion, but leave a localized mode at the site of the defect.

In this paper, we have continued our numerical studies to investigate the behaviour of solitons in a linear lattice in which the limiting optical mode becomes soft. This can be done by introducing an additional term $(-A\Sigma u_n^2)$ in the Hamiltonian so that the limiting optical frequency diminishes from its harmonic approximation value to zero. By giving various values for A from zero to the square of the frequency of the limiting optical mode, the lattice can be made unstable and the frequency of the optical mode ultimately tends to zero. The propagation of a soliton in such an unstable lattice could yield valuable information on displacive phase transitions in ferroelectrics as well as the emergence of domain walls in various contexts during phase transitions. Earlier the statistical mechanics of one-dimensional lattices for structural phase transitions has been studied by Krumhansl and Schrieffer (1975). By using a quartic anharmonic term and an additional negative quadratic term to represent the soft mode, they had studied analytically under various approximations the displacement pattern of the lattice and the emergence of domain walls. The principal interest of Krumhansl and Schrieffer has been the central peak in the neutron scattering experiments, which defies explanation through conventional perturbative anharmonic phonon calculations. Our interest, however, here is to investigate the nature of the displacement pattern and the characteristics of a soliton in a lattice that is susceptible to instability through a soft mode.

In the present paper, we assume that the neighbouring atoms of the lattice interact through strong anharmonic forces represented by a Morse Potential but we make the optical mode soft by introducing an additional term $(-A\Sigma u_n^2)$ in the Hamiltonian. The lattice is otherwise assumed to be uniform and without defects. The results of the computer calculations are presented in §3.

2. Mathematical formulations

We consider a linear lattice consisting of N atoms and denote the displacement of the nth atom from its equilibrium position by u_n.

We assume that the neighbouring atoms interact through a potential of the form

$$\phi_n = k[1-\exp(-\beta r_n)]^2 - Au_n^2, \tag{1}$$

where $r_n = (u_n - u_{n-1})$ and k and β are constants.

The first term is the Morse potential which is highly anharmonic. The second term in which A is kept positive, has a tendency to reduce the frequency of the limiting optical mode and to make it soft and ultimately when $A = k\beta^2$, the coefficient of u_n^2 in ϕ_n will vanish. We assume that a force $f_n(t)$ is applied to the nth particle.

Denoting the relative displacement by $r_n = (u_n - u_{n-1})$, the momentum conjugate to r_n by s_n, the potential energy of the system by U and the kinetic energy of the system by K, we get

$$U = \sum_{n=1}^{N} [\phi_n - r_n f_n(t)]. \tag{2}$$

$$K = \frac{m}{2}\sum_{n=1}^{N} \dot{u}_n^2 = \frac{m}{2}\sum_{n=1}^{N}\left(\sum_{j=1}^{n} \dot{r}_j\right)^2. \tag{3}$$

$$s_n = \frac{\partial K}{\partial \dot{r}_n} = m\sum_{j=n}^{N}\left(\sum_{i=1}^{j} \dot{r}_i\right). \tag{4}$$

The boundary conditions $r_1 = u_1$ and $s_{N+1} = 0$ are to be noted.

The Hamiltonian of the system can be expressed as a function of r_n and s_n as

$$H = \frac{1}{2m} \sum_{n=1}^{N} (s_n - s_{n+1})^2 + \sum_{n=1}^{N} [\phi_n - r_n f_n(t)]. \tag{5}$$

The Hamiltonian equations of motion are given by

$$\begin{aligned} \dot{s}_1 &= -2k\beta[\exp(-\beta u_1) - \exp(-2\beta u_1)] + 2A \sum_{j=1}^{N} u_j + f_1(t), \\ \dot{s}_n &= -2k\beta[\exp\{-\beta(u_n - u_{n-1})\} - \exp\{-2\beta(u_n - u_{n-1})\}] \\ &\quad + 2A \sum_{j=n}^{N} u_j + f_n(t), \quad (n = 2, 3, 4, \ldots N) \\ \dot{u}_n &= \frac{1}{m}(s_n - s_{n+1}), \quad n = 1, 2, 3, 4, \ldots (N-1), \\ \dot{u}_N &= s_N/m. \end{aligned} \tag{6}$$

The above equations will reduce to (11) of our earlier paper, if we set $A = 0$.

Equations (6) represent a set of $2N$ simultaneous equations in the variables u_n and s_n. They are a set of first order differential equations and can be solved using a computer under given initial or boundary conditions.

We give an impulse to the first atom of magnitude $F_0 = 4 \times 10^4$ units, so that

$$f_n(t) = F_0 \cdot \delta_{n,1} \cdot \exp(-t^2/2\sigma). \tag{7}$$

By choosing $\sigma = 0{\cdot}001$, the exponential term can be approximated to a delta function, $\delta_{n,1}$ being the Kronecker delta function.

The equations were written in the non-dimensional form using $T = 10^{-12}$ sec; displacement unit $= 10^{-8}$ cm; mass unit $= 10^{-24}$ g and force unit $= 10^{12}$ dynes.

The equations were solved by fourth order Runge-Kutta formulae with modification due to Gill.

The parameter A was given successively the values $0{\cdot}025\, k\beta^2$, $0{\cdot}125\, k\beta^2$, $0{\cdot}833\, k\beta^2$ and $0{\cdot}999\, k\beta^2$, to study the evolution of the vibrational instability of the lattice.

Other values assumed are given below:

$$m = 1,\ k = 0{\cdot}3;\ \beta = 3{\cdot}333;\ N = 60;$$

$$u_1 = u_2 = u_3 = \cdots = u_N = \dot{u}_1 = \dot{u}_2 = \ldots = \dot{u}_N = 0 \text{ at time } t = 0.$$

3. Numerical results and conclusions

The nature of the vibrational state of a linear lattice in which neighbouring atoms are bound by strong anharmonic Morse Potential under the influence of a strong initial impulse has been described in § 1. It is shown that the displacement pattern of the various atoms at any instant of time is like an heavyside step function, being a constant up to a certain atom and then dropping down to zero. The relative displacements $(u_n - u_{n-1})$ of the atoms at any instant exhibit a finite amplitude sharp pulse or soliton, which progresses uniformly with time.

In figure 1, we plot the graph of the relative displacement for the case $A = 0{\cdot}025\, k\beta^2$. The ratio $(A/k\beta^2)$ is too small to distort the coefficient of the harmonic term in the

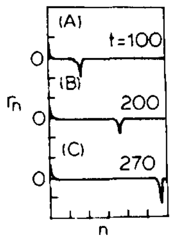

Figure 1. For $A = 0{\cdot}025\ k\beta^2$, the relative displacements of atoms at the instants **A.** $t = 100$, **B.** $t = 200$ and **C.** $t = 270$ are shown.

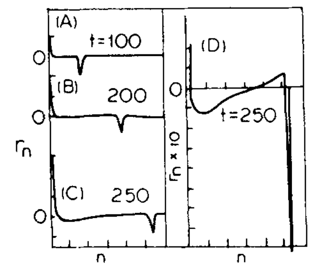

Figure 2. The relative displacements of atoms corresponding to $A = 0{\cdot}125\ k\beta^2$, are shown at instants **A.** $t = 100$ **B.** $t = 200$ and **C.** $= 250$. In 2**D** the relative displacements of C have been magnified 10 times so as to depict the disturbance clearly in the region to the left of the soliton.

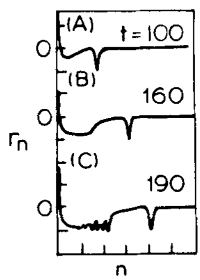

Figure 3. For $A = 0{\cdot}833\ k\beta^2$, the relative displacements of atoms at the instants **A.** $t = 100$, **B.** $t = 160$ and **C.** $t = 190$ are shown.

potential and the influence of the damping term, therefore, is negligible on the propagation of the solitary waves. A soliton propagates freely in the lattice.

In figure 2, we plot the relative displacements of atoms when $A = 0{\cdot}125\ k\beta^2$. Here again the soliton propagates freely, but the region through which the soliton has passed earlier has been found to be disturbed slightly even long after the passage of the soliton through that site. In figure 2d, we have reproduced the relative displacements at $t = 250$, magnified ten times.

We now pass on to the case when the frequency of the mode is reduced significantly and this mode tends to become soft. Figure 3 depicts the relative displacements at $t = 100$, 160 and 190 corresponding to the ratio $A/k\beta^2 = 0{\cdot}833$. The coefficient of the quadratic term has now been reduced from $k\beta^2$ to $(0{\cdot}167\ k\beta^2)$ in the potential and the frequency of the limiting optical mode in the harmonic approximation, then gets reduced to 0·41 ω_{lim}.

Figure 3a shows that a soliton is propagating through the lattice at $t = 100$, but the relative displacement of the atoms in the distorted region preceding the soliton is not zero. The relative displacement first increases and then reduces to zero just before the soliton. Figure 3b shows the relative displacement of the atoms at $t = 160$. Here we notice that the relative displacements have assumed a large value almost equivalent to the amplitude of the soliton itself and further a small ripple has just emerged. As time passes, the relative displacements in the region preceding the soliton show large scale oscillations and further the maximum magnitude of the relative displacement in this region is nearly equal to the amplitude of the soliton. The linear lattice in this case displays three regions. Firstly, a region having large relative displacements which shows large amplitude oscillations. This is followed by a domain in which the relative displacements of the atom are negligible and finally this domain is followed by the soliton. The emergence of a domain exhibiting large relative displacements as well as fluctuations in them followed by a region with no relative displacement at all has similarities with displacive ferroelectric phase transition and the phenomena of domain walls in the ferromagnetic phase transition. It is, therefore, suggested that solitons should play an important role on ferroelectric phase transitions near the critical temperature and the subject approached in this way, can throw more light both on solitons and their role in phase transitions.

In figure 4(a, b, c) we give the displacement pattern of the atoms at different instants of time, after the initial impulse is imparted to the boundary atom, for the case $A = 0{\cdot}833\ k\beta^2$. We may recall that when $A = 0$, the displacement pattern is in the form of a step function, being constant up to a certain atom and the falling down to zero steeply at the site of the soliton. In contrast to this, we also find from that the displacement of the atoms steadily falls down almost linearly first, then parabolically

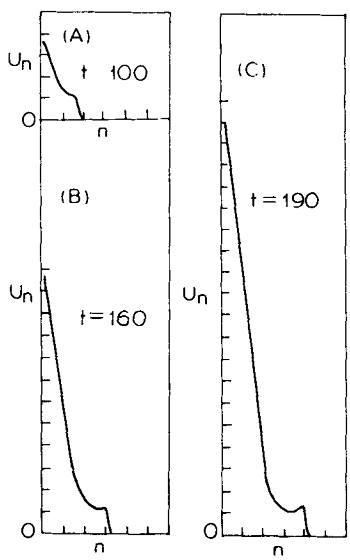

Figure 4. For $A = 0{\cdot}833\ k\beta^2$, the displacements of atoms at times **A.** $t = 100$, **B.** $t = 160$ and **C.** $t = 190$ are shown.

and finally reaches a constant value. Later the displacement jumps to zero at the position of the soliton.

In figure 5(a, b) we show the relative displacements for the case $A = 0{\cdot}999\,k\beta^2$. In this case the frequency of the limiting optical mode in the harmonic approximations would be very nearly equal to zero. Even though these figures are similar to 3(a, b, c), the fluctuations in the domains of the largest relative displacements are very much pronounced here at $t = 200$. These figures convincingly show that the system consists of three domains, sharply separated by either a domain wall or a soliton. Firstly, there is a region in which the relative displacements are large and exhibit large amplitude oscillations. This is followed by a region of negligible relative displacements, but the actual displacement of the atoms in this region is nevertheless finite. Finally the soliton separates this region from the undisturbed part of the linear lattice.

Figure 6(a, b, c) which give the displacement patterns of this unstable lattice are interesting and revealing. Figure 6(a, b) representing the vibrational state of the system at $t = 100$ and 140 respectively show that the displacement of the atoms decrease

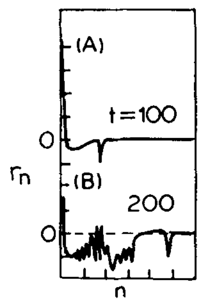

Figure 5. The relative displacements of atoms corresponding to $A = 0{\cdot}999\,k\beta^2$ at **A.** $t = 100$ and **B.** $t = 200$ are shown.

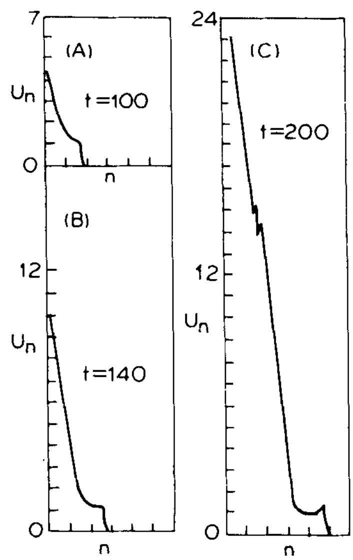

Figure 6. The displacements of atoms corresponding to $A = 0{\cdot}999\,k\beta^2$ at **A.** $t = 100$, **B.** $t = 140$ and **C.** at $t = 200$ are depicted. The incomplete devil's stair case is seen in figure 6 (C).

drastically as well as linearly first, parabolically next and finally become nearly steady. The displacement finally shows a discontinuity and reduces to zero at the site of the soliton. Figure 6(c) shows, in addition, that the displacement pattern exhibits "stair cases", though they are very steep in this case. Such 'stair cases' have been earlier investigated by several workers (Aubry 1978; Fisher *et al* 1978) and have been reviewed by Per Bak (1982). They are known as the devil's stair case and are supposed to play an important role in the transitions, between commensurate to incommensurate systems, hysteresis and phase transitions. A comparison of figure 5(b) with figure 6(c) shows that obviously the devil's stair cases are the cause for the large scale oscillations seen in figure 5(b) for the relative displacements of the atoms.

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