THE CHARACTERISTIC VIBRATIONS OF A RECTANGULAR LATTICE

By K. S. Viswanathan
(*From the Raman Research Institute, Bangalore*)

Received September 16, 1952
(Communicated by Sir C. V. Raman, F.R.S., N.L.)

A. Introduction

In a previous paper,[1] the author had shown that for a linear lattice with p atoms in its unit cell, there are $(2p-1)$ frequencies for which the group velocity of the waves traversing along the lattice vanish, and it was further proved that any arbitrary initial disturbance ultimately settles into a superposition of these $(2p-1)$ characteristic vibrations, the amplitudes of vibrations at any instant being proportional to the square root of the time elapsed. These results, however are not peculiar to linear lattices alone and we have reason to believe that for periodic lattices in two and three dimensions,[2] there are $(8p-2)$ and $(24p-3)$ frequencies respectively for which the group velocity of the waves associated with them vanish, p in each case representing the number of atoms in an unit cell of the lattice. It is the object of the present paper to prove the above statement and extend the results of the previous paper to the case of a rectangular lattice, which for simplicity is assumed to consist of one particle in each of its unit cells.

1. The Characteristic Frequencies

We shall denote the lattice distances by d_1 and d_2 and let $\tan\lambda = \frac{d_2}{d_1}$. The position of any particle is specified by means of the ordered pair of integers (l, m) and the components of the displacements of the particles along the x and y directions are denoted by $x_{l,m}$ and $y_{l,m}$. We restrict the interaction of any particle to its immediate and diagonal neighbours only and neglect the effect of the forces caused on it by the displacements of the more distant neighbours. Since the interacting forces are assumed to be central, this assumption places a restriction on the magnitudes of d_1 and d_2 and implies that $(d_1^2 + d_2^2)^{\frac{1}{2}}$ is less than both $2d_1$ and $2d_2$. The potential energy of the lattice now becomes a function of three force constants α, β, γ and as $(x_{l,m} \cos\lambda + y_{l,m} \sin\lambda)$ is the resolved part of the displacement of the particle (l, m) along the diagonal joining it to the particle $(l+1, m+1)$, we have the following expressions for the potential and kinetic energies of the lattice.

$$2T = M \sum_{l,m} (\dot{x}_{l,m}^2 + \dot{y}^2_{l,m}) \tag{1}$$

$$2V = \alpha \sum_{l,m} (x_{l,m} - x_{l+1,m})^2 + \beta \sum_{l,m} (y_{l,m} - y_{l,m+1})^2$$

$$+ \gamma \sum_{l,m} (x_{l,m} \cos\lambda + y_{l,m} \sin\lambda - x_{l+1,m+1} \cos\lambda - y_{l+1,m+1} \sin\lambda)^2$$

$$+ \gamma \sum_{l,m} (x_{l,m} \cos\lambda - y_{l,m} \sin\lambda - x_{l-1,m+1} \cos\lambda + y_{l-1,m+1} \sin\lambda)^2,$$

the summation extending over all the particles of the lattice.

When the lattice extends indefinitely along both sides, it is necessary to assume the convergence of the series (1); this, however, would be secured in the problem which we consider since the total energy of the lattice, which is due to an initial disturbance imparted to a finite region of the lattice, is a constant.

The equations of motion of the particles are now given by

$$-M\ddot{x}_{l,m} = \alpha (2x_{l,m} - x_{l+1,m} - x_{l-1,m}) \tag{2}$$

$$+ \gamma \cos\lambda \begin{Bmatrix} 4x_{l,m} \cos\lambda - x_{l+1,m+1} \cos\lambda - y_{l+1,m+1} \sin\lambda \\ - x_{l-1,m+1} \cos\lambda + y_{l-1,m+1} \sin\lambda - x_{l+1,m-1} \cos\lambda \\ + y_{l+1,m-1} \sin\lambda - x_{l-1,m-1} \cos\lambda - y_{l-1,m-1} \sin\lambda \end{Bmatrix}$$

$$-M\ddot{y}_{l,m} = \beta (2y_{l,m} - y_{l,m+1} - y_{l,m-1}),$$

$$+ \gamma \sin\lambda \begin{Bmatrix} 4y_{l,m} \sin\lambda - x_{l+1,m+1} \cos\lambda - y_{l+1,m+1} \sin\lambda \\ + x_{l-1,m+1} \cos\lambda - y_{l-1,m+1} \sin\lambda + x_{l+1\,m-1} \cos\lambda \\ - y_{l+1,m-1} \sin\lambda - x_{l-1,m-1} \cos\lambda - y_{l-1,m-1} \sin\lambda \end{Bmatrix}$$

We shall assume wave solutions for these equations of the type

$$x_{l,m} = f_1 e^{i(\omega t + l\theta_1 + m\theta_2)}$$

$$y_{l,m} = f_2 e^{i(\omega t + l\theta_1 + m\theta_2)}, \tag{3}$$

where f_1 and f_2 are functions of the two variables θ_1 and θ_2.

Substituting equations (3) in (2), we get

$$f_1 [f(\theta_1\theta_2) - M\omega^2] + f_2\psi(\theta_1\theta_2) = 0$$

$$f_1 \psi(\theta_1\theta_2) + f_2 [\phi(\theta_1\theta_2) - M\omega^2] = 0, \tag{4}$$

where

$$f(\theta_1\theta_2) = 2\alpha(1 - \cos\theta_1) + 4\gamma\cos^2\lambda(1 - \cos\theta_1\cos\theta_2)$$

$$\phi(\theta_1\theta_2) = 2\beta(1 - \cos\theta_2) + 4\gamma\sin^2\lambda(1 - \cos\theta_1\cos\theta_2) \quad (5)$$

and $\psi(\theta_1\theta_2) = 4\gamma\sin\lambda\cos\lambda\sin\theta_1\sin\theta_2$.

Eliminating f_1 and f_2 from equations (4) we get

$$M^2\omega^4 - M\omega^2[f(\theta_1\theta_2) + \phi(\theta_1\theta_2)] + f(\theta_1\theta_2)\phi(\theta_1\theta_2) - \psi^2(\theta_1\theta_2) = 0 \quad (6)$$

Since from (6), ω is a periodic function of θ_1 and θ_2, we shall consider only the values of θ_1 and θ_2 lying inside the intervals $0 \leqslant \theta_1 \leqslant 2\pi$; and $0 \leqslant \theta_2 \leqslant 2\pi$. Also, by a comparison of (3) with the usual form of the wave function, we get $k = \frac{1}{\lambda} = \frac{1}{2\pi}\sqrt{\frac{\theta_1^2}{d_1^2} + \frac{\theta_2^2}{d_2^2}}$, where λ is the wavelength of a wave. More than the individual waves, greater importance attaches to the groups of waves and their velocities since it is only these physical entities that are accessible to any observation and measurement. The group velocity of the waves defined by $\frac{d\nu}{dk}$ will vanish when both $\frac{\partial\omega}{\partial\theta_1}$ and $\frac{\partial\omega}{\partial\theta_2}$ are equal to zero.

We have now from (6)

$$A\frac{\partial\omega}{\partial\theta_1} = K_1\sin\theta_1, \quad (7a)$$

where

$$A = M\omega[2M\omega^2 - f(\theta_1\theta_2) - \phi(\theta_1\theta_2)]$$

$$K_1 = \alpha[M\omega^2 - \phi(\theta_1\theta_2)] + 2\gamma\cos\theta_2[M\omega^2 - f(\theta_1\theta_2)\sin^2\lambda - \phi(\theta_1\theta_2)\cos^2\lambda] + 16\gamma^2\sin^2\lambda\cos^2\lambda\sin^2\theta_2\cos\theta_1 \quad (8)$$

and $A\frac{\partial\omega}{\partial\theta_2} = K_2\sin\theta_2$. (7b)

where K_2 is defined in a similar manner as (8).

It can therefore easily be seen that both $\frac{\partial\omega}{\partial\theta_1}$ and $\frac{\partial\omega}{\partial\theta_2}$ vanish for the set of points (0, 0); (0, π); (π, 0) and (π, π). Excluding the point (0, 0) which corresponds to a translation of the entire lattice, we have for the frequencies associated with the remaining three points the following expressions:

$$\begin{aligned}
&(1)\ \mathrm{M}u_1^2 = f(0, \pi) = 8\gamma \cos^2 \lambda \\
&\quad\ \mathrm{M}u_2^2 = \phi(0, \pi) = 4(\beta + 2\gamma \sin^2 \lambda) \\
&(2)\ \mathrm{M}v_1^2 = f(\pi, 0) = 4(\alpha + 2\gamma \cos^2 \lambda) \\
&\quad\ \mathrm{M}v_2^2 = \phi(\pi, 0) = 8\gamma \sin^2 \lambda \\
&(3)\ \mathrm{M}w_1^2 = f(\pi, \pi) = 4\alpha \text{ and} \\
&\quad\ \mathrm{M}w_2^2 = \phi(\pi, \pi) = 4\beta.
\end{aligned} \tag{9}$$

It follows now from (7) that the group velocity of the waves associated with each of these six characteristic frequencies is equal to zero.

The case of a square lattice is particularly simple and interesting. Here we have $\alpha = \beta$ and $\lambda = \frac{\pi}{4}$ and only three of the six frequencies given above are distinct.

2. The Effect of an Initial Disturbance

We shall suppose that initially the particle at the origin receives a small displacement whose components parallel to the axes are a and b respectively and that all other particles are at rest.

$$(i.e.)\quad x_{l,m}(0) = a\delta_{l0}\delta_{m0} \tag{10}$$

$$y_{l,m}(0) = b\delta_{l0}\,\delta_{m0} \text{ and } \dot{x}_{l,m}(0) = \dot{y}_{l,m}(0) = 0$$

for all l and m. If the values of f_r $(r = 1, 2)$ corresponding to the frequencies $\pm\,\omega_s$ $(s = 1, 2)$ are denoted by $f_{r,s}$ and $f_{r,2+s}$, following Nagendra Nath,[3] we obtain the general expressions for the displacements of the particles at any time by superposing wave solutions of the type (3) for all values of θ_1 and θ_2 lying in the interval $(0, 2\pi)$. We get

$$\begin{aligned}
x_{l,m} = {} & \frac{1}{8\pi^2}\int_0^{2\pi}\!\!\int_0^{2\pi} (f_{11}\,e^{i\omega_1 t} + f_{13}e^{-i\omega_1 t}) \exp.\, i\,(l\theta_1 + m\theta_2)\, d\theta_1 d\theta_2 \\
& + \frac{1}{8\pi^2}\int_0^{2\pi}\!\!\int_0^{2\pi} (f_{12}\,e^{i\omega_2 t} + f_{14}e^{-i\omega_2 t}) \exp.\, i\,(l\theta_1 + m\theta_2)\, d\theta_1 d\theta_2
\end{aligned} \tag{11}$$

$$\begin{aligned}
y_{l,m} = {} & \frac{1}{8\pi^2}\int_0^{2\pi}\!\!\int_0^{2\pi} (f_{21}\,e^{i\omega_1 t} + f_{23}\,e^{-i\omega_1 t}) \exp.\, i\,(l\theta_1 + m\theta_2)\, d\theta_1 d\theta_2 \\
& + \frac{1}{8\pi^2}\int_0^{2\pi}\!\!\int_0^{2\pi} (f_{22}\,e^{i\omega_2 t} + f_{24}e^{-i\omega_2 t}) \exp.\, i\,(l\theta_1 + m\theta_2)\, d\theta_1 d\theta_2
\end{aligned} \tag{12}$$

With the help of equations (4) and the initial conditions (10), we can express the values of f_{rs} as functions of θ_1 and θ_2. We have from (11)

$$x_{l,m}(0) = \frac{1}{8\pi^2}\int_0^{2\pi}\int_0^{2\pi}(f_{11}+f_{12}+f_{13}+f_{14})\ \text{exp.}\ i\,(l\theta_1+m\theta_2)\,d\theta_1\,d\theta_2$$

$$\dot{x}_{l,m}(0) = \frac{i}{8\pi^2}\int_0^{2\pi}\int_0^{2\pi}\{\omega_1(f_{11}-f_{13})+\omega_2(f_{12}-f_{14})\}\ \text{exp.}\ i\,(l\theta_1+m\theta_2)\,d\theta_1 d\theta_2$$

By expanding $\sum_{r=1}^{4} f_{1r}$ as a Fourier series in θ_1 and θ_2 in the form

$$\sum_{r=1}^{4} f_{1r} = \sum_{+\infty}^{-\infty}\sum_{+\infty}^{-\infty} A_{jk}\, e^{i(j\theta_1+k\theta_2)} \tag{14}$$

we get on substituting (14) in (13)

$$\begin{aligned} x_{l,m}(0) &= \frac{1}{8\pi^2}\sum_{-\infty}^{+\infty}\sum_{-\infty}^{+\infty} A_{jk}\, I_{jl}\, I_{km} \\ &= \tfrac{1}{2}\sum_{-\infty}^{+\infty}\sum_{-\infty}^{+\infty} A_{jk}\,\delta_{-jl}\,\delta_{-km} \\ &= \tfrac{1}{2} A_{-l,-m},\ \text{where we write} \end{aligned}$$

$$I_{lm} = \int_0^{2\pi} e^{i(l+m)\theta} d\theta$$

Hence we get $\sum_{r=1}^{4} f_{1r} = 2a$ (15)

Similarly we have $\sum_{r=1}^{4} f_{2r} = 2b$ (16)

and $\sum_{r=1,2} \omega_r (f_{1r} - f_{1,2+r}) = \sum_{r=1,2} \omega_r (f_{2r} - f_{2,2+r}) = 0$ (17)

Now we get from (4), $f_{2r}\,\psi(\theta_1\theta_2) = f_{1r}\,[M\omega_r^2 - f(\theta_1\theta_2)]$ and hence from (16) and (17) we have

$$\sum_{r=1,2} \omega_r^2 (f_{1,r} + f_{1,2+r}) = 2\,\frac{(\psi b + fa)}{M} \tag{18}$$

and

$$\sum_{r=1,2} \omega_r^3 (f_{1r} - f_{1,2+r}) = 0 \tag{19}$$

Solving these equations we get,

$$f_{11} = f_{13} = \frac{a\,(M\omega_2^2 - f) - \psi b}{M\,(\omega_2^2 - \omega_1^2)} \tag{20}$$

$$f_{12} = f_{14} = \frac{a\,(M\omega_1^2 - f) - \psi b}{M\,(\omega_1^2 - \omega_2^2)}$$

and two similar expressions for f_{21} and f_{22}.

With these values for f_{11} and f_{12}, equation (17) can now be rewritten as

$$x_{l,m} = \frac{1}{8\pi^2}\int_0^{2\pi}\int_0^{2\pi} f_{11}\,(e^{i\omega_1 t} + e^{-i\omega_1 t})\, e^{i(l\theta_1 + m\theta_2)}\, d\theta_1\, d\theta_2 \tag{21}$$

$$+ \frac{1}{8\pi^2}\int_0^{2\pi}\int_0^{2\pi} f_{12}\,(e^{i\omega_2 t} + e^{-i\omega_2 t})\, e^{i(l\theta_1 + m\theta_2)}\, d\theta_1 d\theta_2$$

The asymptotic value of the above integral for large values of t can be obtained by means of an extension of Kelvin's method of stationary phases for double integrals. We shall consider the integral

$$I = \int_\Delta f(x,\ y)\ \text{exp.}\ i\,[\omega\,(x,\ y)\ t + lx + my]\ dx\, dy, \tag{A}$$

where $f(x, y)$ is integrable in Δ and t is large compared to l and m (*i.e.*) $t = 0\,(l^2 + m^2)$. We shall assume that the region of integration contains only one stationary point of $\omega\,(x, y)$ at $(x_0 y_0)$. When the region of integration contains several stationary points of $\omega\,(x, y)$, it can be split up into subregions such that $\omega\,(x, y)$ has only one stationary point in each of these subregions. Since the exponent in the integrand is a very rapidly fluctuating function when t is large, the most important contribution to the integral arises only from a region in the neighbourhood of $(x_0 y_0)$ at which $\omega\,(x, y)$ is stationary. We have, if $x - x_0 = \xi$ and $y - y_0 = \eta$, for small values of ξ and η,

$\omega\,(x, y) = \omega\,(x_0 y_0) + \frac{1}{2}\,(a\xi^2 + 2h\xi\eta + b\eta^2)$, where a, h, b are the values of $\frac{\partial^2\omega}{\partial x^2}, \frac{\partial^2\omega}{\partial x \partial y}, \frac{\partial^2\omega}{\partial y^2}$ at the point $(x_0 y_0)$. Hence (A) can be written as

$$I \sim f(x_0 y_0)\ \text{exp.}\ i\,[\omega\,(x_0 y_0)\ t + lx_0 + my_0] \int_{-\xi_0}^{+\xi_0}\int_{-\eta_0}^{+\eta_0} e^{\frac{it}{2}(a\xi^2 + 2h\xi\eta + b\eta^2)}\, d\xi d\eta \tag{22}$$

We transform the variables ξ, η to a new set of variables σ and ρ given by

$$ta\left(\xi + \frac{h}{a}\eta\right)^2 = \sigma^2$$

$$\frac{(ab - h^2)}{a} t\eta^2 = \rho^2;$$

the limits for σ and ρ can be taken to be $\pm\infty$ without any appreciable error. Hence if $ab > h^2$, and $a > 0$ (22) becomes

$$\mathrm{I} \sim \frac{f(x_0 y_0)}{t(ab - h^2)^{\frac{1}{2}}} \exp. i\left[\omega(x_0 y_0) t + l x_0 + m y_0\right] \int_{-\infty}^{+\infty} e^{-\sigma^2/2i} d\sigma \int_{-\infty}^{+\infty} e^{-\rho^2/2i} d\rho$$

$$= \frac{2\pi f(x_0 y_0)}{t(ab - h^2)^{\frac{1}{2}}} \exp. i\left[\omega(x_0 y_0) t + l x_0 + m y_0 + \pi/2\right)$$

If $(ab - h^2)$ is negative, then we have

$$\mathrm{I} \sim \frac{2\pi f(x_0 y_0)}{t(h^2 - ab)^{\frac{1}{2}}} \exp. i\left[\omega(x_0 y_0) t + l x_0 + m y_0\right]. \tag{23}$$

In a similar way, the value of the integral $\mathrm{I}_1 = \int_\Delta f(x, y) \exp. i\left[-\omega(x, y)t + lx + my\right] dx\, dy$ for large values of t is given by

$$\mathrm{I} = \frac{2\pi f(x_0 y_0)}{t\,|\,ab - h^2\,|^{\frac{1}{2}}} \exp. i\left[-\omega(x_0 y_0) t + l x_0 + m y_0 - \epsilon_{ab}\frac{\pi}{2}\right] \tag{24}$$

where ϵ_{ab} takes the values 1 or 0 according as $ab \gtrless h^2$.

Turning to the integral (21) we note that when θ_1 and θ_2 take any of the values

$(0, \pi)$; $(\pi, 0)$ and (π, π), we have

$$f_{11}(\theta_1\theta_2) = a; \quad f_{22}(\theta_1\theta_2) = b$$

$$f_{12}(\theta_1\theta_2) = f_{21}(\theta_1\theta_2) = 0.$$

Also at these points,

$$2\mathrm{M}\omega_1 \frac{\partial^2\omega_1}{\partial\theta_r^2} = \frac{\partial^2 f}{\partial\theta_r^2}; \quad 2\mathrm{M}\omega_2 \frac{\partial^2\omega_2}{\partial\theta_r^2} = \frac{\partial^2\phi}{\partial\theta_r} \quad (r = 1, 2)$$

and $\dfrac{\partial^2\omega_r}{\partial\theta_1\partial\theta_2} = 0.$

Hence if $w_1 > u_1$, and $w_2 > v_2$, applying the results (23) and (24) to the integral (21) we get

$$x_{l,m} = \frac{2a}{\pi t}\left[\frac{(-1)^m \cos u_1 t}{(w_1^2 - u_1^2)^{\frac{1}{2}}} + \frac{(-1)^{l+1}\sin v_1 t}{u_1} + \frac{(-1)^{l+m} w_1 \cos w_1 t}{u_1(w_1^2 - u_1^2)^{\frac{1}{2}}}\right. \tag{I}$$

Similarly,

$$y_{l,m} = \frac{2b}{\pi t}\left[\frac{(-1)^{m+1}\sin u_2 t}{v_2} + \frac{(-1)^l \cos v_2 t}{(w_2^2 - v_2^2)^{\frac{1}{2}}} + \frac{(-1)^{l+m} w_2 \cos w_2 t}{v_2 (w_2^2 - v_2^2)^{\frac{1}{2}}}\right]$$

Two similar expressions can be derived if the initial conditions are slightly modified. If we have initially $x_{l,m}(0) = y_{l,m}(0) = 0$ and $\dot{x}_{l,m}(0) = u\delta_{l0}\delta_{m0}$; $\dot{y}_{l,m}(0) = v\delta_{l0}\,\delta_{m0}$ for all l and m, we get by an exactly similar procedure the following expressions for the displacements of the particles from their equilibrium positions.

$$x_{l,m} = \frac{2u}{\pi t}\left[\frac{(-1)^m \sin u_1 t}{u_1 (w_1^2 - u_1^2)^{\frac{1}{2}}} + \frac{(-1)^l \cos v_1 t}{u_1 v_1} + \frac{(-1)^{l+m}\sin w_1 t}{u_1 (w_1^2 - u_1^2)^{\frac{1}{2}}}\right] \qquad \text{(II)}$$

$$y_{l,m} = \frac{2v}{\pi t}\left[\frac{(-1)^m \cos u_2 t}{u_2 v_2} + \frac{(-1)^l \sin v_2 t}{v_2 (w_2^2 - v_2^2)^{\frac{1}{2}}} + \frac{(-1)^{l+m}\sin w_2 t}{v_2 (w_2^2 - v_2^2)^{\frac{1}{2}}}\right]$$

When initially, a displacement combined with a small velocity is imparted to the particle at the origin, then the components of the displacements along the x- and y-directions are given by the sum of the x and y components of the displacements in (I) and (II); this result follows from the principle of superposition.

3. Physical Interpretations

The expressions (I) and (II) clearly indicate that the movements of the particles tend asymptotically to a superposition of the six characteristic vibrations of the lattice, with a slowly diminishing amplitude which varies inversely as the time elapsed. It is interesting to note that the x-components of the displacements of the particles depend only on three of these modes which may be pictured as the movements of, (1) the y-lines moving normally against each other, (2) the x-lines moving tangentially in opposite directions, and (3) as the oscillations of the diagonal lines against each other along the x-axis. Similarly, the y-components of the displacements of the particles depend on three different modes of vibrations which are the tangential oscillation of the y-lines, the normal oscillation of the x-lines against each other and the movements of the diagonal lines along the y-axis, the frequencies of vibrations of both the diagonal lines being the same.

The decay of the vibrations according to the law t^{-1} can be understood physically also. Since the initial disturbance is progressively transmitted to all the atoms around the origin, the amplitudes of the particles in the region where their movements are represented by (I) should vary approximately as the inverse square root of the area of this region and hence are inversely proportional to the time elapsed from the instant of the initial disturbance.

All these results were arrived at under the assumption that the lattice is unbounded. If however, we confine our observations to a time-interval which is large compared to the individual periods of the eigen-vibrations, but still small in comparison with the time taken by the fastest wave to reach the boundary, the above restriction can be removed and the results of the preceding sections can be seen to hold good for a finite lattice also, provided its dimensions are very large compared to that of its unit cells.

My sincere thanks are due to Professor Sir C. V. Raman, F.R.S., N.L., for the valuable suggestions and encouragement he gave, during the course of this work.

SUMMARY

For a rectangular lattice with one particle in each unit cell, it is shown that the group velocity of the waves vanishes for the six characteristic frequencies and that the state of movements of the particles arising out of an initial disturbance tends to a superposition of these six characteristic vibrations of the lattice. These six frequencies would reduce to three for a square lattice on account of its symmetry; in all these two cases however, the amplitudes of vibrations of the particles vary inversely as the time elapsed from the instant of the initial disturbance. The physical interpretation of these results and their applicability to the case of a finite lattice are discussed.

REFERENCES

1. Viswanathan, K. S. .. *Proc. Ind. Acad. Sci.*, 1952, **35**, 265.
2. Raman, C. V. .. *Ibid.*, 1943, **18**, 237.
3. Nagendra Nath, N. S. and Roy, S. K. .. *Ibid.*, 1948, **28**, 289.

878-52 Printed at The Bangalore Press, Bangalore City, by G. Srinivasa Rao, Superintendent, and Published by The Indian Academy of Sciences, Bangalore