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# Vibration of Two Coupled Linear Atomic Chains

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## ABSTRACT

By method of difference equations an equation of motion have been calculated for two coupled linear chains with different atoms. Special cases are discussed and shows full agreement with the above results.

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# اهتزازات سلسلتين ذريتين مرتبطتين مع بعضهما

## الملخص

لقد تم في هذا البحث مناقشة اهتزازات سلسلتين خطيتين مختلفتي الذرات مرتبطة مع بعضهما. كما تم وضع معادلة الحركة لاهتزاز ذرات السلسلتين عندما تصبح سلسلة واحدة. وتم مناقشة الحالات الخاصة لذلك أيضاً. كانت النتائج مطابقة للأبحاث التي أجريت سابقاً على السلاسل الخطية.

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## INTRODUCTION

The study of lattice dynamics now forms an important part of any course in solid state physics (Ruvalds and Zavadovsky,1970; Agranovich,1970; Kimball et al.,1981). The vibration of atoms in crystal not only determine its thermal properties but also govern phenomena like diffuse scattering of x-ray, neutron scattering, spin lattice relaxation, etc. (Ghatak and Kothari,1972). In order to understand any of these phenomena it is necessary to develop the theory of vibration of atoms, that is, the theory of lattice dynamic. The atom vibration in crystal can be quantized, and this given rise to quasi-particles called phonons (Valenta and Jager,1977; Kittel, 1976; Jager et al.,1988; Jager and Mossa,1986; Gasagrande et al., 1977). Neutron scattering from a crystal is usually analized in terms of the number of phonons exchanged with the crystal.

Zero phonon process corresponds to elastic scattering, since no energy change of the crystal is involved. In elastic scattering, that is,the scattering process in which one or more phonons are either created or absorbed in crystal,gives us information about lattice dynamics.

This work represents an attempt to carry out farther calculation related to the theory of lattice dynamics, under the harmonic approximation, that is, in writing the potential energy of the vibrating atom. We retain atoms only up to the second power in the displacement for the atom. This implies that there is no phonon-phonon interaction and hence these quasi-particles have an infinite life time. This time. This also means, that the energy of a phonon is exactly defined. The neglect of higher-order terms will prevent us from discussing anharmonic effects, that is, the phonon-phonon interaction which leads to finite life time for a phonon. The finite life time of a phonon implies a spread in its energy and when a neutron with a well-defined energy is scattered by the absorption or emission of a phonon, it will also show a spread in energy corresponding to the spread in energy of the phonon.

## EQUATION OF MOTION

Let us consider a lattice consisting of two linear chains of equally spaced atoms bound together and lying at a straight line, fig. (1).

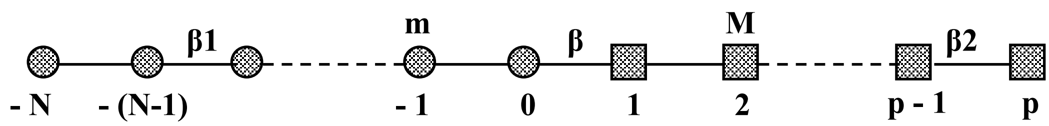


Fig.1: Linear model of two atomic chains coupled through nearest-neighbor forces.

We assume that the atoms are held together by elastic forces obeying Hook's law. The first chain consist from (N+1) identical particles of mass m with coupling constant β1 . The second chain constant from p identical particles of mass M, with coupling constant β2. The coupling constant between the two chains is denoted by β. We may choose 0 number particle as the origin. The particles on the right are successively numberd 1, 2, 3, …, p. and those on the left of the origin are numbered –1, -2, -3, …, -N. We consider that these particles can vibrate longitudinally.

The displacement of the $n^{th}$ particle from its equilibrium position will be denoted by $u_n$.

Since we have assumed that the force between particles obeys Hook's law, the energy of interaction between any two neighbor particles will be a function only of distance between them. So that the equations of motion of these particles at any instant of time build a system of (N+p+1) homogenous difference equations.

$$m\frac{d^2u_{-N}}{dt^2} = -\beta_1\,(u_{-N} - u_{-N+1}) \tag{1}$$

$$m\frac{d^2u_n}{dt^2} = -\beta_1\,(2u_n - u_{n+1} - u_{n-1}) \quad ; \quad -(N-1) \le n \le -1 \tag{2}$$

$$m\frac{d^2u_0}{dt^2} = -\beta_1\,(u_0 - u_{-1}) - \beta\,(u_0 - u_1) \tag{3}$$

$$M\frac{d^2u_1}{dt^2} = -\beta\,(u_1 - u_0) - \beta_2\,(u_1 - u_2) \tag{4}$$

$$M\frac{d^2u_n}{dt^2} = -\beta_2\,(2u_n - u_{n+1} - u_{n-1}) \quad ; \quad 2 \le n \le p-1 \tag{5}$$

$$M \frac{d^2u_p}{dt^2} = -\beta_2 (u_p - u_{p-1}) \tag{6}$$

For the time dependence of $u_n$ we take the factor exp(-iωt), then we get the following time independent difference equations:

From equation (1) we get:

$$u_{n+1} + \left( \frac{m\,\omega^2}{\beta_1} - 2 \right) u_n + u_{-n+1} = 0 \tag{7}$$

From equation (2) we obtain:

$$u_{n+1} + \left( \frac{m\,\omega^2}{\beta_1} - 2 \right) u_n + u_{n-1} = 0 \tag{8}$$

By using the relation $\omega_{max}^2 = \frac{4\beta_1}{m}$, we can write the above difference equation as following characteristic equation:

$$\lambda^{n+1} + \left( \frac{4\,\omega^2}{\beta_1} - 2 \right) \lambda^n + \lambda^{n-1} = 0 \tag{9}$$

And by dividing this equation by $\lambda^{n-1}$, we get:

$$\lambda^2 + \left( \frac{4\,\omega^2}{\omega_{max}^2} - 2 \right) \lambda + 1 = 0 \tag{10}$$

with the following solution:

$$\lambda_{1,2} = \left( 1 + \frac{4\,\omega^2}{\omega_{max}^2} \right) \pm \frac{2\,\omega}{\omega_{max}^2} \sqrt{\omega^2 - \omega_{max}^2} \tag{11}$$

Which is conjugate complex relation. And by using the general theory of (Valenta and Jager, 1977 ; Berg, 1979), we obtain the angle $\theta$ in the following:

$$\tan\theta = \frac{\left( \frac{4\,\omega^2}{\omega_{max}^2} - \frac{4\,\omega^4}{\omega_{max}^4} \right)^{1/2}}{\left( 1 - \frac{2\,\omega^2}{\omega_{max}^2} \right)} \tag{12}$$

Then the general solution for the above difference equation for the first chain is given as (Valenta and Jager, 1977, 1981; Mossa, 1986) by the following equation:

$$u_n = c_1\, e^{i\theta n} + c_2\, e^{-i\theta n} \tag{13}$$

where $c_1$ and $c_2$ are constants.

From equations (3) and (4) we get the following equations:

$$(m\,\omega^2 - \beta_1 - \beta)\, u_0 + \beta_1\, u_{-1} + \beta\, u_1 = 0 \tag{14}$$

$$(M\,\omega^2 - \beta_2 - \beta)\, u_1 + \beta\, u_0 + \beta_2\, u_2 = 0 \tag{15}$$

from equation (5) we get:

$$(M\,\omega^2 - 2\,\beta_2)\,u_n + \beta_2\,u_{n+1} + \beta_2\,u_{n-1} = 0 \tag{16}$$

we can write this equation as follows:

$$u_{n+1} + \left(\frac{M\,\omega^2}{\beta_2} - 2\right) u_n + u_{n-1} = 0 \tag{17}$$

And by using the relation $\varpi^2_{max} = \dfrac{4\,\beta_2}{M}$ , then we can write the above difference equation as following characteristic equation:

$$\lambda^{n+1} + \left(\frac{4\,\omega^2}{\varpi^2_{max}} - 2\right)\lambda^n + \lambda^{n-1} = 0 \tag{18}$$

by dividing by $\lambda^{n-1}$ , we obtain:

$$\lambda^2 + \left(\frac{4\,\omega^2}{\varpi^2_{max}} - 2\right)\lambda + 1 = 0 \tag{19}$$

and its solution is:

$$\lambda_{1,2} = \left(1 + \frac{2\,\omega^2}{\omega^2_{max}}\right) \pm \frac{2\,\omega}{\varpi^2_{max}} \sqrt{\omega^2 - \omega^2_{max}} \tag{20}$$

Which is conjugate complex equation. By using the general theory of (Valenta and Jager, 1977 ; Berg, 1979), we obtain the angle $\phi$ in the following:

$$\tan\phi = \frac{\left(\dfrac{4\,\omega^2}{\varpi^2_{max}} - \dfrac{4\,\omega^4}{\varpi^4_{max}}\right)^{1/2}}{\left(1 - \dfrac{2\,\omega^2}{\varpi^2_{max}}\right)} \tag{21}$$

Then the general solution for the above difference equation is given as (Valenta and Jager, 1977 , 1981) by the following form:

$$u_n = c_1^1\,e^{i\phi n} + c_2^1\,e^{-i\phi n} \tag{22}$$

where $c_1^1$ and $c_2^1$ are constants.

And for equation (6) we obtain:

$$(M^2\,\omega - \beta_2)\,u_p + \beta_2\,u_{p-1} = 0 \tag{23}$$

When we substitute the general solution of the first chain from equation (13) into the boundary particle equation of this chain, i.e. in (-N) number particle equation, and solving, we obtain a relation between the two constants $c_1$ and $c_2$ in the following manner:

$$c_2 = c_1\,e^{-i\theta(2N+1)} \tag{24}$$

In the same way, when we substitute the general solution of the second chain from equation (22) into the boundary particle equation of the chain, i.e. in (p) number particle equation, and solving it, we obtain a relation between the two constants $c_1^1$ and $c_2^1$ in the following manner:

$$c_2^1 = c_1^1 \, e^{-i\phi(2p+1)} \tag{25}$$

Then when we substitute the general solutions from equations (13) and (22) in the boundary particles equations, i.e. equations (14) and (15) and using the two free boundary equations (24) and (25) and solving together, we obtain the general equation of motion for the system as follows:

$$2 \,\mathrm{Sin}\frac{\theta}{2} \,\mathrm{Sin}\,\theta\,(N+1)\,\mathrm{Sin}\frac{\phi}{2}\,\mathrm{Sin}\,\phi(p) - \frac{\beta}{\beta_1}\,\mathrm{Sin}\frac{\phi}{2}\,\mathrm{Sin}\,\phi\,\mathrm{Cos}\,\theta\left(N+\frac{1}{2}\right)$$
$$-\frac{\beta}{\beta_2}\,\mathrm{Sin}\frac{\theta}{2}\,\mathrm{Sin}\,\theta\,(N+1)\,\mathrm{Cos}\left(p-\frac{1}{2}\right)\phi = 0 \qquad \ldots (26)$$

Relation (26) is an equation of motion for two linear chains with different atoms and different force constants coupled together and forming a system of one linear chain, this equation is valid for any particular atom in the system.

## SPECIAL CASES

**1) For $\beta = 0$:**

This means our coupled chains divided into two finite chains, then we get from equation (26) two equations as in (Wallis, 1956) for finite atomic chain as follows:

$$\mathrm{Sin}\frac{\theta}{2}\,\mathrm{Sin}\,\theta\,(N+1) = 0 \tag{27}$$

and

$$\mathrm{Sin}\frac{\phi}{2}\,\mathrm{Sin}\,\phi\,p = 0 \tag{28}$$

From this two equations one can obtain the optics and acoustics branches of the frequencies.

**2)** When the coupling constants $\beta_1$ , $\beta_2$ & $\beta$ are equal and m=M , p=N+1 , this means $\theta = \phi$ , then we get (26) in the following forms:

$$\mathrm{Sin}^2\frac{\theta}{2}\,\mathrm{Sin}^2\,p\theta\;\mathrm{Sin}\frac{\theta}{2}\,\mathrm{Sin}\,p\theta\,\mathrm{Cos}\left(p+\frac{1}{2}\right)\theta = 0 \tag{29}$$

Which is the equation of motion of a finite chain with (p+N+1) particles.

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