Pramāṇa, Vol. 20, No. 5, May 1983, pp. 415–427. © Printed in India

Solitons in a linear lattice with defects

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MS received 11 August 1982; revised 8 March 1983

Abstract. Solitons are generated in an anharmonic linear lattice in which neighbouring atoms interact through a Morse potential by giving either a strong initial impulse or a large displacement to an end atom. Studies on the variation of the characteristic properties of the soliton with the strength of the initial pulse show that the velocity and the amplitude of the soliton increase with the strength of the initial impulse, but below a certain critical value for the initial impulse, only an oscillatory tail is generated. It is shown that when a defect is present in the lattice, a localised mode appears at the site of the defect and additional solitons travelling forward or even backwards, are generated. When two solitons collide at a defect region, they reemerge but leave a localised mode at the site of the defect. If an initial velocity is imparted to a particular particle, synchronously with the crossing of the particle by the soliton, a localised mode emerges at the site of the particle and additional solitons are also generated. When a soliton moves from a denser to a rarer medium, a strong localised pulse is created near the region of the density discontinuity and additional solitons appear; and further a weak oscillatory tail is left behind in the denser medium. On the other hand, if a soliton moves from a rarer to a denser medium, it is reflected back and a small localised mode is generated at the site of the density discontinuity. The variation of amplitude of the soliton with the velocity of propagation is also studied.

Keywords. Soliton; linear lattice; defects; localised mode; equation of motion.

1. Introduction

Solitons are finite amplitude waves having remarkable stability and can propagate in a medium without distortion or change of shape. Solitons have been either observed or studied in a variety of contexts, such as solid state, plasma or elementary particle physics. Russell (1844) first noticed the remarkable stability of the solitary wave in shallow water and also the break-up of an initial pulse into two solitons. Korteweg and DeVries (1895) derived the nonlinear differential equation satisfied by the solitary waves. Interest in the subject revived after the classical work of Zabusky and Kruskal (1965) who showed by a series of numerical experiments that solitons are extremely stable on collision. In the field of condensed matter physics, solitons find applications in different topics such as phase transitions and critical phenomena, spin waves, dislocations, defects in crystals and one dimensional metals. The diverse applications of solitons in solid state physics have been reported in the excellent review of Bishop and Schneider (1978).

A linear lattice bound by anharmonic forces had been studied by Fermi *et al* (1955), Toda (1970), Zabusky and Kruskal (1965). 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. They also studied the scattering of solitons by mass inhomogeneities and showed that when the mass ratio is 13/12 a solitary wave survives at least 500 collisions and its energy is modulated cyclically. In the present paper we generate solitons in an anharmonic lattice by giving a strong initial impulse as well as a large displacement to a boundary atom. That the disturbance propagating through the lattice represented in reality a soliton was verified from the characteristic properties of the soliton, such as its stability, retention of shape through propagation or re-emergence after collision with little distortion. We have investigated in particular the effect of varying the initial impulse on the characteristic properties of the soliton and the scattering of a soliton by a defect. The problems investigated in the paper are different from those studied by Rolfe and Rice (1980). It is shown that when a defect is present in the lattice, a localised mode is generated at the site of the defect; additional solitons are also created at the site of the defect, some travelling even backwards. The velocities of propagation and amplitudes of the additional solitons have been found to be different from the original soliton. When two solitons collide at the site of a defect, they re-emerge without much distortion but leave the trail of a localised mode at the site of a defect. If the initial force imparted to the boundary atom is increased, both the amplitude as well as the velocity of the solitons increase. If an initial velocity is imparted synchronously with the crossing of a particular particle by the soliton, a localised mode is produced at the site of this particle, and besides additional solitons are generated. Several initial or boundary value problems relating to the propagation of solitons in a linear chain are also presented.

2. Equation of motion

We consider a linear lattice of N atoms each separated from its neighbour by an equilibrium distance a. We restrict the interaction to the first neighbours only and assume that the interaction potential between the neighbouring atoms is described by the Morse potential of the form

$$V_{n+1,n} = k\{1 - \exp\left[-\beta\left(u_{n+1} - u_n\right)\right]\}^2 \tag{1}$$

where u_n represents the instantaneous displacement of the nth atom from its equilibrium position; β and k are constants. The kinetic energy of the system is given by

$$K = \frac{m}{2} \sum_{N=1}^{N} \dot{u}_n^2. \tag{2}$$

The relative displacement between two neighbours is denoted by

$$r_n = (u_n - u_{n-1}) \tag{3}$$

Taking $r_1 = u_1$ and using (3), the kinetic energy of the system can be expressed as

$$K = \frac{m}{2} \sum_{n=1}^{N} \left(\sum_{j=1}^{n} \dot{r}_j \right)^2. \tag{4}$$

We assume that a force $f_n(t)$ is applied to the nth particle. The potential energy of the system is given by

$$U = \sum_{n=1}^{N} [\phi_n - r_n f_n(t)], \tag{5}$$

where $$\phi_n = V_{n,n-1} = k\,[1 - \exp(-\beta\, r_n)]^2. \tag{6}$$

The momentum conjugate for r_n is denoted by s_n and is given by

$$s_n = \frac{\partial K}{\partial r_n} = m \sum_{j=n}^{N} \left(\sum_{l=1}^{j} r_l \right). \tag{7}$$

The Hamiltonian is a function of r_n and s_n, and may be written as

$$H = \frac{1}{2m} \sum_{n=1}^{N} (s_n - s_{n+1})^2 + \sum_{n=1}^{N} (\phi_n - r_n f_n(t)). \tag{8}$$

The Hamiltonian equations of motion are given by

$$\dot{r}_n = \frac{\partial H}{\partial s_n} = \frac{1}{m}(2s_n - s_{n-1} - s_{n+1}), \tag{9}$$

$$\dot{s}_n = -\frac{\partial H}{\partial r_n} = -\left(\frac{\partial \Phi}{\partial r_n} - f_n(t)\right), \tag{10}$$

where $$\Phi = \sum_{n=1}^{N} \phi_n.$$

Equations (9) and (10) constitute a set of $2N$ equations in the variables r_n and s_n which can be solved with the aid of a computer. For analysing our computational results and for physical visualisation, it is necessary to return to the actual displacement u_n. In terms of u_n, (9) and (10) may be written as

$$\dot{s}_1 = -2k\beta\,[1 - \exp(-\beta\, u_1)]\,\exp(-\beta\, u_1) + f_1(t),$$

$$\dot{s}_n = -2k\beta\,[1 - \exp(-\beta(u_n - u_{n-1}))]\exp[-\beta(u_n - u_{n-1})] + f_n(t)$$

$$(n = 2, 3, \ldots, N) \tag{11}$$

$$\dot{u}_n = \frac{1}{m}(s_n - s_{n+1}) \cdot [n = 1, 2, 3, \ldots (N-1)],$$

$$\dot{u}_N = \frac{1}{m} s_N.$$

Equation (11) 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 different initial and boundary conditions. We considered a lattice consisting of 60 atoms. A computer program was written to solve the set of $2N$ equations. The numerical method of solving (11) is different from the algorithm mentioned by Rice *et al* (1979). We have solved the set of equations by fourth order Runge-Kutta formulae with the modification due to Gill. The computer was instructed to print the displacements u_n, the relative displacements r_n and the velocities $\dot{u}_n$ of the set of N atoms at different periods of time at intervals of 2 units. The equations were rewritten in non-dimensional form using $T=10^{-12}$ sec; displacement unit$=10^{-8}$ cm, mass unit$=10^{-24}$ g and force unit$=10^{12}$ dynes.

Solitons were generated in the lattice by giving a large initial displacement to the boundary atom and subjecting the atom to a force of infinitesimal duration. Mathematically this can be achieved by treating the initial impulse as a delta function. The remaining atoms are kept unaffected. Several numerical experiments were conducted by modifying the initial and boundary conditions, as well as by introducing defects in the lattice, some of which are as follows:

(i) A large initial impulse was given to the first atom alone. The boundary conditions are

$$f_n(t) = F_0\,\Delta_{n,1}\,[\exp(-t^2/2\sigma)]$$

where $\Delta_{n,1}$ is the Kronecker delta function. By taking $\sigma=0{\cdot}001$, the Gaussian distribution can be made to approximate a delta function. F_0 was given values of the order 10^4 and 10^3 and β was given different values ranging from $\frac{1}{2}(3{\cdot}333)$ to $(3{\cdot}333)$ at $t = 0$; $u_i = \dot{u}_i = 0$ for all $i = 1, N$.

(ii) A soliton was produced as above by introducing a large initial impulse to the first atom and a vacancy was created at the 13th place of the linear chain.

(iii) The crossing of 2 solitons at the site of a defect was investigated.

(iv) The parameters m, k and β were kept constant for $n=21$ to 60, but were changed to $2m$, $2k$ and 3β respectively for $n=1, 20$. The lattice corresponds to a medium with different densities and the propagation of solitons in this lattice corresponds to propagation in a medium with a discontinuous change of density at some point.

(v) When the soliton is crossing a particular atom, say the 48th atom, an instantaneous velocity was given to this particle. The effect of this on the future time development was studied.

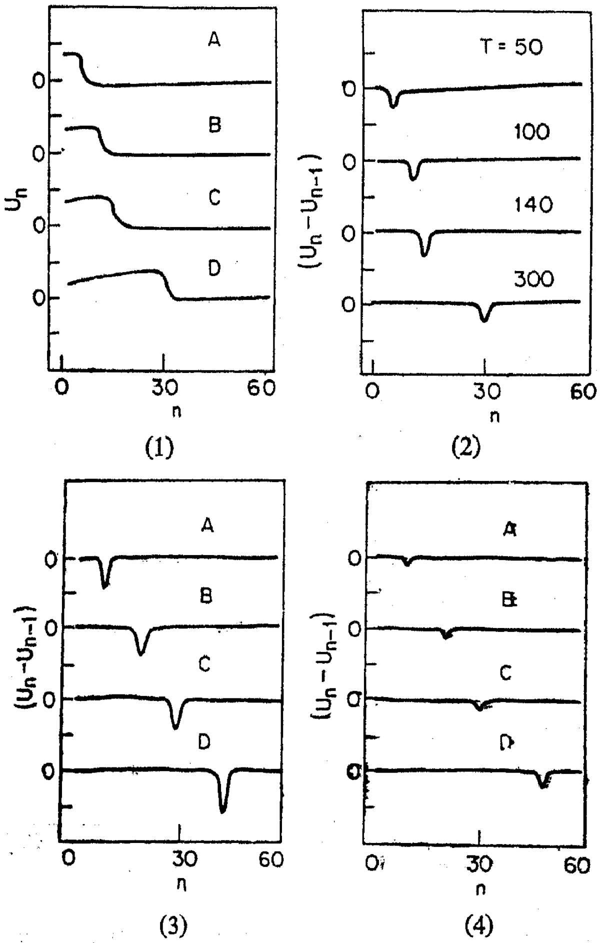
(vi) The nature of propagation of the disturbance, when the initial force F_0 was reduced by a factor of 10 to 10^3 from 10^4 was studied.

(vii) In addition to the impulse, an initial displacement of the order of the interatomic spacing was given to the first atom.

3. Solitons produced by an initial impulse

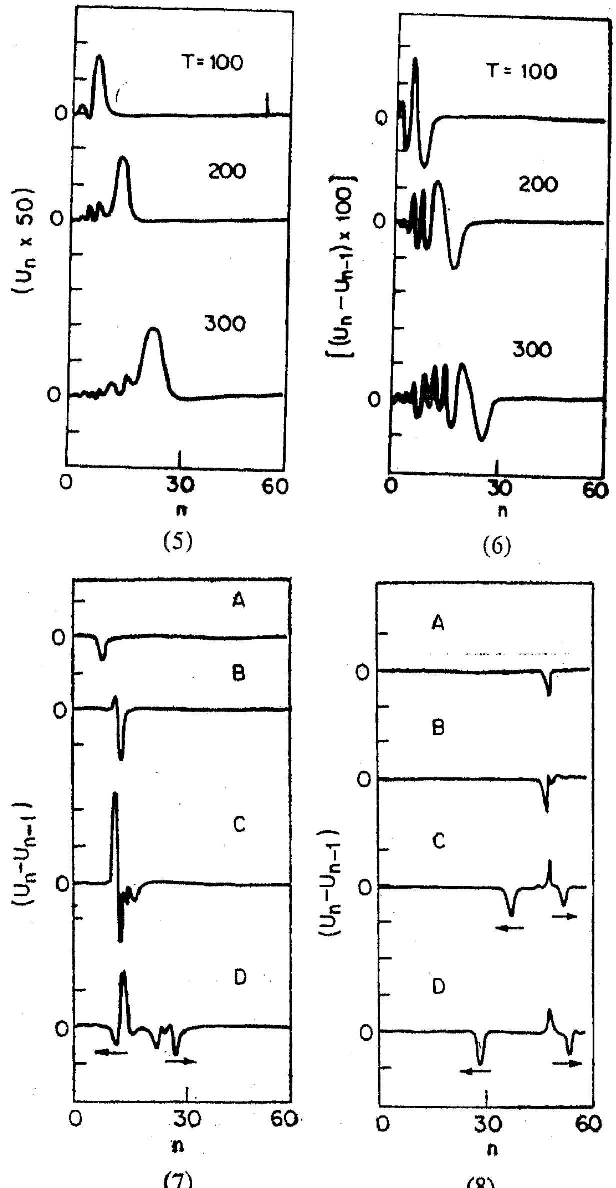
Solitons were produced by giving a strong initial impulse characterised by the parameters $F_0 = 2 \times 10^4$, $\beta = 3{\cdot}333$, to one end of a chain containing 60 atoms. The disturbance thus generated represented a soliton and this was verified by the fact that the pulse travelled with unifoım velocity and retained its height as well as width without any distortion throughout the propagation up to the end of the chain. Further two solitons generated at both ends of the lattice crossed each other without any change of shape or velocity of propagation.

In figure 1 (A-D) is given the displacement pattern of the lattice at four different



Figures 1-4. **1.** Displacement *vs* atom number. Parameters $F_0 = 2 \times 10^4$, $\beta = 3{\cdot}333$; $k = 0{\cdot}3$; $T = 50$ (for A), 100(for B); 140 (for C) and 300 (for D). **2.** Relative displacement *vs* atom number. Parameters same as that for figure 1. **3.** Parameters $F_0 = 5 \times 10^4$; $\beta = 3.333$; $k = 0{\cdot}3$. **4.** Parameters $F_0 = 2 \times 10^4$; $\beta = 2 \times 3{\cdot}333$; $k = 0.3$. X axis 1 cm=10 atoms, Y axis=1 Å.

instants of time for a chain of 60 particles, when the first atom was given an initial force $F_0=2\times10^4$. The parameter β characterising the oscillation period was given the value $\beta=3{\cdot}333$. It is seen that a shock propagates in the lattice and the displacement suffers a steep drop in value at a particular point in the lattice at any instant of time. Figure 2, gives the plot of the relative displacement (u_n-u_{n-1}) of the neighbouring atoms at four different periods of time. It is seen that a soliton is generated in the lattice and it travels forward in the lattice without any distortion or change of shape. In figure 3, we consider the effect of increasing the strength of the initial force to understand how the soliton parameters such as the pulse height, width and velocity of propagation depend on the initial force. When the force is increased to 4×10^4, both the amplitude and the velocity of propagation increase. The amplitude increases by a factor of



Figures 5-8. **5.** Displacement *vs* atom number. Parameters $F_0=1000{\cdot}0$; $\beta=3\times3{\cdot}333$; $k=0{\cdot}333$. **6.** Relative displacement *vs* atom number. Parameters same as for figure 5. **7.** The case of a vacancy at the place of 13th atom. Parameters $F_0=3\times10^4$; $\beta\times3{\cdot}333$; $k=0{\cdot}333$. **8.** The case of crossing of an excited atom by a soliton. A backward moving soliton crosses the 48th atom which is just excited. X axis 1 cm=10 atoms, Y axis=1 Å

nearly $\sqrt{5}/2 \sim 1\cdot 6$, equal to the square-root of the ratio of the initial forces, whereas the velocity increases by a factor approximately equal to the ratio of the initial forces. In figure 4, we compare the effect of increasing the parameter β by a factor 2. In the absence of anharmonicity, β is proportional to the frequency of the zone edge mode. It is seen that as β increases by a factor 2, the pulse height decreases but the velocity of propagation of the soliton increases rapidly. In figure 5, we show the nature of displacement of the atoms when the initial force was reduced by a factor of twenty. This figure corresponds to the case $F_0=10^3$ and $\beta'=3\beta$. The increase in the β value will ensure that the disturbance travels fast. The figure shows that the solution is no longer of the soliton type. It is seen that the displacement consists of a leading wave followed by a train of waves or an oscillating tail. When soliton solutions are present, the displacement has the character of a step-like function and figure 5 compared with figure 1 will show the difference between the two cases. In figure 6, we plot the relative displacements $(u_n - u_{n-1})$. It is seen that instead of a pulse, we obtain an oscillating solution. It is clear from these figures that the emergence of solitons depends on the magnitude of the initial impulse and for values of F_0 below a critical value, one obtains a train of waves instead of a solitary wave.

4. Interaction of a soliton with a defect

We next consider the case in which there is a vacancy in the lattice, say at the position of the 13th atom. In order that the lattice may not break up, we assume a weak coupling force between the 12th atom and the next atom (designated as 13th) at the 14th place in the lattice, the distance between these two atoms being twice the lattice spacing. Alternatively our model corresponds to a lattice in which one bond in the chain has a structure and strength different from the rest. While the equation of motion of the atoms from 1 to 12 and from 14 to 60 remains unaltered, the equation of motion of the atoms 12 and 13 near the vacancy gets altered. It can be shown that the set of equations (11) undergo only a single change *viz.*

$$\dot{s}_{13} = -2k'\beta'(1-\exp[-\beta'(u_{13}-u_{12})])\exp[-\beta'(u_{13}-u_{12})] \tag{12}$$

where k' and β' are constants of the Morse potential for the pair of atoms 12 and 13. We are justified in taking $k' < k$ and $\beta' < \beta$ and for our calculation we have chosen $\beta' = \beta/4$ and $k' = 2k/5$.

Figure 7 (A-D), gives the plot of the time development of a solitary wave in a lattice with a vacancy. The soliton was generated as before by giving a strong initial impulse at one end of the chain with $F_0=3\times 10^4$ and $\beta=3\cdot 333$. It is seen from figure 7a that a soliton is travelling along the lattice at $t=60$; (7B) shows the nature of the relative displacements of the atoms at time $t=100$ when the soliton has just touched a vacancy. In addition to the forward-moving soliton, a localised mode is produced at the site of the vacancy. Our computer calculations show that for another 80 units of time, the lattice undergoes a non-equilibrium phase and this can be seen from figure 7c corresponding to $t=160$. The vacancy in fact arrests the free propagation of the soliton. At time $t=160$, two additional solitons have been produced and these travel forward along the lattice. Figure 7D representing $t=250$ shows that the vacancy produces in addition a soliton travelling backwards. It is clear that a vacancy arrests the free propagation of a soliton and scatters it. At the site of a vacancy a strong localised mode is generated. Further additional solitons travelling both forward as well as backwards are created by the vacancy and these seem to be a general characteristic of the collision of a soliton with a vacancy.

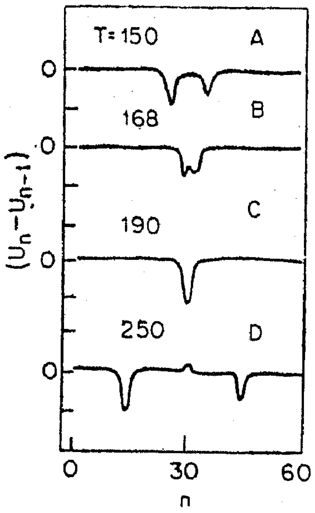
Time development of the interaction of the soliton with a vacancy for various other cases also have been studied with F_0 ranging from 1×10^4 to 5×10^4, but are not reproduced in this paper. It is found that when the initial force is reduced to 1×10^4, the soliton and the additional solitons created at the vacancy travel slowly. On the other hand when the force is increased to 5×10^4, the initial soliton travels faster and the vacancy generates two other solitons travelling forward and one soliton travelling backward. The amplitudes of the additional solitons are different and they travel with different velocities. The leading soliton always travels faster.

5. Interaction of a soliton with other excitations

What will happen when the atom that has been hit by the soliton is simultaneously subjected to an increase in its velocity? In figure 8, the soliton was generated by giving an initial impulse to the last atom and it travels backwards. It was observed that the soliton crossed the 48th atom at time $t = 72$. An initial velocity of 10^5 cm/sec was given to this atom at $t = 72$, when the soliton crossed it. The initial velocity given is of the order of the velocities of the various atoms in the chain after the soliton has crossed them. The time development of the relative displacements of the various atoms in the chain is given in figure 8(b, c, d). It is seen that the initial velocity given synchronously with the crossing of the soliton produces a localised mode and also generates an additional soliton propagating in the opposite direction. The figure also shows that the original soliton has gained both in its amplitude and the velocity of propagation.

6. Collision of two solitons at a defect

It is well-known that two solitons can collide and cross each other but they recover their shape later. How far does this property hold good when they collide at the site of a defect? To verify this, we generated two solitons from both the ends of a chain in which the mid atom happened to be a vacancy. The time development of the system is given in figure 9 (a–d). At time $t = 150$ (figure 9a) the 2 solitons approached each other close to the site of the defect. Figure 9b represents the system at the instant of the collision and shows that there is a single soliton which has a double peak or an internal structure. At time $t = 172$, (figure 9c) the 2 solitons have merged into each other resulting in a single soliton of large amplitude. The system has been found to be in a non-equilibrium phase from $t = 170$ to 190 with the amplitudes of the atoms surrounding the defect undergoing large oscillations, but thereafter settles to a uniform state. Figure 9d, corresponding to $t = 250$, shows that the two solitons re-emerge after the collision without much distortion but a small trail consisting of a localised mode is left at the site of the defect.



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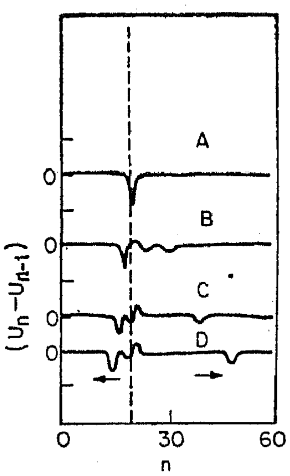

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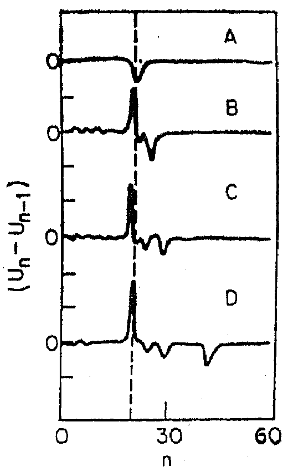


(11)

Figures 9-11. **9.** Collision of two solitons at a vacancy at the place of 30th atom in the chain of 60 atoms. **10, 11.** Propagation of soliton in a medium with density discontinuity. **10.** Propagation of soliton from a rarer to denser medium **11.** Propagation from a denser to rarer medium. X axis 1 cm=10 atoms, Y axis=1 Å

7. Propagation of a soliton in a medium with a density discontinuity

There are several situations in physics in which a wave encounters a discontinuity in the density of the medium as it propagates. To understand qualitatively the nature of propagation of a soliton in a medium with density changes, we studied the case of a linear lattice in which the atoms 1 to 20 have a mass m whereas the atoms from 21 to 60 had a different mass m'. The parameters chosen were $F_0 = 3 \times 10^4$ and m, k and β for atoms 1 to 20 and $2m$, $2k$ and 3β for 21 to 60. The soliton was produced by an initial impulse to the boundary atom. Figure 10 (a–d) denotes the time development of the disturbance in such a hypothetical chain. The soliton reaches the region of density change at $t = 150$, and its propagation is smooth till then. The subsequent figures show that the soliton gets reflected at the discontinuity. Further as before, a localised mode of moderate amplitude is created at the region of density discontinuity and another soliton is created which moves forward. The amplitude of the additional soliton created is much smaller than the original one, this is because energy has to be imparted to a medium with higher density. The denser medium could thus reflect a soliton. We then investigated the case of the propagation of a soliton from a denser to a rarer medium and for this we exchanged the parameters mentioned above. The propagation of the soliton in this case is depicted in figure 11(A–D). It is seen that a strong localised mode, with a height greater than in the preceding case is created near the discontinuity at the denser medium region. The presence of a localised mode at the site of the discontinuity is reminiscent of the creation of a shock during supersonic flow past an obstacle. Further two additional solitons are created. The state of vibration in the region between atoms 1 and 19 is drawn as a zig-zag line in the figure as the amplitudes of these atoms are small, but the same relative displacement when magnified by a factor of 50 is shown in figure 12. When a soliton moves from a denser to a rarer medium, a strong localised pulse is generated at the site of density change on the denser medium side and additional solitons are generated. Further the trail left by the soliton in the denser medium consists of an oscillatory tail.

8. Solitons produced by an initial displacement

We have generated the solitons in all the above numerical experiments by imparting a strong initial impulse to the boundary atom of the linear chain. Solitons can alternatively be produced by giving an initial displacement, smaller but of the order of the lattice spacing, to the boundary atom.

In figure 13, we draw the relative displacement pattern of the chain in which the first atom is subjected to an initial displacement $u_1 = 1{\cdot}0$ at $t = 0$. It is seen that two solitons freely propagate in the lattice.

In this section we study the interaction of the soliton with a defect, situated at the centre of the chain at the 30th place and having a mass different from the rest ($m' = m/2$). The defect mass interacts with both its neighbours with a force different from the rest of the pairs. Let k', β' be the constants of the Morse potential for the pairs of atoms (29, 30) and (30, 31) of the lattice. It is seen that three of the set of equations (11) are to be modified as

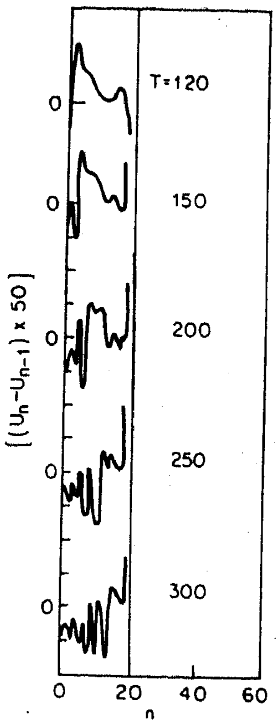
$$\dot{s}_{30} = -2k'\beta' \{1 - \exp[-\beta'(u_{30} - u_{29})]\} \exp[-\beta'(u_{30} - u_{29})]$$

$$s_{31} = -2k'\beta' (1 - \exp[-\beta'(u_{31} - u_{30})]) \exp[-\beta'(u_{31} - u_{30})]$$

and $\dot{u}_{30} = (s_{30} - s_{31})/m'$

the other equations of the set (11) remaining the same.

Figure (13A–C) represents the state of disturbance in the lattice. Figure (13B) corresponds to $t = 180$, when the pair of solitons have touched the defect site. It is seen that there are two strong localised modes of opposite amplitude at the site of the defect atom. Figure (13C) corresponding to $t = 300$, shows that in addition to the



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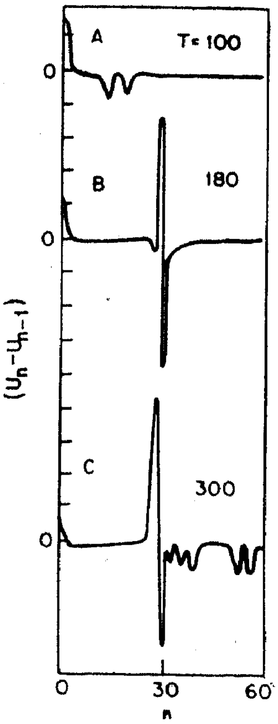

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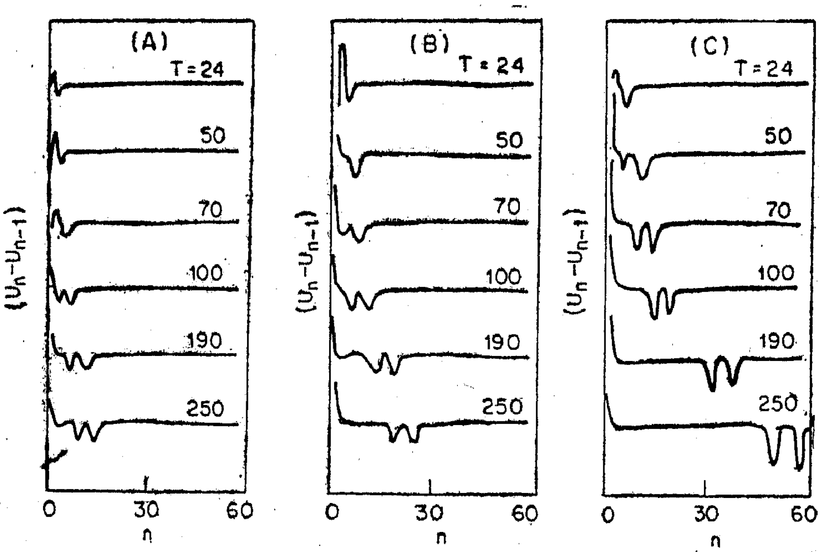

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Figures 12-14. **12.** The trail left by the soliton in the denser medium as it passes from denser to rarer medium. **13.** Crossing of soliton through a defect mass placed at the 30th place. The defect mass is taken as $m/2$ where m is the mass of every other atom except the 30th. **14.** A. $u_1 = 0{\cdot}5$ at $t = 0$; *B.* $u_1 = 0.75$ at $t = 0$; *C.* $u_1 = 1.0$ at $t = 0$. X axis 1 cm=10 atoms, Y axis=1 Å

two solitons which have travelled from the defect site, a few other solitons have been generated close to the defect site. Our numerical data for different instants of time suggest that the additional solitons in the system travel with a velocity different from the original solitons and are slower. It may be seen that the soliton close to the defect site has an internal structure with an additional peak. It is noticed that whenever

Table 1. Velocity-amplitude relationship.

Amplitude of soliton waves (Å)	Distance moved by the peak in terms of lattice spacing (Å)	Time of travel (10^{-12} sec)	Velocity* (cms/sec)
3	9 a	180	500 a
5·5	22 a	250	800 a
7·0	6 a	38	1578 a
7·5	27 a	140	1928 a

*Velocity expressed in terms of a where the lattice spacing is a Au.

Common for all figures: Scale along X axis 1 cm = 10 atoms
Scale along Y axis 1 cm = 1 Å

a soliton shows an internal structure, it is in a non-equilibrium phase and it later disintegrates into two or more solitons.

9. The velocity amplitude dependence

An important property of the soliton is that its velocity of propagation is dependent on the amplitude. No experimental or numerical work seems to have been carried out to verify this property. We have generated solitons of different amplitudes and calculated their velocities of propagation in a chain of 60 atoms. The consolidated result is given in figure 14, which clearly depicts the velocity dependence of the solitons on their amplitudes. To achieve this, we changed the values of the initial displacement u_1 ($u_1 = 0{\cdot}5, 0{\cdot}75, 1{\cdot}0$, etc.,) at $t = 0$. The amplitude or pulse height of a soliton can be controlled by varying the initial displacement of the end atom. The velocity of a soliton can be easily calculated by measuring the distance travelled by a soliton in two adjacent intervals of time and dividing it by the time interval. The amplitude *vs* velocity chart containing four different cases was thus obtained and is reproduced in table 1.

The velocity of a sound wave in the lattice can easily be obtained from the equations of motion by ignoring the anharmonicity and for our lattice ($\beta = 3{\cdot}333$), it is given by $v = (447{\cdot}2a)$ where a is the lattice spacing in Angström units. It is seen from table 1 that a soliton always travels with a velocity greater than the sound wave velocity in the medium and that the velocity of a soliton is an increasing function of the amplitude. It also shows that the relationship between velocity and amplitude is parabolic.

Acknowledgement

One of the authors (VNI) would like to thank the University Grants Commission for a fellowship.

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