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FINITE AMPLITUDE LONGITUDINAL WAVES IN LATTICES*

R. MANVI,† G. E. DUVALL and S. C. LOWELL

Shock Dynamics Laboratory, Department of Physics, Washington State University, Pullman, Washington

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Summary—The system analyzed in this paper consists of a semi-infinite chain of mass points with linear and nonlinear nearest neighbor interaction. There is no dissipation in the system. A finite velocity step is applied at the first mass point at zero time to generate a shock-like disturbance in the system. Explicit solution of the linear case is extended to the nonlinear case by a time-averaging procedure. The approximate solution thus obtained compares favorably with numerical solutions and provides enhanced understanding of the physics of the system.

NOTATION

X_N	dimensionless position of Nth mass point = position co-ordinate/reference length
T	dimensionless time = (time) × (reference frequency)
$F_{N,N+1}$	dimensionless interaction force between mass points N and $N+1$ = (force)/(reference force)
α	coefficient of nonlinearity (nondimensional)
$\bar{U}_s$	dimensionless average shock velocity = (shock velocity)/(reference sound speed)
u_1	dimensionless velocity step at $N = 1$ = (velocity)/(reference sound speed)
S_N	dimensionless displacement from equilibrium of the Nth mass point = (displacement)/(reference length)
d_1	reference length: the equilibrium separation at zero time, for convenience taken to be 1 cm
ω_1	reference frequency: $\sqrt{(K/m)}$ in a linear lattice. K is the spring stiffness and m is the mass of each particle in the chain
$\omega_1 d_1$	reference sound speed in the lattice = D_0, Newtonian sound speed
Kd_1	reference force
N, L, K, M	integers
y	dummy variable
$u_p(N, T)$	dimensionless velocity of Nth mass point = (velocity of Nth mass point)/(reference velocity)
$\sigma(N, T)$	defined in equation (16)
B^2	defined in equation (18)
J_L	Bessel function of first kind
Y_L	Bessel function of second kind

INTRODUCTION

IT IS known from sub-microscopic physical studies that a solid is better represented in the small by a lattice of interacting mass points than by a

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† Present address: Department of Mechanical Engineering, California State College, Los Angeles, California.

continuum. One of the common interests of the engineer and physicist is to determine what properties of the lattice influence macroscopic behavior of the solid and how macroscopic properties of a solid can be used to infer various features of atomic interactions. Of special interest in this regard is the structure of a shock wave propagating in a solid, since it may relate directly to fundamental dissipative processes. The state of such investigations in solids is far behind that for gases.

Unfortunately the analytical and numerical tools available to us are completely inadequate for dealing with a multidimensional lattice in which each atom interacts with many neighbors through nonlinear forces. It has been found, however, that an understanding of the mechanics of a one-dimensional lattice of mass points interacting only with nearest neighbors often leads to a conceptual understanding of the more general three-dimensional lattice. For this reason the lattice illustrated in Fig. 1 has been used to study finite amplitude wave propagation.[1] It is a one-dimensional semi-infinite chain located on the positive side of the X-axis in cartesian co-ordinates. The chain is assumed perfect, having only one kind of mass point at each lattice point. The free surface is located at $N = 1$. This initially is at $X = 0$, i.e. $X_1(0) = 0$.

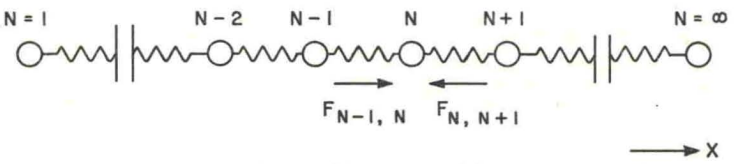

FIG. 1. Lattice model.

In the present study, all mass points are assumed to be constrained to move only in the X-direction. With this assumption, questions of transverse waves do not arise.

For initial conditions we assume that all mass points are at rest in their equilibrium positions, i.e. at $T = 0$ the displacements from equilibrium position, velocity and acceleration of every mass point equal zero.

Disturbance in the chain is created by forcing the first mass point, $N = 1$, to move with a constant velocity u_1 from zero time onwards. This finite velocity step forces a compressive wave, which we call a "shock wave", to propagate in the chain. Shock velocity is defined to be the velocity at which the head of the disturbance propagates in the chain. A "shock profile" is the plot of particle velocity $u_p(N)$, or of some related quantity, versus mass point N.

EQUATION OF MOTION

A nonlinear nearest neighbor interaction of the type

$$F_{N,N+1} = -(S_{N+1} - S_N) + \alpha(S_{N+1} - S_N)^2 \tag{1}$$

leads to an equation of motion for the mass point N of the following form

$$S''_N(T) = \{(S_{N+1} - 2S_N + S_{N-1})\,[1 - \alpha(S_{N+1} - S_{N-1})]\} \tag{2}$$

In the above equation prime denotes differentiation with respect to T. We seek a solution of the above equation for the initial conditions

$$S_N(0) = 0; \quad S'_N(0) = 0 \quad \text{for all } N \geqslant 2 \tag{3}$$

The boundary condition for $N = 1$ is

$$S_1(T) = u_1 T \quad \text{for} \quad T \geqslant 0 \tag{4}$$

The results of numerical integrations of equation (2) are described in Ref. 1 for various values of u_1 and α, including the linear case, $\alpha = 0$. They will be used in the following sections for comparison with analytical results.

SHOCK IN A LINEAR CHAIN

The dimensionless equation of motion for the linear chain is obtained by setting $\alpha = 0$ in equation (2). Hence we have

$$S''_N(T) = S_{N+1} - 2S_N + S_{N-1} \tag{5}$$

A solution of equation (5) which satisfies the initial and boundary conditions of equations (3) and (4) can be obtained in terms of Bessel functions of the first kind. This ensures that the solution remains finite for all values of $T \geqslant 0$. Equation (5) is satisfied by solutions of the form[2]

$$S_N(T) = \text{constant} \,.\, J_{2(N-1)+L}(2T) \tag{6}$$

To satisfy boundary and initial conditions, constants have to be fixed and solutions superposed. The required solution is

$$S_N(T) = u_1 \,.\, \sum_{K=0}^{\infty} (2K+1)\, J_{2(N-1)+2K+1}\,(2T), \quad \text{for } N \geqslant 1, \text{ and } T \geqslant 0 \tag{7}$$

To verify that boundary condition (4) is satisfied, we substitute $N = 1$ in the above to get

$$S_1(T) = u_1 \,.\, \sum_{K=0}^{\infty} (2K+1)\, J_{2K+1}(2T) = u_1 \,.\, \tfrac{1}{2}(2T) = u_1\, T \tag{8}$$

In the above equation, we have made use of the identity,[2]

$$\sum_{K=0}^{\infty} (2K+1)\, J_{2K+1}(y) = \tfrac{1}{2} y \tag{9}$$

The solution (7) also satisfies the initial conditions of equation (3) because, for $N \geqslant 2$, and $K \geqslant 0$, we have

$$2(N-1)+2K+1 \geqslant 3, \quad 2N+2K-2 \geqslant 2, \quad 2N+2K \geqslant 4$$

and equation (7) and its derivative are zero at $T = 0$, since

$$J_L(0) = 0, \quad \text{for} \quad L > 0 \tag{10}$$

It is shown in equation (34) of the Appendix that solution (7), when substituted into equation (5), leads to the form

$$S''_N(T) = 2u_1 \,.\, (N-1)/T \,.\, J_{2(N-1)}(2T) \quad \text{for} \quad N \geqslant 2 \tag{11}$$

Therefore the velocity profile is given by

$$S'_N(T) = u_p(N, T) = 2u_1 \,.\, (N-1) \,.\, \int_0^T \frac{1}{y} \,.\, J_{2(N-1)}(2y) \,.\, \mathrm{d}y \tag{12}$$

Displacement from initial equilibrium position is obtained from another integration of the above equation or directly from equation (7).

Equation (11) is illustrated in Fig. 2 along with the results of numerical integration of equation (5) for the same boundary and initial conditions. We note the following: the maximum acceleration of each mass point decreases with time after the first maximum.

This follows from the asymptotic behavior

$$|J_{2(N-1)}(2T)| < 1/(2T)^{1/2}, \quad T \gg N-1$$

Hence,

$$|S''_N(T)| < \text{constant}/T^{3/2}, \quad T \gg N-1 \tag{13}$$

Vanishing of the acceleration as $T \to \infty$ ensures that the mass point velocity approaches a constant value. We can thus conclude that the dynamics of the chain is responsible for decay of oscillations with time even in the absence of dissipation. This point is particularly important in evaluating numerical solutions.[6] Since such solutions are inexact, it is difficult to determine whether decaying behavior represents the physical behavior of the original system or is an artifact introduced by the neglect of higher-order differences.

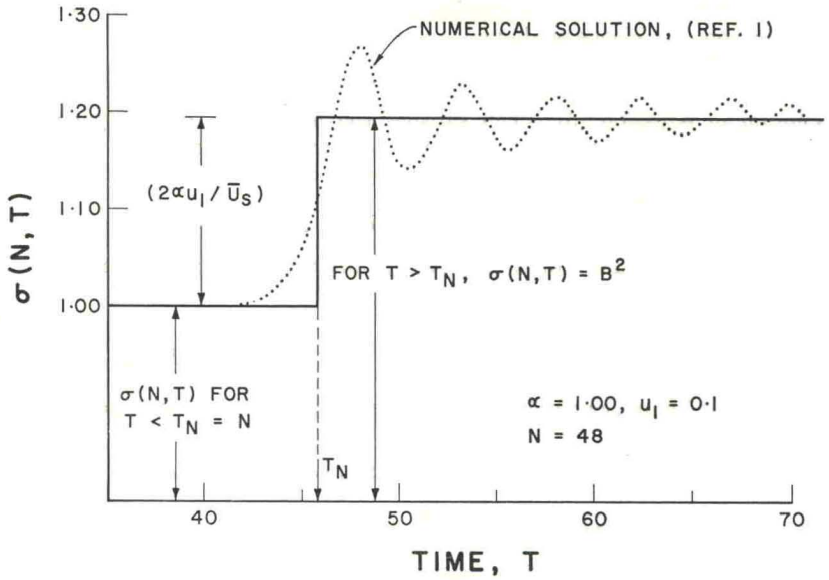

FIG. 2. Acceleration of a mass point in a linear chain.

For large order L, the Bessel functions $J_L(y)$ will be zero essentially until the argument equals the order. From equation (11) we see that

$$S''_N(T) \simeq 0 \quad \text{until} \quad 2T \simeq 2(N-1) \tag{14}$$

Since the dimensionless distance of the Nth mass point from the free surface is $(N-1)$, the relation in equation (14) indicates that the head of the disturbance in the linear chain propagates at an average velocity $\bar{U}_s \simeq 1$. We have nondimensionalized all velocities with respect to the Newtonian sound speed[4] in a chain, $(\omega_1 d_1)$. This is the propagation speed for infinitely long waves corresponding to the low frequency limit. Hence the leading disturbance propagates at an average velocity equal to the Newtonian sound speed in a linear chain independent of the amplitude of the disturbance.

SHOCK IN A NONLINEAR CHAIN

In the previous section it was found possible to obtain the solution for a shock in a linear chain by superposition of elementary solutions. When the governing equation of motion is nonlinear, as in equation (2), such superposition is no longer possible. For the present the only possible approaches seem to be numerical integration and approximate analytic techniques based on time averaging.[5] In this section we propose to extend the analysis of the previous section to the nonlinear problem by a time averaging procedure.

We rewrite equation (2) as

$$\frac{S''_N(T)}{(S_{N+1}-2S_N+S_{N-1})} = 1-\alpha(S_{N+1}-S_{N-1}) \tag{15}$$

If α is very small, then the behavior of the above equation is expected to be analogous to that of equation (5), as illustrated in equation (7). The expression on the right-hand side of equation (15) is a function of mass point N and time T.

We define

$$\sigma(N, T) \equiv 1-\alpha(S_{N+1}-S_{N-1}) \tag{16}$$

and illustrate this function in Fig. 3 for a particular case. Until the arrival of the disturbance at the $(N-1)$th mass point, both the displacements S_{N+1}, S_{N-1} are zero and hence the value of $\sigma(N, T)$ equals unity. Numerical results[1] show that the disturbance propagates at uniform average velocity $\bar{U}_s > 1$. For times greater than the time of arrival of the disturbance at the $(N-1)$th mass point, the value of $\sigma(N, T)$ oscillates about a mean value greater than unity with decreasing amplitude.

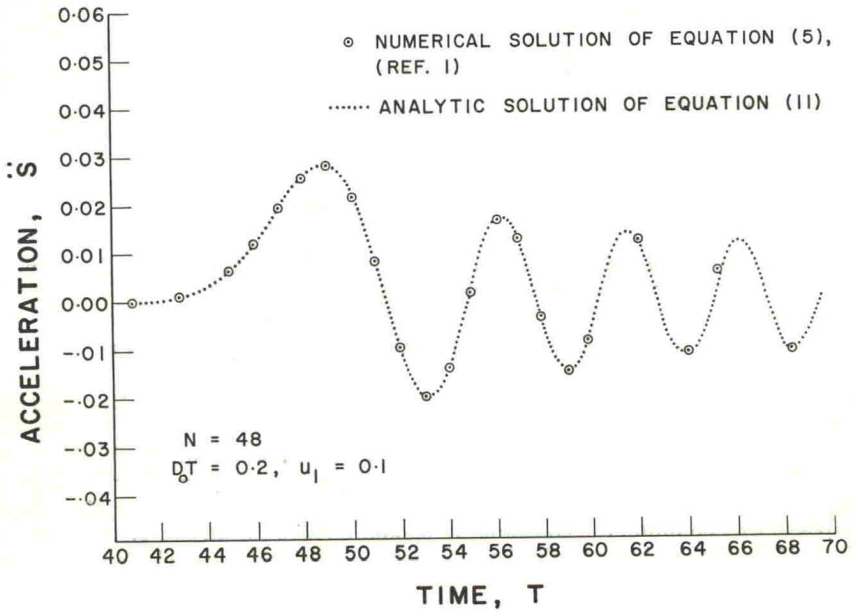

FIG. 3. $\sigma(N, T)$ as defined in equation (16).

To obtain an approximate solution to equation (15) for the initial conditions of equation (3) and boundary condition of equation (4), we approximate the time-dependent function $\sigma(N, T)$ by a step function representing a time average:

$$\sigma(N, T) = \begin{cases} 1 & \text{for} \quad T < T_N \\ B^2 & \text{for} \quad T > T_N \end{cases} \tag{17}$$

where $T_N = (N-1)\bar{U}_s$ and T_N is arrival time of the disturbance at the Nth mass point, illustrated in Fig. 3. In Ref. 1 it is shown that the constant B^2 is

$$B^2 = 1+2\alpha(u_1/\bar{U}_s) \tag{18}$$

We are therefore led to replace equation (15) by two approximate linear equations

$$\frac{S''_N(T)}{S_{N+1}-2S_N+S_{N-1}} = 1, \quad \text{for} \quad T < T_N \tag{19}$$

and

$$\frac{S''_N(T)}{S_{N+1}-2S_N+S_{N-1}} = B^2 \quad \text{for} \quad T > T_N \tag{20}$$

The initial and boundary conditions of equations (3) and (4) remain the same for the differential difference equation (19), whereas the initial conditions for equation (20) are provided by the solution of equation (19) at time $T = T_N$. We denote the solution of equation (19) by $S_{N,1}(T)$ and that of equation (20) by $S_{N,2}(T)$. The physical conditions of continuity of displacement and velocity at T_N imply

$$S_{N,1}(T_N) = S_{N,2}(T_N) \tag{21}$$

and

$$S'_{N,1}(T_N) = S'_{N,2}(T_N) \tag{22}$$

These conditions of continuity are satisfied trivially by the physics of the system. T_N is the arrival time of the disturbance at the Nth mass point, and at this time we require that displacement and velocity be zero. The situation represented by equation (20) is that of replacing the spring in equation (19) by a spring of stiffness B^2 times the original.

The solution of equation (19) was obtained in the previous section as equation (7).

From equation (20) we have

$$\left(\frac{\mathrm{d}^2 S_N}{\mathrm{d}T^2}\right)/(S_{N+1}-2S_N+S_{N-1}) = B^2 \tag{20a}$$

Define a new variable

$$y = BT \tag{23}$$

Then equation (20a) becomes

$$\frac{\mathrm{d}^2 S_N}{\mathrm{d}y^2} = S_{N+1}-2S_N+S_{N-1} \tag{24}$$

We can write the general solution of equation (24) in terms of Bessel functions. This follows from our previous work. The solution for $T \geqslant T_N$ is

$$S_{N,2}(T) = \sum_{K=0}^{\infty} [A_K J_{2(N-1)+2K+1}(2BT) + B_K Y_{2(N-1)+2K+1}(2BT)] \tag{25}$$

where A_K and B_K are constants depending on the summation index K. Then can be evaluated as follows.

From equation (17), T_N is of the order of $(N-1)$, and B is of the order of unity 1. Hence $(2BT_N) < 2(N-1)+2K+1$ for $K \geqslant 0$. The Bessel functions $Y_L(y)$ are very large when the argument is less than the order 3. Therefore to satisfy our requirement that for all N the displacement be finite, the constant B_K should be zero for all $K \geqslant 0$. In addition, the solution (25) is required to satisfy the boundary condition (4), which fixes the constant A_K as

$$A_K = \frac{u_1(2K+1)}{B} \tag{26}$$

Hence the solution to equation (20) is

$$S_{N,2}(T) = (u_1/B) \sum_{K=0}^{\infty} (2K+1)\, J_{2(N-1)+2K+1}(2BT) \quad \text{for} \quad N \geqslant 1,\ T \geqslant T_N \tag{27}$$

From the above equation we obtain

$$S''_{N,2}(T) = \frac{2u_1(N-1)}{T} . J_{2(N-1)}(2BT) \quad \text{for} \quad N \geqslant 2,\ T \geqslant T_N \tag{28}$$

The velocity profile is obtained by an integration of the above equation as

$$S'_{N,2}(T) = 2u_1(N-1) \int_{T_N}^{T} \frac{1}{y} . J_{2(N-1)}(2By)\, \mathrm{d}y$$

The average shock velocity, $\bar{U}_s$, appearing in equation (18) for computing the constant B is given by[1]

$$\bar{U}_s = \sqrt{[1+\alpha(u_1/\bar{U}_s)]} \tag{29}$$

Equation (28) is plotted in Fig. 4 for a case where $\alpha = 1$ and $u_1 = 0{\cdot}1$, along with the numerical solution of equation (2) for the same constants. The assumptions made to obtain the approximate solution appear reasonable since the approximate analytic solution shows a behavior similar to that of the numerical solution. It yields a solution which has

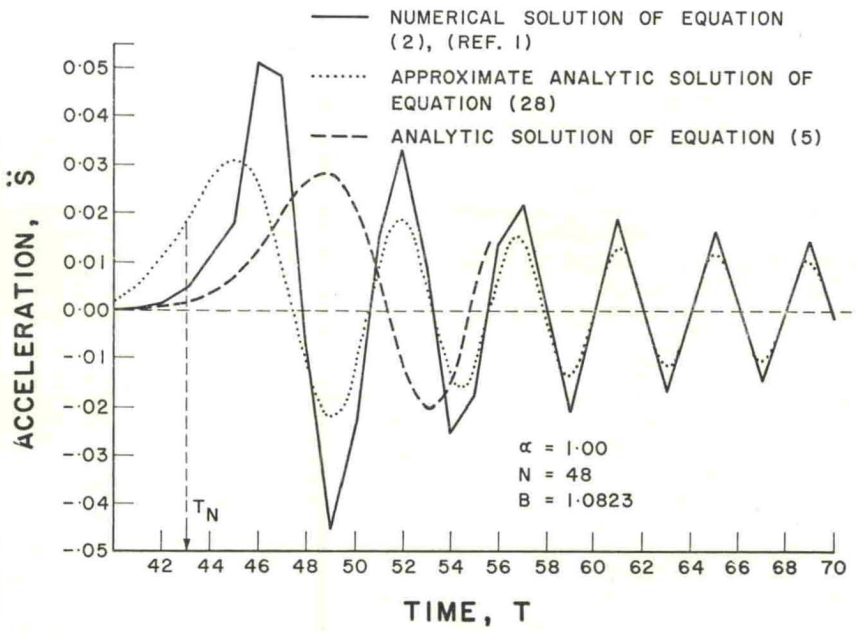

FIG. 4. Acceleration of a mass point in a nonlinear chain.

about the same period as the numerical solution, but a different amplitude; the most important result is verification of the decay of oscillations shown in Fig. 3 without introduction of damping.

CONCLUSIONS

We have studied the propagation of finite amplitude waves in one-dimensional linear and nonlinear chains. A disturbance was created by application of a velocity step to the mass point in the free surface. Only nearest neighbor interactions were considered and no dissipation exists in the chains.

Our analysis shows that

(1) A simple time-averaging of nonlinear force terms in the equation of motion produces a solution which agrees reasonably well with numerical computations and is significantly better than a linear approximation.

(2) A typical displacement path ($S_N(T)$ vs. T) is oscillatory. As T increases, the particle performs oscillations of decreasing amplitude and period about a mean displacement represented by a line of slope $\mathrm{d}S_N/\mathrm{d}T = u_1$ in the S–T plane.

(3) The approximate solution for the nonlinear chain shows that the Nth mass point has an acceleration which oscillates with decreasing amplitude about zero after arrival of the leading disturbance. The rate of decrease of

amplitude ensures that mass-point velocity becomes constant at very large times without the presence of dissipative forces.

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APPENDIX

Simplified difference equation

Substitution of the solution of equation (7) into the equation of motion (5) gives

$$S''_N(T) = u_1 \cdot \Big[\sum_{K=0}^{\infty} (2K+1)\, J_{2N+2K-3}(2T) - 2 \sum_{K=0}^{\infty} (2K+1)\, J_{2N+2K-1}(2T) + \sum_{K=0}^{\infty} (2K+1)\, J_{2N+2K+1}(2T) \Big] \tag{30}$$

By defining a dummy variable of summation, M, such that $2M+1 = 2N+2K-3$ for the first sum on the right, $2M+1 = 2N+2K-1$ for the second sum on the right and $2M+1 = 2N+2K+1$ for the third sum on the right, equation (30) becomes

$$S''_N(T) = u_1 \cdot \Big\{ \sum_{M=N-2}^{\infty} [(2M-2N+5)\, J_{2M+1}(2T)] - 2 \cdot \sum_{M=N-1}^{\infty} [(2M-2N+3)\, J_{2M+1}(2T)] + \sum_{M=N}^{\infty} [(2M-2N+1)\, J_{2M+1}(2T)] \Big\} \tag{31}$$

Simplifying

$$S''_N(T) = u_1 \cdot [J_{2N-1}(2T) + J_{2N-3}(2T)] \tag{32}$$

But we have the identity for Bessel functions,[3]

$$\frac{2M}{y} J_M(y) = J_{M-1}(y) + J_{M+1}(y) \tag{33}$$

With the above identity, $M = 2N-2$ and $y = 2T$, equation (32) becomes

$$S''_N(T) = \frac{2u_1(N-1)}{T} \cdot J_{2(N-1)}(2T) \tag{34}$$