

## Normal modes of oscillations of one-dimensional monoatomic and diatomic lattices

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**Abstract.** A polynomial equation is obtained for the solutions of the vibrational frequencies of one-dimensional monoatomic and diatomic lattices with particles connected by identical springs, but with arbitrary springs connecting the end particles to rigid walls. The exact expressions of the different normal modes of oscillations of the linear chain of particles for monoatomic, diatomic and defective lattices are derived in a straightforward way. As special cases of our problem we have considered the effects of different end springs on the vibrational frequencies. One interesting result is that very high frequencies are allowed when the ends of the diatomic lattice are rigidly fixed with the boundary walls.

**Keyword.** Lattice oscillations.

### 1. Introduction

The normal modes of oscillations of a chain of finite number of particles have been investigated by a number of authors using either the cyclic boundary condition or the free end condition of the lattices. Born (1942) and Halford (1951) have shown that the frequency distribution function of a monoatomic one-dimensional lattice is the same in both the approaches as  $N \rightarrow \infty$ , where  $N$  is the number of point masses in the lattice. However, it has been pointed out that the use of the cyclic condition may not give the correct result for the surface effects of a thin film and the infrared absorption spectrum of an ionic lattice (Rosenstock 1955). This is due to the differences in the phases of the atomic displacements for a cyclic lattice compared to a lattice with free ends.

The vibration frequencies of one-dimensional lattices with two kinds of point masses arranged in an alternating array have been discussed in detail by Wallis (1957). Assuming nearest neighbour Hooke's law interactions and free ends, he has shown that this type of diatomic lattice may possess surface modes of vibration (Lifshitz and Pekar 1955) with frequencies in the forbidden gap between the optical and acoustical branches. These surface modes are very important in the investigation of surface phenomena such as adsorption and heterogeneous catalysis. On the contrary, Born (1942) has found that all modes are wave-like in character with frequencies in either the optical branch or the acoustical branch. Born has considered the motion of  $2N$  particles with cyclic boundary

conditions, whereas Wallis (1957) has assumed that the end atoms interact only with their nearest neighbours on the interior of the lattice and are otherwise free. Wallis has obtained a set of  $2N$  linear homogeneous equations in terms of the vibrational amplitudes, which has been solved subsequently by evaluating a determinant of order  $2N$ . In an alternative simpler matrix procedure where a  $2 \times 2$  matrix is multiplied  $N$  times, Louck (1962) has obtained the amplitude and vibrational frequencies of a linear chain of  $N$  identical particles with the end particles connected to rigid walls by arbitrary forces. Recently, this method has been extended by Malik *et al* (1973) for the case of a diatomic lattice. Their calculation, however, does not contain the proper end conditions.

In this paper we consider the problem of vibration of one-dimensional monoatomic and diatomic lattices in a frame which is easily tractable. Like Louck (1962) we assume that the end particles are connected to the rigid walls by arbitrary forces. It is well known that the amplitudes of vibration of different particles in normal modes of oscillation satisfy a set of second order difference equations. We have solved the set of difference equations by using an iterative technique without using the complicated matrix algebra. The results obtained by us in the case of a monoatomic lattice are exactly the same as given by Louck. Next we have shown that this technique of iteration of a difference equation can be applied successfully to a lattice having one or more defective atoms. We then apply the same method to the problem of diatomic lattices for two different cases: (i) end atoms are not alike, (ii) end atoms are alike. We have studied the variation of the frequencies with different end forces. We observe one interesting phenomenon when the ends of the diatomic lattice are rigidly fixed. We find that the lattice in this case can vibrate with high frequencies.

## 2. One-dimensional monoatomic lattices

We consider a monoatomic lattice consisting of  $N$  identical particles of mass  $m_1$ . The particles are connected with identical Hooke's law springs with force constant  $k$ , whereas the two end particles are connected to rigid walls by springs with arbitrary force constants  $K$  and  $K'$  respectively (figure 1). Let  $x_1, x_2, \dots, x_N$  be the displacements from the equilibrium positions of the masses at time  $t$ , and let the atoms interact only through their nearest neighbours. The equations of motion for small vibrations may be written as

$$\left. \begin{aligned} m_1 \ddot{x}_1 &= -(K + k)x_1 + kx_2 \\ m_1 \ddot{x}_j &= k(x_{j+1} - 2x_j + x_{j-1}) \\ & \quad j = 2, 3, \dots, N-1 \\ m_1 \ddot{x}_N &= kx_{N-1} - (K' + k)x_N \end{aligned} \right\} \quad (1)$$

We seek normal-mode solutions of (1) having the form

$$x_j = a_j \cos(\omega t + \delta) \quad (2)$$

where  $\delta$  is an arbitrary constant phase and  $a_j$  is the amplitude or the maximum

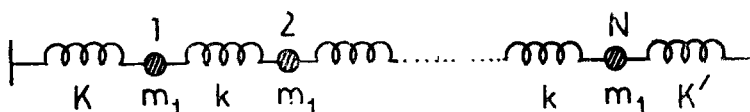


Figure 1. One-dimensional monoatomic lattice with arbitrary end forces.

displacement of the  $j$ th particle. The system of second order differential equations (1) is then transformed into a set of second order difference equations:

$$a_{j+1} = \beta a_j - a_{j-1}, \quad j = 1, 2, \dots, N \quad (3)$$

where

$$\beta = 2 - \alpha_1^2 \quad (4 a)$$

$$\alpha_1^2 = m_1 \omega^2 / k \quad (4 b)$$

$$a_0 = -s a_1 \quad (4 c)$$

$$a_{N+1} = -s' a_N \quad (4 d)$$

with

$$s = K/k - 1, \quad s' = K'/k - 1.$$

Equations (3) can now be solved immediately by iteration:

$$a_j = a_1 [f_j(\beta) + s f_{j-1}(\beta)] \quad (5)$$

where  $f_j(\beta)$  is defined in Appendix 1.

Next we determine the allowed frequencies of vibration of the lattice by imposing the end condition (4 d) which yields

$$f_{N+1}(\beta) + (s + s') f_N(\beta) + s s' f_{N-1}(\beta) = 0 \quad (6)$$

where (7) and (A7) have been used. Equation (6) can be rewritten in terms of the variable  $\lambda$  by using (A4) and the resulting equation comes out to be identically same as that given by Louck (1962) in the matrix procedure.

### 3. Lattice defect

We now consider that the atom at the  $l$ th position is replaced by a different atom of mass  $m_2$  so that the force constant for the interactions of this atom with its nearest neighbours is  $\gamma k$  where  $\gamma$  is any number. In this case the set of difference equations satisfied by the amplitudes of the various atoms will be as follows:

$$a_{j+1} = (2 - \alpha_1^2) a_j - a_{j-1} \quad (7 a)$$

$$j = 1, 2, \dots, l-2, l+2, \dots, N$$

$$\gamma a_l = (1 + \gamma - \alpha_1^2) a_{l-1} - a_{l-2} \quad (7 b)$$

$$\gamma a_{l+1} = (2\gamma - \alpha_2^2) a_l - \gamma a_{l-1} \quad (7 c)$$

$$a_{l+2} = (1 + \gamma - \alpha_1^2) a_{l+1} - \gamma a_l \quad (7 d)$$

where  $\alpha_2^2 = m_2 \omega^2 / k$ , and other quantities are defined in equations (4).

Now (7 a) can be iterated in a simple way as described in the previous section to get  $a_{l-2}$  and  $a_{l-1}$  in terms of  $a_1$ . Starting with  $j = l + 2$  onwards the set of equations (7 a) is iterated to obtain  $a_N$  and  $a_{N+1}$  in terms of  $a_{l+2}$  and  $a_{l+1}$ . With the help of these equations and (7 b-7 c) all the amplitudes  $a_j$ 's can be expressed in terms of  $a_1$ . Finally we impose the end condition (4 d) to get the allowed frequencies of vibration of a defective lattice. The equation for  $\gamma = 1$  has the following simple form

$$\begin{aligned} & J_{N+1}(\beta) + (s + s') f_N(\beta) + s s' f_{N-1}(\beta) \\ & = (\alpha_2^2 - \alpha_1^2) [f_{N-l+1}(\beta) + s' f_{N-l}(\beta)] [f_l(\beta) + s f_{l-1}(\beta)] \end{aligned} \quad (8)$$

where we have used the relations (A8d) and (A8e).  $\gamma = 1$  corresponds to the situation where the force constant for the interactions of the defective atom with its neighbours is same as that of normal atoms. This can be realised in practice by assuming that the defective atom is an isotope of the other atoms. But the procedure described here is quite general and one may obtain the allowed frequency condition for any arbitrary value of  $\gamma$ .

Since the method described here is essentially a method of iteration of a difference equation, this technique can be applied successfully to find the vibrational modes of one-dimensional lattice with more than one defect, and with arbitrary force constant for interactions of the defective atoms with their neighbours.

#### 4. One-dimensional diatomic lattices

In this section we study the vibration frequencies of a diatomic one-dimensional lattice in which the point masses alternately have the values  $m_1$  and  $m_2$ ,  $m_1 < m_2$ . We will consider two cases:

(i) *End atoms are not alike*—Considering  $N$  atoms of mass  $m_1$  and  $N$  atoms of mass  $m_2$  we find the following set of difference equations for the amplitudes of the atoms:

$$\left. \begin{aligned} (2 - \alpha_1^2) a_1 &= -s a_1 + a_2 \\ (2 - \alpha_2^2) a_{2j} &= a_{2j-1} + a_{2j+1}, \quad j = 1, 2, \dots, N-1 \\ (2 - \alpha_1^2) a_{2j-1} &= a_{2j-2} + a_{2j}, \quad j = 2, 3, \dots, N \\ (2 - \alpha_2^2) a_{2N} &= a_{2N-1} - s' a_{2N} \end{aligned} \right\} \quad (9)$$

By means of a little manipulation the even and odd amplitudes of (9) can be separated out:

$$\left. \begin{aligned} \beta a_{2j} &= a_{2j-2} + a_{2j+2}, \quad j = 1, 2, \dots, N-1 \\ \beta a_{2j-1} &= a_{2j-3} + a_{2j+1}, \quad j = 1, 2, \dots, N-1 \end{aligned} \right\} \quad (10)$$

where

$$\beta = (2 - \alpha_1^2)(2 - \alpha_2^2) - 2 \quad (11 a)$$

$$(2 - \alpha_1^2 + s) a_0 = -s a_2 \quad (11 b)$$

$$a_{-1} = -[s(2 - \alpha_2^2) + 1] a_1 \quad (11 c)$$

One can see that (10) does not imply (9) unless it is augmented with the following two equations

$$(2 - \alpha_1^2 + s) a_1 = a_2 \quad (12 a)$$

$$(2 - \alpha_2^2 + s') a_{2N} = a_{2N-1} \quad (12 b)$$

By the method employed in section 2, the system of difference equations (10) can be solved:

$$a_{2j} = a_1 [(2 - \alpha_1^2 + s) f_j(\beta) + s f_{j-1}(\beta)] \quad (13 a)$$

$$j = 1, 2, \dots, N$$

$$a_{2j-1} = a_1 [f_j(\beta) + \{s(2 - \alpha_2^2) + 1\} f_{j-1}(\beta)] \quad (13 b)$$

$$j = 1, 2, \dots, N$$

where (11 b), (11 c) and (12 d) have been used.

**Table 1.** Vibrational frequencies  $\omega_r^2$  of a diatomic lattice with  $\delta = \frac{1}{2}$ ,  $N = 10$ , when the end atoms are not alike

(a) Frequencies in the optical branch											
$S=S'=-1$		$S=S'=-0.6$		$S=S'=-0.3$		$S=S'=0$		$S=S'=1$		$S=S'=10$	
$\phi_r$	$\omega_r^2/\sigma$	$\phi_r$	$\omega_r^2/\sigma$	$\phi_r$	$\omega_r^2/\sigma$	$\phi_r$	$\omega_r^2/\sigma$	$\phi_r$	$\omega_r^2/\sigma$	$\phi_r$	$\omega_r^2/\sigma$
0.31	1.99	0.31	1.99	0.31	1.99	0.30	1.99	0.31	1.99	0.34	1.99
0.63	1.96	0.63	1.96	0.61	1.96	0.60	1.96	0.63	1.96	0.67	1.95
0.94	1.90	0.93	1.91	0.92	1.91	0.90	1.91	0.94	1.90	1.01	1.89
1.26	1.83	1.24	1.84	1.23	1.84	1.20	1.85	1.26	1.83	1.34	1.81
1.57	1.75	1.56	1.78	1.54	1.76	1.50	1.77	1.57	1.75	1.68	1.71
1.88	1.65	1.87	1.68	1.84	1.66	1.80	1.67	1.88	1.65	2.01	1.60
2.20	1.54	2.18	1.55	2.15	1.56	2.09	1.58	2.20	1.54	2.35	1.49
2.51	1.44	2.49	1.45	2.46	1.46	2.39	1.48	2.51	1.44	2.70	1.39
2.83	1.36	2.81	1.37	2.81	1.37	2.69	1.39	2.83	1.36		
						2.99	1.34				

(b) Frequencies in the acoustical branch											
$S=S'=-1$		$S=S'=-0.6$		$S=S'=-0.3$		$S=S'=0$		$S=S'=1$		$S=S'=10$	
$\phi_r$	$\omega_r^2/\sigma$	$\phi_r$	$\omega_r^2/\sigma$	$\phi_r$	$\omega_r^2/\sigma$	$\phi_r$	$\omega_r^2/\sigma$	$\phi_r$	$\omega_r^2/\sigma$	$\phi_r$	$\omega_r^2/\sigma$
0	0	0.27	0.01	0.29	0.01	0.30	0.01	0.31	0.01	0.33	0.01
0.31	0.01	0.53	0.03	0.58	0.04	0.60	0.04	0.63	0.04	0.65	0.05
0.63	0.04	0.80	0.07	0.86	0.08	0.90	0.09	0.94	0.10	0.97	0.11
0.94	0.10	1.09	0.13	1.16	0.14	1.20	0.15	1.26	0.17	1.31	0.18
1.26	0.17	1.37	0.20	1.45	0.22	1.50	0.23	1.57	0.25	1.64	0.28
1.57	0.25	1.66	0.28	1.74	0.31	1.80	0.32	1.88	0.35	1.97	0.38
1.88	0.35	1.97	0.38	2.03	0.40	2.09	0.42	2.20	0.46	2.30	0.49
2.20	0.46	2.26	0.48	2.33	0.50	2.39	0.52	2.51	0.56	2.62	0.59
2.51	0.56	2.56	0.57	2.61	0.59	2.69	0.61	2.83	0.64	2.93	0.65
2.83	0.64	2.85	0.64	2.89	0.65	2.99	0.66				

The allowed frequencies are obtained from (12 *b*). Using the recurrence relations (A 7) we have from (12 *b*), (13 *a*) and (13 *b*)

$$g_{N+1}(\lambda) + [s(2 - \alpha_2^2) + s'(2 - \alpha_1^2) + ss' + 1]g_N(\lambda) + ss'g_{N-1}(\lambda) = 0 \quad (14)$$

Due to the relation (A8 *a*) we see that if  $\lambda_r$  is a root of (14), then  $\lambda_r^{-1}$  is also a root of (14), and for a pair of roots we have

$$\omega_r^2 = \sigma [1 \pm (\cos^2(\phi_r/2) + \epsilon^2 \sin^2(\phi_r/2))^{1/2}] \quad (15 a)$$

or,

$$\omega_r^2 = \sigma \left[ 1 \pm \left\{ 1 + \frac{\delta}{\lambda_r} \left( \frac{\lambda_r - 1}{\delta + 1} \right)^2 \right\}^{1/2} \right] \quad (15 b)$$

with

$$\delta = m_1/m_2$$

$$\sigma = k \left( \frac{1}{m_1} + \frac{1}{m_2} \right)$$

$$\epsilon = (m_2 - m_1)/(m_2 + m_1)$$

Thus for each pair of roots  $\lambda_r$  and  $\lambda_r^{-1}$  of (14) we have two frequencies given by (15) and  $N$  pairs of roots yield  $2N$  allowed values of  $\omega^2$ .

We have to find out only the roots of (14). From the definition of  $\lambda$  [A 3 *a*] we know that  $\lambda$  becomes complex when  $-2 < \beta < 2$  and for complex roots  $\phi_r$ 's are real. The allowed values of  $\phi_r$ 's are given by

$$[\sin(N+1)\phi_r + \{s(2 - \alpha_2^2) + s'(2 - \alpha_1^2) + ss' + 1\} \sin(N\phi_r) + ss' \sin(N-1)\phi_r] / \sin\phi_r = 0 \quad (16)$$

If we replace  $\phi_r$  by  $2\pi - \phi_r$ , we see that both (16) and (15 *a*) remain unchanged. Therefore, the roots lie symmetrically with respect to the line  $\phi_r = \pi$  and the frequencies for  $\phi_r$  and  $2\pi - \phi_r$  are same, and it is sufficient to determine those values of  $\phi_r$  which lie between 0 and  $\pi$  and which satisfy (16).

It is interesting to study the variation of the frequencies when the lattice is changing gradually from the cyclic boundary condition ( $S = S' = 0$ ) to the free end condition ( $S = S' = -1$ ). In the present paper the variation of frequencies lying in the optical and acoustical branches with the different end conditions are shown in table 1. One can see from table 1 and from figure 2 that when  $S$  and  $S'$  change from  $-1$  to 0 gradually the forbidden gap frequency gradually moves towards the optical branch and in the limit when  $S = S' = 0$ , there is no forbidden gap frequency and there are equal number of frequencies in the optical and acoustical branches. The variation of the forbidden gap frequency with the end forces is shown in figure 2. The curve I is present for all values of  $S'$  (the results have been obtained here for  $S'$  varying from  $-1$  to 10). The lines parallel to the  $s$ -axis show that there are forbidden gap frequencies for different values of  $S'$ , which do not depend on  $S$ . Therefore, for  $S' > 0.2$  and  $S < 0$ , there are two forbidden gap frequencies for the vibration of a diatomic lattice with ten atoms of each kind. These forbidden gap frequencies always correspond to real negative roots of (14). The real positive roots of (14) on the other hand yield high frequencies. Figure 3

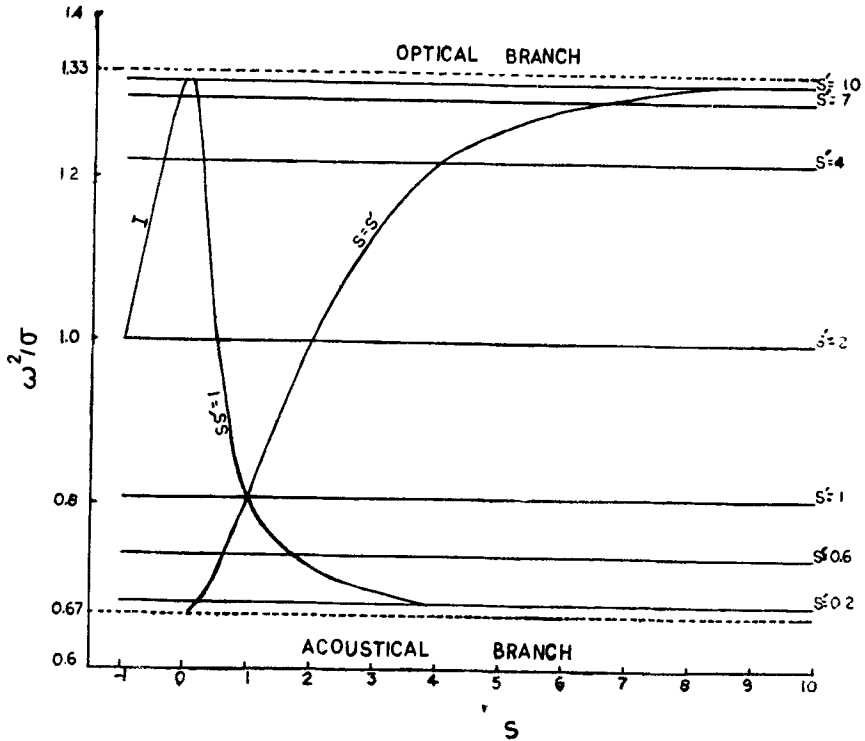


Figure 2. Variation of the forbidden gap frequencies with the end forces for a diatomic lattice with  $\delta = m_1/m_2 = \frac{1}{2}$ ,  $N = 10$ , when the end atoms are not alike. The curve I is present for all values of  $s'$  from  $-1$  to  $10$ .

represents the variation of these special frequencies with the end forces. Here again the curve I is present for all values of  $S'$  ranging from  $-1$  to  $10$ . When  $S > 0.6$  and  $S' > 3$  there are two special frequencies and the frequencies are quite high when both  $S$  and  $S'$  are large. In the special case when  $SS' = 1$ , (14) yields the following solutions

$$\omega_r^2/\sigma = 1 \pm \left[ 1 - \frac{4\delta}{(1+\delta)^2} \sin^2(\phi_r/2) \right]^{1/2} \tag{17 a}$$

with

$$\phi_r = r\pi/N, \quad r = 1, 2, \dots, N - 1$$

and

$$\omega^2/\sigma = \frac{1}{2(1+\delta)} \left[ (2+s) + \delta(2+s') \pm \{(2+s)^2 + \delta^2(2+s')^2 - 2\delta(3+2s+2s')\}^{1/2} \right] \tag{17 b}$$

Equation (17 b) admits high frequencies for high values of  $S$  or  $S'$  with the constraint  $SS' = 1$ .

For mixed cases (e.g.,  $S = 0, S' = -1$ ;  $S = -1, S' = 0$ ), eq. (14) does not give closed form solutions for the normal frequencies.

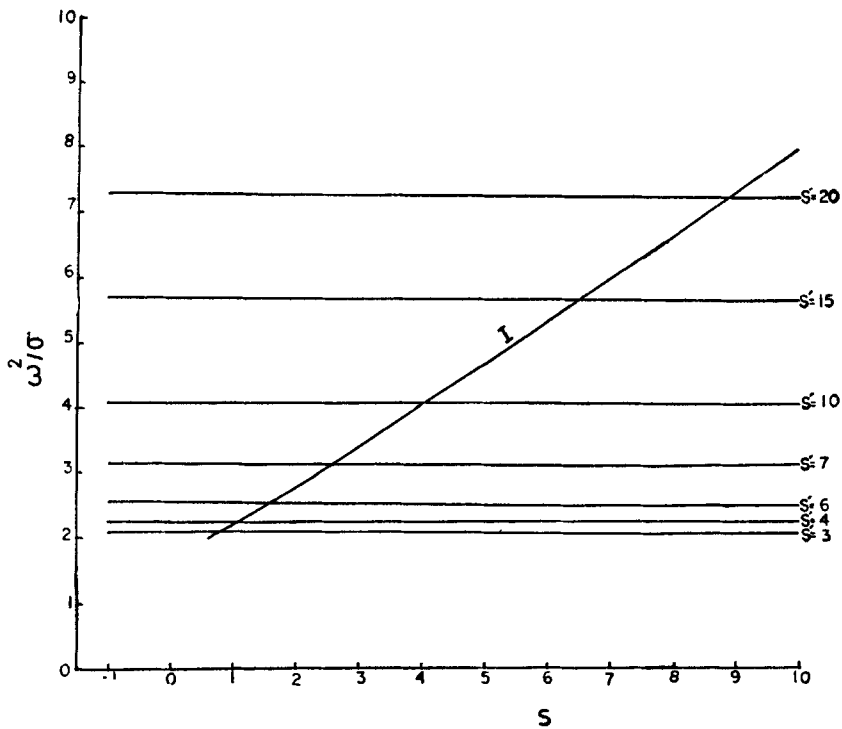


Figure 3. Variation of the special frequencies corresponding to the real positive roots of (14) with  $S$  and  $S'$  for a diatomic lattice with  $\delta = m_1/m_2 = \frac{1}{2}$ ,  $N = 10$ , when the end atoms are not alike. The curve I is present for all values of  $s'$  from  $-1$  to  $10$ .

(ii) *End atoms are alike*—We consider a linear diatomic lattice with  $2N + 1$  atoms where both the end positions are occupied by lighter atoms. The equations for the amplitudes of vibration are given by (9)–(11) with slight modifications. In particular, equations (10) take the following forms:

$$\left. \begin{aligned} \beta a_{2j} &= a_{2j-2} + a_{2j+2}, & j &= 1, 2, \dots, N-1 \\ \beta a_{2j-1} &= a_{2j-3} + a_{2j+1}, & j &= 1, 2, \dots, N \end{aligned} \right\} \quad (18)$$

where  $\beta$ ,  $a_0$  and  $a_{-1}$  are defined by (11). Here the set of equations (18) must be augmented with the end conditions

$$(2 - \alpha_1^2 + s) a_1 = a_2 \quad (19 a)$$

$$(2 - \alpha_1^2 + s') a_{2N+1} = a_{2N} \quad (19 b)$$

Following the procedure of section (4i) step by step, one may easily obtain different amplitudes in terms of  $a_1$ . The allowed frequencies may also be obtained by solving the following equation:

$$(2 - \alpha_1^2 + s + s') g_{N+1}(\lambda) + [s + s' + ss'(2 - \alpha_2^2)] g_N(\lambda) = 0 \quad (20)$$

which reduces to

$$\alpha_1^2 g_{N+1}(\lambda) + \alpha_2^2 g_N(\lambda) = 0 \quad (21)$$

for the free boundary condition ( $S = S' = -1$ ). Equation (21) shows that  $\omega = 0$



is a solution which corresponds to the translation of the lattice. Other solutions are obtained from (21) which may be rewritten as

$$(\lambda^2 - 1)^{-1} [\delta (\lambda^{2N+2} - 1) + \lambda (\lambda^{2N} - 1)] = 0 \quad (22)$$

Equation (22) can be solved numerically for different values of the mass ratio  $\delta$  and the number of atoms  $2N + 1$ . It allows both real and complex roots. Complex roots correspond to the real values of  $\phi_r$ , satisfying the equation

$$[\delta \sin(N + 1)\phi_r + \sin(N\phi_r)]/\sin\phi_r = 0 \quad (23)$$

whereas the real roots of (22) correspond to the complex values of  $\phi_r$ .

The real values of  $\phi_r$  obtained from (23) correspond to the wave-like modes and the frequencies are then given by (15 a). When the mass ratio tends to unity the surface modes obtained from the real roots of (22) pass to the wave-like modes as usual.

It should be mentioned that all the allowed values of the frequencies are obtained here from the solutions of a single equation (eq. 21) whereas Wallis in a completely different approach has found a set of two equations. It has been checked by numerical computations that the results are same in both the approaches. For the frequencies in the forbidden gap one may have the analytical expressions for the roots of (22) which lead to

$$\omega^2/\sigma \approx 1 \pm \delta^N(1 - \delta), \quad \delta^{2N} \ll 1 \quad (24)$$

Finally we mention that the different modes of oscillation of a diatomic lattice with heavy atoms at the ends may also be obtained in a simple way by just interchanging the roles of  $m_1$  and  $m_2$ .

## 5. Discussion

We have shown that the problem of vibration of monoatomic and diatomic lattices can be solved in a unified approach where simply a solution of a second order difference equation is required.

For a diatomic lattice we obtain the surface modes of oscillation with frequencies lying in the forbidden gap between the acoustical and optical branches. This is in agreement with the observation of Wallis. We also obtain the exact expressions for the amplitudes of the different particles in the various vibration modes. These amplitudes are of great importance in different branches of solid state and molecular physics. With the help of these amplitudes one may find the mean square velocities and displacements of different particles, which in turn give an estimate of the Mössbauer fractions for different nuclei in the optical and acoustical regions.

Finally, we mention the presence of some special positive roots of the polynomial equation when the ends of the diatomic lattice are rigidly fixed to the boundary walls. These special roots correspond to high frequencies for the vibration of the lattice.

## Appendix 1

*Some properties of the polynomial  $f_j(\beta)$ :*

The polynomial  $f_j(\beta)$  in  $\beta$  of degree  $j - 1$  is defined by

$$f_j(\beta) = 2^{-j+1} \sum_{r=0}^M \binom{j}{2r+1} \beta^{j-2r-1} (\beta^2 - 4)^r \quad (\text{A1})$$

with  $M = j/2$  or  $(j-1)/2$  whichever is an integer.

The expression (A1) can be written in the following simple form:

$$f_j(\beta) = 2^{-j} (\beta^2 - 4)^{-1/2} \{[\beta + (\beta^2 - 4)^{1/2}]^j - [\beta - (\beta^2 - 4)^{1/2}]^j\} \quad (\text{A2})$$

where the summation in (A1) has been removed.

Further if we define

$$\lambda = \frac{1}{2} [\beta + (\beta^2 - 4)^{1/2}] \quad (\text{A3 a})$$

then

$$\lambda^{-1} = \frac{1}{2} [\beta - (\beta^2 - 4)^{1/2}] \quad (\text{A3 b})$$

and (A2) reduces to

$$f_j(\beta) \equiv g_j(\lambda) = (\lambda^j - \lambda^{-j})/(\lambda - \lambda^{-1}) = \sin(j\phi)/\sin\phi \quad (\text{A4})$$

where we have put

$$\lambda = \exp(i\phi) \quad (\text{A5})$$

It is obvious from (A3 a) that  $\lambda$  can never vanish.

We can easily verify from (A4) that  $g_j(\lambda)$  satisfies the following recurrence relation:

$$(1 + \lambda^2) g_j(\lambda) = \lambda [g_{j+1}(\lambda) + g_{j-1}(\lambda)] \quad (\text{A6})$$

In terms of the variable  $\beta$  the recurrence relation (A6) becomes

$$\beta f_j(\beta) = f_{j+1}(\beta) + f_{j-1}(\beta) \quad (\text{A7})$$

Thus, we see that the polynomial  $f_j(\beta)$  introduced in (A1) is the solution of the difference equation (A7). Although the structure of  $f_j(\beta)$  is a little complicated it satisfies a simple recurrence relation (A7).

The following properties of  $f_j(\beta)$  or  $g_j(\lambda)$  should be noted:

$$g_j(\lambda^{-1}) = g_j(\lambda) \quad (\text{A8 a})$$

$$g_j(1) = f_j(2) = j \quad (\text{A8 b})$$

$$g_0(\lambda) = 0, \quad g_1(\lambda) = 1 \quad (\text{A8 c})$$

$$f_{N-1}(\beta) f_{i+1}(\beta) - f_{N-i-1}(\beta) f_1(\beta) = f_N(\beta) \quad (\text{A8 d})$$

$$f_{N-i+1}(\beta) f_i(\beta) - f_{N-i}(\beta) f_{i-1}(\beta) = f_N(\beta) \quad (\text{A8 e})$$

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