

16/04/25

## Lecture - 20

Revanth Reddy Pannala  
EBIT, Unibo  
స్టోర్స్ బెర్జు

→ continuing from the last lecture on calculation  
of Normal coordinates for Elastic Matrix.

### Diagonalization of the Hamiltonian Function — V

From

$$T_a + V_a - V_{a0} = \sum_{\sigma=1}^{3N} H_{\sigma},$$

where each  $H_{\sigma}$  corresponds to one degree of freedom, it follows that the system is completely separable in the normal coordinates, and that each normal coordinate evolves as a linear harmonic oscillator. The total energy can be expressed in terms of the initial conditions as

$$T_a + V_a = V_{a0} + \sum_{\sigma=1}^{3N} E_{\sigma}, \quad E_{\sigma} = \frac{1}{2} \dot{b}_{\sigma}^2(0) + \frac{1}{2} \omega_{\sigma}^2 b_{\sigma}^2(0).$$

One also sees that to calculate the displacements it is necessary to preliminarily determine the eigenvalues  $\omega_{\sigma}^2$  and the eigenvectors  $\eta_{\sigma}$ . For this, one must solve the eigenvalue equation

\*  $C \eta_{\sigma} = \omega_{\sigma}^2 M \eta_{\sigma}, \quad [C]_{kn} = \left( \frac{\partial^2 V_a}{\partial \xi_k \partial \xi_n} \right)_0, \quad [M]_{kn} = \mu_n \delta_{kn}.$

$\omega$  = angular frequency  
i.e oscillation frequency  
of lattice vibrations

### Calculation of the Normal Coordinates — V

• In the new indices the eigenvalue equation to be solved becomes

$$\sum_{n\beta w} c_{m\alpha u}^{n\beta w} \eta_{n\beta w} = \omega^2 \mu_{\alpha} \eta_{m\alpha u},$$

where  $m, n = 1, \dots, N_c$ ;  $\alpha, \beta = 1, \dots, N_b$ ;  $u, w = 1, 2, 3$ . The indices of the eigenvalue and eigenvector have been omitted for simplicity. Letting

$$\sum_{n\beta w} d_{m\alpha u}^{n\beta w} \zeta_{n\beta w} = \omega^2 \zeta_{m\alpha u},$$

$$d_{m\alpha u}^{n\beta w} \doteq \frac{c_{m\alpha u}^{n\beta w}}{\sqrt{\mu_{\alpha} \mu_{\beta}}}, \quad \zeta_{m\alpha u} \doteq \sqrt{\mu_{\alpha}} \eta_{m\alpha u}, \quad \zeta_{n\beta w} \doteq \sqrt{\mu_{\beta}} \eta_{n\beta w}.$$

• Where the coefficient  $\mu_{\alpha}$  has been eliminated from the right hand side, and the above has the standard form of an eigenvalue equation.

• The matrix  $D$  of entries  $d_{m\alpha u}^{n\beta w}$  is called **dynamical matrix** and, after the properties of  $C$ , is symmetrical ( $d_{m\alpha u}^{n\beta w} = d_{n\beta w}^{m\alpha u}$ ) and translationally invariant:

$$d_{m\alpha u}^{n\beta w} = d_{\alpha u}^{\beta w}(\mathbf{l}_m, \mathbf{l}_n) = d_{\alpha u}^{\beta w}(\mathbf{l}_m - \mathbf{l}_n, 0) = d_{\alpha u}^{\beta w}(\mathbf{l}_m - \mathbf{l}_n).$$

→ The presence of mass  $m_\alpha$  on the RHS of Eigen value equation is inconvenient.

→ yes by defining a scaled Eigen vector

$$l_{\max u} = \sqrt{\mu_\alpha} n_{\max u}$$

→ Bloch Theorem

## Calculation of the Normal Coordinates — VI

As a consequence of the translational invariance of  $\mathbf{D}$ , Bloch theorem applies, namely, for any eigenvector of indices  $k\gamma e$  and letting  $\mathbf{l}_0 = 0$ , the following holds:

Selecting the origin

$$\zeta_{\gamma e}(\mathbf{l}_k) = \exp(\mathbf{c} \cdot \mathbf{l}_k) \zeta_{\gamma e}(0),$$



Eigenvalue of  
cell near  
the origin

where  $\mathbf{c}$  is any complex vector of the reciprocal lattice, and  $k = 0, \dots, N_c - 1; \gamma = 1, \dots, N_b; e = 1, 2, 3$ .

→ One should notice that the real eigenvectors used so far are being replaced for convenience by complex quantities. At the end of the calculation, a set of real eigenvectors can be recovered by suitable combinations of the complex ones. Using the Born-von Karman boundary conditions,  $\mathbf{c}$  is found to be purely Imaginary

$$\mathbf{c} = j\mathbf{q}, \quad \mathbf{q} = \sum_{s=1}^3 \frac{\nu_s}{N_s} 2\pi \mathbf{b}_s,$$

where  $N_1, N_2, N_3$  are the number of cells along the directions of the characteristic vectors of the direct lattice,  $\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3$  are the characteristic vectors of the reciprocal lattice, and  $\nu_1, \nu_2, \nu_3$  are integers, with  $\nu_s = 0, 1, \dots, N_s - 1$ . The total number of distinct  $\mathbf{q}$  vectors is thus  $N_1 N_2 N_3 = N_c$ .

Block Theorem:

$$\zeta_{re}(l_k) = \underbrace{\exp(c \cdot l_k)}_{\text{multiplying factor}} \zeta_{re}^{(0)}$$

$\zeta_{re}^{(0)}$   $\Rightarrow$  Eigen vector of cell centered with origin

\* The Block Theorem states that if we have found the Eigen vector corresponding to the cell centered at origin we can find the Eigen vector corresponding to any other cell of the crystal by multiplying eigen vector of origin by some factor.

\* This theorem is extremely powerful if you succeed in solving for one cell and then thanks to periodicity we can find immediately by multiplication the Eigen vector of any other cell of the crystal.



## Calculation of the Normal Coordinates — VII

Eigen Vectors  
at the origin

- The line of indices  $m\alpha u$  of the eigenvalue equation then reads

$$\sum_{n\beta w} d_{m\alpha u}^{n\beta w} \zeta_{n\beta w} = \omega^2 \zeta_{m\alpha u} \Rightarrow \sum_{n\beta w} A_{m\alpha u}^{n\beta w} \zeta_{\beta w}(0) = \omega^2 \zeta_{m\alpha u}(0),$$

$$A_{m\alpha u}^{n\beta w} \doteq \frac{1}{\sqrt{\mu_\alpha \mu_\beta}} c_{\alpha u}^{\beta w} (\mathbf{l}_m - \mathbf{l}_n) \exp[j \mathbf{q} \bullet (\mathbf{l}_n - \mathbf{l}_m)].$$

- As the eigenvalues  $\omega^2$  are real, the matrix made of the entries  $A_{m\alpha u}^{n\beta w}$  must be Hermitian, as is easily found by remembering that  $\mathbf{D}$  is real and symmetrical:

\*  $A_{n\beta w}^{m\alpha u} = d_{\beta w}^{\alpha u} (\mathbf{l}_n - \mathbf{l}_m) \exp[j \mathbf{q} \bullet (\mathbf{l}_m - \mathbf{l}_n)] = (A_{m\alpha u}^{n\beta w})^*$ .

- Another important observation stems from the expression at the left hand side,  $\sum_{n\beta w} A_{m\alpha u}^{n\beta w} \zeta_{\beta w}(0) = \sum_{\beta w} (\sum_n A_{m\alpha u}^{n\beta w}) \zeta_{\beta w}(0)$ , where  $A_{m\alpha u}^{n\beta w}$  is translationally invariant because it depends on the cell indices only through the difference  $\mathbf{l}_m - \mathbf{l}_n$ . It follows that the sum  $\sum_n A_{m\alpha u}^{n\beta w}$  does not depend on  $m$ . This can easily be verified by performing the sum first with, say,  $m = 1$ , then with  $m = 2$ , and observing that the terms of the second sum are the same as in the first one, but displaced by one position.



## Calculation of the Normal Coordinates — VIII

*object The problem to be solved*

- Letting  $\mathbf{A}$  be the  $3N_b \times 3N_b$  matrix of entries

$$A_{\alpha u}^{\beta w}(\mathbf{q}) \doteq \sum_{n=1}^{N_c} d_{\alpha u}^{\beta w}(\mathbf{l}_m - \mathbf{l}_n) \exp[j\mathbf{q} \bullet (\mathbf{l}_n - \mathbf{l}_m)],$$

which is obviously Hermitean, yields

$$\sum_{\beta w} A_{\alpha u}^{\beta w}(\mathbf{q}) \zeta_{\beta w}(0) = \omega^2 \zeta_{\alpha u}(0).$$

- For a given  $\mathbf{q}$ , the above is an eigenvalue equation of order  $3N_b$ , whose  $3N_b$  eigenvalues are found by solving the algebraic equation

$$\det(\mathbf{A} - \omega^2 \mathbf{I}) = 0.$$

- As the entries of  $\mathbf{A}$  depend on  $\mathbf{q}$ , the calculation of the  $3N_b$  eigenvalues must be repeated for each distinct value of  $\mathbf{q}$ , namely,  $N_c$  times. The total number of eigenvalues thus found is  $3N_b \times N_c = 3N$ , as should be.

- The above result shows that, while the translational invariance eliminates the dependence on  $\mathbf{l}_m$ , it introduces that on  $\mathbf{q}$ . As the number of different determinations of the two vectors is the same, namely,  $N_c$ , the total number of eigenvalues is not affected.



## Calculation of the Normal Coordinates — XIII

- Due to the above considerations, and remembering that

$$\zeta_{\gamma e}^{\alpha u}(\mathbf{l}_m, \mathbf{q}_k) = \exp(j\mathbf{q}_k \bullet \mathbf{l}_m) \zeta_{\gamma e}^{\alpha u}(0, \mathbf{q}_k),$$

one recovers a set of real eigenvectors of the dynamical matrix:

$$\begin{aligned} & \zeta_{\gamma e}^{\alpha u}(\mathbf{l}_m, \mathbf{q}_k) + \zeta_{\gamma e}^{\alpha u}(\mathbf{l}_m, -\mathbf{q}_k) = \\ & = \zeta_{\gamma e}^{\alpha u}(0, \mathbf{q}_k) \exp(j\mathbf{q}_k \bullet \mathbf{l}_m) + \zeta_{\gamma e}^{*\alpha u}(0, \mathbf{q}_k) \exp(-j\mathbf{q}_k \bullet \mathbf{l}_m) \end{aligned}$$

where, as usual, the indices  $k\gamma e$  count the eigenvectors and the indices  $m\alpha u$  count the entries.

- The displacements of the particles from the equilibrium position are given by  $\xi = \mathbf{G}\mathbf{b}$ , where the entries of  $\mathbf{b}$  have the form

$$b_{k\gamma e}(t) = \frac{1}{2} \left\{ \tilde{b}_{k\gamma e 0} \exp[-j\omega_{\gamma e}(\mathbf{q}_k)t] + \tilde{b}_{k\gamma e 0}^* \exp[j\omega_{\gamma e}(\mathbf{q}_k)t] \right\},$$

with  $\tilde{b}_{k\gamma e 0}$  depending on the initial conditions  $b_{k\gamma e 0}(0)$ ,  $\dot{b}_{k\gamma e 0}(0)$ . In turn, the entries of matrix  $\mathbf{G}$  are  $\eta_{k\gamma e}^{m\alpha u}$ , where the lower indices refer to the columns and count the eigenvectors, the upper ones refer to the rows and count the entries of each eigenvector.



## Calculation of the Normal Coordinates — XIV

The quantities  $\eta_{k\gamma e}^{mau}$  equal the corresponding terms of the real eigenvector of the dynamical matrix, divided by  $\sqrt{\mu_\alpha}$ .

Note that once the real eigenvectors  $\eta_{k\gamma e}$  are determined, one must check that they are orthonormal with respect to  $\mathbf{M}$ . In conclusion, from

$$\xi = \mathbf{G}\mathbf{b} \implies \xi_{mau} = \sum_{k\gamma e} \eta_{k\gamma e}^{mau} b_{k\gamma e},$$

the displacements are given by

$$\begin{aligned} \xi_{mau} &= \sum_{k\gamma e} \frac{1}{\sqrt{\mu_\alpha}} \zeta_{k\gamma e}^{mau} b_{k\gamma e} = \frac{1}{\sqrt{\mu_\alpha}} \times \\ &\times \Re \sum_{k\gamma e} \zeta_{k\gamma e}^{\alpha u}(0, \mathbf{q}_k) [\tilde{b}_{k\gamma e 0} \exp(j\Phi_{k\gamma e}^m) + \tilde{b}_{k\gamma e 0}^* \exp(j\Psi_{k\gamma e}^m)], \end{aligned}$$

where the phases are defined by

$$\Phi_{k\gamma e}^m \doteq \mathbf{q}_k \bullet \mathbf{l}_m - \omega_{\gamma e}(\mathbf{q}_k) t, \quad \Psi_{k\gamma e}^m \doteq \mathbf{q}_k \bullet \mathbf{l}_m + \omega_{\gamma e}(\mathbf{q}_k) t.$$

The above result shows that, in the harmonic approximation, the displacements have the form of a superposition of plane and monochromatic waves, with a wave vector  $\mathbf{q}_k$  and an angular frequency  $\omega_{\gamma e}(\mathbf{q}_k)$ .

The relation  $\omega \propto \mathbf{q}_k$  is Non-linear

The problem is solved, showing that the vibrational state of the crystal can be described as a superposition of planar and monochromatic waves



## Calculation of the Normal Coordinates — XV

- The wave corresponding to a given  $\mathbf{q}_k$  is called *vibrational mode*. Typically, the number of  $\mathbf{q}_k$  vectors is so high that they are considered as a continuous variable  $\mathbf{q}$  ranging over the first Brillouin zone.
- The function  $\omega_{\gamma e}(\mathbf{q})$  is also called *dispersion relation*, and is viewed as a multi-valued function of  $\mathbf{q}$  with  $3N_b$  branches.
- For each branch, letting  $q = |\mathbf{q}|$ , the wave length is defined by  $\lambda = 2\pi/q$  and the phase velocity by  $u_f = \omega/q = \lambda\nu$ , with  $\nu = \omega/(2\pi)$  the frequency. The group velocity is given by  $\mathbf{u} = \text{grad}_{\mathbf{q}}\omega$ .
- The total energy of the system is the sum of the mode energies. In turn, the energy quantization shows that each mode energy is made of terms of the form  $\hbar\omega_{\gamma e}(\mathbf{q})$ , this leading to the concept of phonon.
- Note the analogy with the expression of the e.m. as a superposition of modes—which, however, does not require the harmonic approximation, and also the analogy with the dispersion relation  $E(\mathbf{k})$  of the electrons in the crystal—which, however, has infinite branches.

$$\mathbf{q} = \sum_{s=1}^3 \frac{\mathbf{v}_s}{N_s} 2\pi \mathbf{b}_s$$

$\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3$  are the characteristic vectors  
of reciprocal lattice

↑ edge  
Brillouin  
Zone

$\Delta \nu_s$  goes from  $0, 1, \dots, N_s - 1$   
 centred the Brillouin  
 zone

units of  $(q) \Rightarrow \frac{1}{\text{length}}$



One-Dim., Monoatomic Phonon Spectrum — I

- Consider a one-dimensional monatomic lattice made of  $N_c$  cells. Let the lattice be aligned with the  $x$  axis, and the corresponding characteristic vector be  $a = ai$ ,  $a > 0$ , with  $i$  the unit vector of the  $x$  axis. Finally, let the positions of the  $N_c + 1$  nodes be  $0, a, 2a, \dots, na, \dots$ . The translational vector associated to the  $n$ th node is  $l_n = nai$ .
- Due to the periodic boundary conditions the nodes of indices  $n = 0$  and  $n = N_c$  are actually the same node. As a one-dimensional case is considered, with  $N_b = 1$ , the total number of atoms is  $N = N_c$ .
- The number of degrees of freedom of the lattice is  $N_c$ , and the correspondence with the indices used in the general theory is

$m, n = 1, \dots, N_c, \quad \alpha, \beta = 1, \quad u, w = 1.$

As only one atom per cell is present, one may assume that the equilibrium position of each nucleus coincides with that of a node.

→ We remember that the Force is -ve grad of P.E  
 But in Harmonic approximation that we are using  
 the P.E is a Quadratic form in Displacement whose  
 coefficients are the components of an Elastic Matrix.



## One-Dim., Monoatomic Phonon Spectrum — II

- In the harmonic approximation the force acting on the  $r$ th nucleus is a linear function of the displacements:

*Force acting on the Nucleus of Index 'r'*

$$F_r = - \sum_{k=1}^{N_c} c_{rk} \xi_k.$$

*The Force is because of all the other Nuclei*

- In real crystals, the interaction between nuclei becomes rapidly negligible as the distance increases. As a consequence, the dynamics of a nucleus may be tackled in a simplified manner by considering only the interaction with the neighboring nuclei to be effective.

This is equivalent to letting  $c_{rk} = 0$  when  $|r - k| > 1$ , whence

$$F_r = -c_r^{r-1} \xi_{r-1} - c_r^r \xi_r - c_r^{r+1} \xi_{r+1} = F_r(\xi_{r-1}, \xi_r, \xi_{r+1}).$$

*Force because of Atom on the left*

*Force related to central index*

*Force related to Atom on the Right*

$$F_r = -c_r^{r-1} \xi_{r-1} - c_r^r \xi_r - c_r^{r+1} \xi_{r+1} = F_r(\xi_{r-1}, \xi_r, \xi_{r+1}).$$

- When the nuclei of indices  $r - 1, r, r + 1$  are in the equilibrium positions it is obviously  $F_r(0, 0, 0) = 0$ . On the other hand, it is also  $F_r(\delta, \delta, \delta) = 0$ , with  $\delta \neq 0$  an arbitrary displacement. In fact, when all displacements are equal the interatomic distance remains the same as in the equilibrium condition. It follows

$$F_r(\delta, \delta, \delta) = 0 \implies c_r^{r-1} + c_r^r + c_r^{r+1} = 0. \quad \text{--- (1)}$$



## One-Dim., Monoatomic Phonon Spectrum — III

- Moreover, on account of the fact that all atoms are identical and all equilibrium distances are also identical, it is  $F_r(-\delta, 0, \delta) = 0$ ,  $\delta \neq 0$ , whence

$$F_r(-\delta, 0, \delta) = 0 \xrightarrow{\text{from eq-1}} c_r^{r-1} = c_r^{r+1}.$$

*When left atom has  $-\delta$  displacement*

*Right atom has  $+\delta$  displacement*

It follows

$$c_r^r = -c_r^{r-1} - c_r^{r+1} = -2c_r^{r-1} = -2c_r^{r+1}.$$

*Just move the Central Atom + δ*

- Finally, the relation  $F_r(0, \delta, 0) = -c_r^r \delta$  on account of the fact that  $(0, 0, 0)$  is an equilibrium condition, shows that  $c_r^r > 0$ .

If the central atom moves right by  $\delta r$  then force must be to the left to bring it back to equilibrium position  $\therefore C_r^r > 0$

- Due to the lattice periodicity the coefficients should not depend on the index. In conclusion, letting

$$\chi = -c_r^{r-1} = -c_r^{r+1} > 0, \quad c_r^r = 2\chi,$$

and letting  $\mu$  be the common mass of the nuclei, the dynamics of the  $r$ th nucleus is described by the equation

$$\mu \ddot{\xi}_r = -\chi (2\xi_r - \xi_{r+1} - \xi_{r-1})$$

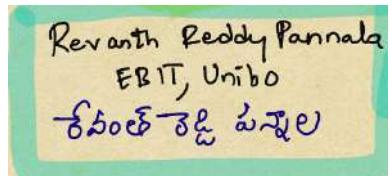
This is the eq<sup>n</sup> that describes the dynamics of any Nuclear Monoatomic chain.

d) How can we solve the above eq<sup>n</sup>?

because it has 3 unknowns  $\xi_r, \xi_{r+1}, \xi_{r-1}$

Ans We already know displacements can be written as a superposition of linear monochromatic waves.

$\therefore \xi_r$  in the form of a Monochromatic wave





*Eqv*

- The general theory shows that the displacement has the form
$$\xi_r = \xi_0 \exp(jqra - j\omega t),$$
where  $\xi_0$  is a complex constant,  $qra = \mathbf{q} \bullet \mathbf{l}_r = q\mathbf{i} \bullet r\mathbf{a}$ , and  $\omega = \omega(q)$ . Replacing the above form in the differential equation and dividing by  $\xi_r$  yields all the time factors are cancelled
$$\begin{aligned} \mu\omega^2 &= \chi [2 - \exp(jqa) - \exp(-jqa)] = \\ &= 2\chi [1 - \cos(qa)] = 4\chi \sin^2(qa/2). \end{aligned}$$
Defining  $\tilde{\omega} = \sqrt{\chi/\mu}$  and remembering that  $\omega$  is non negative, one finds the dispersion relation

$$\dot{\xi}_r = \frac{d^2}{dt^2} \left( \xi_0 \exp(jqra - j\omega t) \right)$$

- Defining  $\tilde{\omega} = \sqrt{\chi/\mu}$  and remembering that  $\omega$  is non negative, one finds the dispersion relation

$$\omega(q) = 2\tilde{\omega} |\sin(qa/2)|$$

- From the periodic boundary condition  $\xi(r = N_c a) = \xi(r = 0)$  one finds, with  $\nu$  an integer,

$$\exp(jqN_c a) = 1 \Rightarrow qN_c a = 2\pi\nu, \quad q = \frac{\nu}{N_c} \frac{2\pi}{a}.$$

- Replacing  $q$  within the expressions of  $\xi_r$  or  $\omega$  one finds that using  $\nu + N_c$  instead of  $\nu$  leaves the result unchanged.

→ we continue with the description of linear Monatomic chain we were considering the Periodic Boundary conditions showing that Thanks to these conditions we have found the

$$\text{vector } \langle q' \rangle = \frac{2\pi}{N_c} \frac{\overrightarrow{a}}{a}$$



## One-Dim., Monoatomic Phonon Spectrum — V

periodicity

- For the above reason, it is sufficient to consider only  $N_c$  consecutive values of  $\nu$ , say  $\nu = 0, 1, \dots, N_c - 1$ , which in turn limit the possible values of  $q$  to an interval of length  $2\pi/a$ .
- One also notices that  $b = 2\pi/a$  is the size of the first Brillouin zone in the one-dimensional case. Typically, the interval of  $q$  is made to coincide with the first Brillouin zone, namely  $-\pi/a \leq q < +\pi/a$ .  
Also, in the practical cases  $q$  is treated as a continuous variable.

The phase velocity is

$$u_f = \frac{\omega}{q} = \pm a\bar{\omega} \frac{\sin(qa/2)}{qa/2}$$

while the group velocity is

$$u = \frac{d\omega}{dq} = \pm a\bar{\omega} \cos(qa/2).$$

• 'q' here is a discrete quantity because it is associated with an Integer index but in general the no. of cells of lattice is so high that we can consider 'q' as continuous so that we can take the Derivatives.



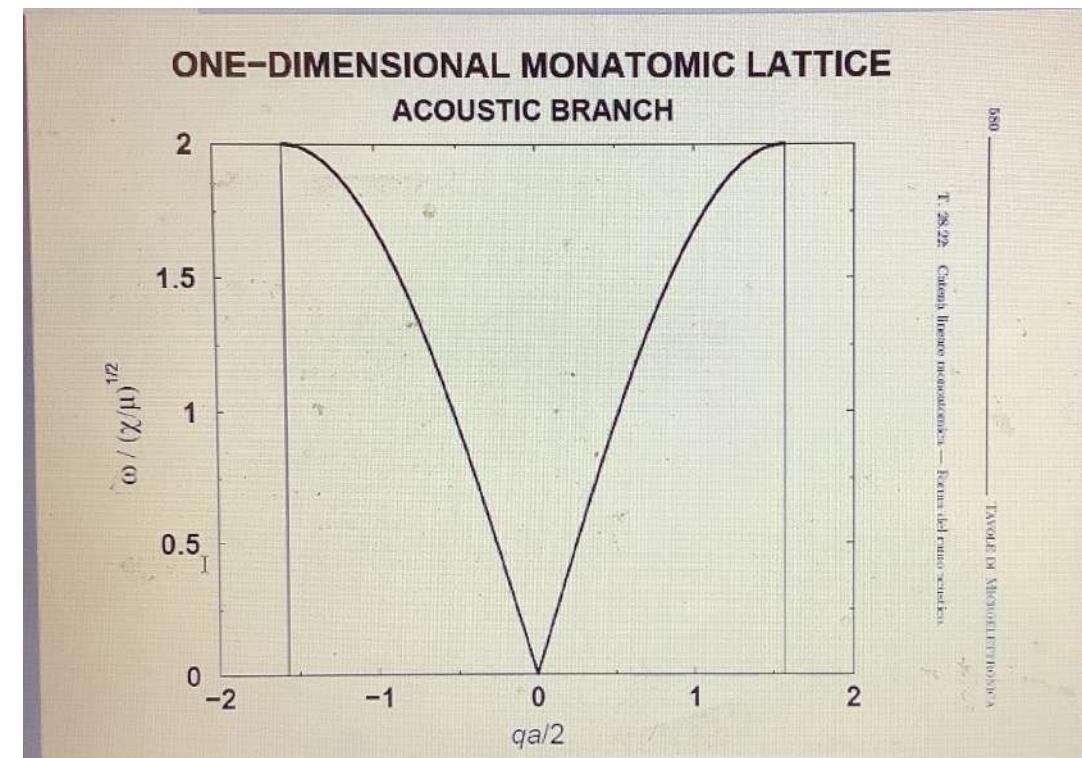
Also, in the practical cases  $q$  is treated as a continuous variable.  
The phase velocity is

$$u_f = \frac{\omega}{q} = \pm a\tilde{\omega} \frac{\sin(qa/2)}{qa/2}$$

while the group velocity is

$$u = \frac{d\omega}{dq} = \pm a\tilde{\omega} \cos(qa/2)$$

where the positive (negative) sign holds when  $q$  is positive (negative). At the boundary of the Brillouin zone it is  $qa/2 = \pi/2$  whence  $\omega = 2\tilde{\omega}$ ,  $u_f = \pm a\tilde{\omega}/\pi$ ,  $u = 0$ . Near the center of the Brillouin zone it is  $\omega = a\tilde{\omega}|q|$ ,  $u_f = u = \pm a\tilde{\omega}$ . At the center it is  $\omega = 0$ .



\* Here essentially we have only one possible Dispersion Relation because we have a One-Dimensional problem and we have only

one atom per cell.

→ In more general case we found there are Branches of Dispersion Relation → These Branches are equal to "3" times  $N_b$  if we are in a 3D case with Basis made of  $N_b$  Atoms.

Q) Why is the Graph of 1D-Monatomic Lattice is called Acoustic Branch?

Ans The Description of Displacements are function of Time essentially provides Description of vibrational modes of the lattice.

- So, it describes How Vibrations propagate inside the Solid!
- Vibrations of low frequency can be perceived by Human Ear as sound

The figure has only one branch and it also crosses zero

\* More complicated than this is a 1D lattice with two atoms/cell and these atoms have different masses and along the chain the atoms alternate.

Obviously the forces in this structure will be a little more complicated



### One-Dim., Diatomic Phonon Spectrum — I

Consider a one-dimensional lattice made of  $N_c$  cells, with a two-atom basis. Let the lattice be aligned with the  $x$  axis, and the corresponding characteristic vector be  $a = ai$ ,  $a > 0$ , with  $i$  the unit vector of the  $x$  axis. Finally, let the positions of the  $N_c + 1$  nodes be  $0, a, 2a, \dots, na, \dots$ . The translational vector associated to the  $n$ th node is  $\mathbf{l}_n = na\mathbf{i}$ .

Due to the periodic boundary conditions the nodes of indices  $n = 0$  and  $n = N_c$  are actually the same node. As a one-dimensional case is considered, with  $N_b = 2$ , the total number of atoms is  $N = 2N_c$ . The number of degrees of freedom of the lattice is  $2N_c$ , and the correspondence with the indices used in the general theory is

$$m, n = 1, \dots, N_c, \quad \alpha, \beta = 1, 2, \quad u, w = 1.$$

As two atoms per cell are present, one may assume that the equilibrium position of one type of nucleus coincides with that of a node. Such nuclei will be given the index  $\alpha, \beta = 1$ . The other nuclei will be given the index  $\alpha, \beta = 2$ .



In this we don't derive the whole eq' but we directly go to the results

Remembering the result  $c_{\text{mou}}^{n\beta w} = c_{n\beta w}^{\text{mou}}$  of the general theory one also finds

$$c_{r,2}^{r,1} = c_{r,1}^{r,2} = -\chi_1, \quad c_{r,2}^{r+1,1} = c_{r+1,1}^{r,2} = c_{r,1}^{r-1,2} = -\chi_2,$$

whence

$$c_{r,1}^{r,1} = c_{r,2}^{r,2} = \chi_1 + \chi_2 > 0.$$

One also notices that, from the relations

$$F_{r,1}(0,0,\delta) = \chi_1 \delta, \quad F_{r,1}(\delta,0,0) = \chi_2 \delta$$

it follows that  $\chi_1 > 0$ ,  $\chi_2 > 0$ , on account of the fact that  $(0,0,0)$  is an equilibrium condition.



Letting  $\mu_1$ ,  $\mu_2$  be the masses of the two types of nuclei, the dynamics of the  $r$ th nuclei is described by the equations

$$\mu_1 \ddot{\xi}_{r,1} = -\chi_1 (\xi_{r,1} - \xi_{r,2}) - \chi_2 (\xi_{r,1} - \xi_{r+1,2}),$$

$$\mu_2 \ddot{\xi}_{r,2} = -\chi_1 (\xi_{r,2} - \xi_{r,1}) - \chi_2 (\xi_{r,2} - \xi_{r+1,1}).$$

- The general theory shows that the displacements have the form  $\xi_r$

$$\xi_{r,1(2)} = \xi_{0,1(2)} \exp(jqra - j\omega t),$$

planar Mono Chirmonic wave

where  $\xi_{0,1}$ ,  $\xi_{0,2}$  are complex constants,  $qra = q \bullet l_r = q i \bullet r a i$ , and  $\omega = \omega(q)$ .

- In this case we have  $2 \times 2$  homogeneous S/S which provides Eigen values as we

expected

Replacing the above forms in the differential equations and dividing by  $\xi_{r,1}$ ,  $\xi_{r,2}$ , respectively, yields

$$\mu_1 \omega^2 \xi_{0,1} = \chi_1 (\xi_{0,1} - \xi_{0,2}) + \chi_2 [\xi_{0,1} - \xi_{0,2} \exp(-jqa)] ,$$

$$\mu_2 \omega^2 \xi_{0,2} = \chi_1 (\xi_{0,2} - \xi_{0,1}) + \chi_2 [\xi_{0,2} - \xi_{0,1} \exp(+jqa)] .$$

Defining  $A_1^1$ ,  $A_1^2$ ,  $A_2^1$ ,  $A_2^2$  such that

$$\mu_1 A_1^1 = \chi_1 + \chi_2 , \quad -\mu_1 A_1^2 = \chi_1 + \chi_2 \exp(-jqa) ,$$

$$\mu_2 A_2^2 = \chi_1 + \chi_2 , \quad -\mu_2 A_2^1 = \chi_1 + \chi_2 \exp(+jqa) ,$$

the homogeneous algebraic system above transforms into

$$(A_1^1 - \omega^2) \xi_{0,1} + A_1^2 \xi_{0,2} = 0 ,$$

$$A_2^1 \xi_{0,1} + (A_2^2 - \omega^2) \xi_{0,2} = 0 .$$

The trace and determinant of the matrix formed by  $A_1^1$ ,  $A_1^2$ ,  $A_2^1$ ,  $A_2^2$  are

$$T = A_1^1 + A_2^2 = \frac{\mu_1 + \mu_2}{\mu_1 \mu_2} (\chi_1 + \chi_2) ,$$

$$D = A_1^1 A_2^2 - A_1^2 A_2^1 = 2 \frac{\chi_1 \chi_2}{\mu_1 \mu_2} [1 - \cos(qa)] .$$



## One-Dim., Diatomic Phonon Spectrum — VII

- The eigenvalues  $\omega^2$  are found by solving

$$i \left( \omega^2 \right)^2 - T\omega^2 + D = 0$$

whose discriminant is

$$\Delta(q) = T^2 - 4D = \left[ \frac{(\chi_1 + \chi_2)(\mu_1 + \mu_2)}{\mu_1 \mu_2} \right]^2 + \\ + 8 \frac{\chi_1 \chi_2}{\mu_1 \mu_2} [\cos(qa) - 1].$$

- Such a discriminant must be non negative because, as shown by the general theory, the eigenvalues  $\omega^2$  are real.
- In fact, the discriminant is non negative. Remembering that  $\chi_1, \chi_2 > 0$  its minimum  $\Delta_m$  occurs for  $q = \pm\pi/2$ . Letting

$$K_\chi \doteq \frac{(\chi_1 - \chi_2)^2}{4\chi_1 \chi_2} \geq 0, \quad K_\mu \doteq \frac{(\mu_1 - \mu_2)^2}{4\mu_1 \mu_2} \geq 0,$$

## One-Dim., Diatomic Phonon Spectrum — VIII

The calculation becomes simpler by taking  $\mu_1 = \mu_2 = \mu$ , to find

$$\Delta(q) = \frac{4}{\mu^2} [\chi_1^2 + \chi_2^2 + 2\chi_1 \chi_2 \cos(qa)],$$

whose minimum is  $\Delta(\pm\pi/a) = 4(\chi_1 - \chi_2)^2/\mu^2 \geq 0$ . In turn, its maximum is  $\Delta(0) = 4(\chi_1 + \chi_2)^2/\mu^2 = T^2$ .

The solution of the algebraic equation provides two branches of the dispersion relation, to be found by taking the square root of

$$\omega^2 = \frac{T}{2} \pm \frac{1}{2} \sqrt{\Delta(q)}.$$

Remembering that  $\Delta(0) = T^2$  one finds that selecting the minus sign provides the branch that crosses the origin. It is called *acoustic branch*.

The resulting expressions can be recast into a simpler form by introducing a parameter

$$\tilde{\omega} = \sqrt{(\chi_1 + \chi_2)/\mu}$$

## One-Dim., Biatomio Phonon Spectrum — IX

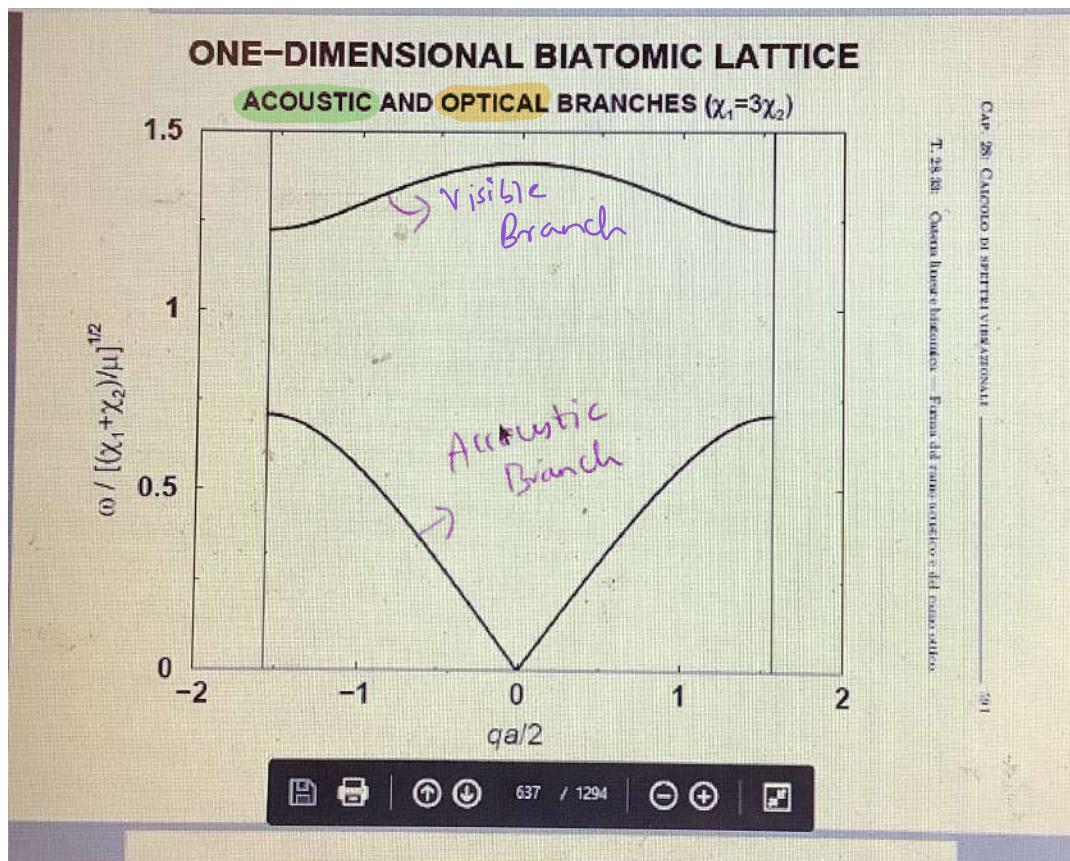
One finds for the acoustic branch

$$\omega_{ac}^2 = \bar{\omega}^2 \left\{ 1 - \left[ 1 - 4 \frac{\chi_1 \chi_2}{(\chi_1 + \chi_2)^2} \sin^2 \left( \frac{qa}{2} \right) \right]^{1/2} \right\}.$$

At the center of the Brillouin zone it is  $\omega_{ac} = 0$ , which is also the minimum. The maximum of  $\omega_{ac}$  is reached at the boundary  $qa/2 = \pm\pi/2$  of the Brillouin zone.

Selecting the plus sign provides a branch that does not cross the origin. It is called *optical branch*. One finds for it

$$\omega_{op}^2 = \bar{\omega}^2 \left\{ 1 + \left[ 1 - 4 \frac{\chi_1 \chi_2}{(\chi_1 + \chi_2)^2} \sin^2 \left( \frac{qa}{2} \right) \right]^{1/2} \right\}.$$



## Properties of the Dispersion Relation — I

The following observations are of interest:

- The eigenvalue  $\omega = 0$  is possible. This apparently contradicts the initial hypothesis that the variation  $V_a - V_{a0}$  in the potential energy of the nuclei is a positive-definite quadratic form. However, the introduction of the periodic boundary conditions at a later stage intrinsically modified the nature of  $V_a - V_{a0}$ , which became a non-negative definite quadratic form. In fact, the periodic boundary conditions allow for a rigid shift of the crystal as a whole, which was instead prohibited when  $V_a - V_{a0}$  was assumed to be positive definite.
- When  $|q|$  is small the dispersion relation  $\omega(q)$  becomes linear, and the group velocity coincides with the phase velocity. This means that a wave packet made of the superposition of low  $|q|$  waves propagates within the crystal without being distorted. Also, a sufficiently small  $|q| = 2\pi/\lambda$  corresponds to a wavelength long enough to have  $\lambda \gg a$ . In this case

it is not necessary to distinguish the

individual atoms within the cell because it is like the cell moves like a unique block inside the crystal which corresponds to the wavelength <sup>that is</sup> much larger than the cell

In this case one can consider the whole crystal as a continuous entity without

Distinguishing anymore among the Atoms.  
In This case one can Apply the Rules  
of Elasticity of Macroscopic Bodies

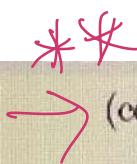


Properties of the Dispersion Relation — II

(cont.)

- The frequency corresponding to  $\omega$  is  $\nu = \bar{\omega}a/\lambda \ll \bar{\omega}$ . In such a condition, the atomic nature of the crystal has little importance for the dynamics of the displacements. The crystal, in fact, may be considered as a continuous medium. Such a situation is typical of the propagation of the sound waves in a solid. For this reason, the branch of the dispersion relation  $\omega(q)$  such that  $\omega(0) = 0$  is called *acoustic branch*.
- There are as many acoustic branches as the dimensions of the domain in the real space. As a consequence, in a general three-dimensional case with  $3N$  degrees of freedom there are  $3$  acoustic branches and  $3N - 3$  non-acoustic branches. The latter are called *optical branches* because, in the ionic crystals, the low- $|q|$  waves of such branches can interact with the electro-

Majority of Branches are Optical and  
only Three Branches are Acoustic  
and in the ionic crystals The Branches  
of optical type can interact with EMF in  
the visible range and for this reason they  
are responsible for the optical properties  
of the crystal.



→ (cont.)

- The motion of the nuclei in the case of the acoustic branches is such, that the nuclei of each elementary cell move as a single block. In contrast, in the case of the optical branches the nuclei belonging to the same elementary cell have also a motion relative to each other.
- As should be expected, the above calculation of  $\omega(q)$  does not provide any information about the complex constants  $\xi_0, \xi_{0,1}, \xi_{0,2}, \dots$ , whose values are to be found at a later stage by determining the eigenvectors of the algebraic system.
- If the hypothesis that a nucleus interacts only with its neighboring nuclei is dropped, one finds that the form of  $\omega(q)$  becomes more complicated, but the essential results shown here still hold.



## General Properties of the Coefficients — I

of elastic matrix

- Consider the expansion of the potential energy of a crystal, truncated to the second order:

$$V_a \simeq V_{a0} + \frac{1}{2} \sum_{m,n=1}^{N_c} \sum_{\alpha,\beta=1}^{N_b} \sum_{u,w=1}^3 c_{mau}^{n\beta w} \xi_{mau} \xi_{n\beta w},$$

where  $N_c$  is the number of cells of the crystal and  $N_b$  the number of atoms of the basis. The symbol  $\xi_{mau}$  indicates the component of the displacement, with respect to the equilibrium position, of the  $\alpha$ th nucleus of the  $m$ th cell along the  $u$ th coordinate axis.

The  $u$ th component of the force acting on the  $\alpha$ th nucleus of the  $m$ th cell is

$$F_{mau} = -\frac{\partial V_a}{\partial \xi_{mau}} = - \sum_{n=1}^{N_c} \sum_{\beta=1}^{N_b} \sum_{w=1}^3 c_{mau}^{n\beta w} \xi_{n\beta w}.$$

(I)

$$F_{m\alpha u} = -\frac{\partial V_a}{\partial \xi_{m\alpha u}} = -\sum_{n=1}^{N_e} \sum_{\beta=1}^{N_b} \sum_{w=1}^3 c_{m\alpha u}^{n\beta w} \xi_{n\beta w}.$$

**Translational invariance:** If all nuclei are in the equilibrium positions it is  $F_{m\alpha u} = 0$ . If, starting from this condition, the crystal is rigidly displaced by a small amount of components  $\delta_1, \delta_2, \delta_3$ , the interatomic distances are left unchanged and it is still  $F_{m\alpha u} = 0$ .

(II)

**Rotational invariance.** To treat the case of the rotation it is useful to remind the definition of the displacements,

$$\xi_{n\beta w} = s_{n\beta w} - s_{n\beta w}^{(0)},$$

where  $s_{n\beta w}^{(0)}$  are the equilibrium positions of the nuclei. If all nuclei are in the equilibrium positions it is  $F_{m\alpha u} = 0$ . If, starting from this condition, the crystal is rigidly rotated by a small amount around a fixed axis, the interatomic distances are left unchanged and it is still  $F_{m\alpha u} = 0$ .

(III)

**Coordinate-inversion invariance.** If the direction of each coordinate axis is inverted, namely,  $x_1 \leftarrow -x_1, x_2 \leftarrow -x_2, x_3 \leftarrow -x_3$ , all components of the displacements and of the forces change sign. As this happens for any value of the displacements, the coefficients

$$c_{m\alpha u}^{n\beta w} = c_{\alpha u}^{\beta w} (l_m - l_n)$$

are invariant for coordinate inversion.



## 2.11 Dynamics of the Nuclei at Large Wavelengths

This section is concerned with the vibrational modes whose wavelength is much larger than the diameter of the elementary cell of the direct lattice. As shown in Sect. 2.9, in the acoustic branches the group velocity coincides with the phase velocity when  $q$  is small; this means that a wave packet made of the superposition of low- $q$  waves propagates within the crystal without being distorted. Also, remembering that  $q = 2\pi/\lambda$ , a small value of  $q$  corresponds to a long wavelength; in such a condition, the atomic nature of the crystal has little importance for the dynamics of the displacements: the crystal, in fact, may be considered as a continuous medium. Such a situation is typical of the propagation of the sound waves in a solid: the motion of the nuclei in the case of acoustic branches is such, that the nuclei of each elementary cell move as a single block.<sup>15</sup> This makes it possible to simplify the description of the dynamics of the nuclei: the starting point is the general expression (2.73) of the force, whence the dynamics of each component  $u$  of the  $\alpha$ th nucleus of the  $m$ th cell is given by

$$\mu_\alpha \ddot{h}_{m\alpha u} = - \sum_{n=1}^{N_c} \sum_{\beta=1}^{N_b} \sum_{w=1}^3 c_m^{n\beta w} h_{n\beta w}. \quad (2.88)$$

For an acoustic mode, the nuclei of each cell move as a single block, whence one may let *we can use only one symbol for Displacement*

$$\psi_{mu} = h_{m1u} = h_{m2u} = \dots, \quad \psi_{nw} = h_{n1w} = h_{n2w} = \dots \quad (2.89)$$

Adding up over  $\alpha$  both sides of (2.89) yields

$$\sum_{\alpha=1}^{N_b} \mu_\alpha \ddot{h}_{m\alpha u} = M \ddot{\psi}_{mu} = - \sum_{n=1}^{N_c} \sum_{\alpha,\beta=1}^{N_b} \sum_{w=1}^3 c_m^{n\beta w} \psi_{nw} = - \sum_{n=1}^{N_c} \sum_{w=1}^3 Q_{mu}^{nw} \psi_{nw}, \quad (2.90)$$

with

$$M = \sum_{\alpha=1}^{N_b} \mu_\alpha, \quad Q_{mu}^{nw} = \sum_{\alpha,\beta=1}^{N_b} c_m^{n\beta w}, \quad (2.91)$$

$M$  being the total mass of each cell: in other terms, the lattice is treated as if it were monatomic. Since the elastic matrix  $\mathbf{C}$ , whose entries are  $c_m^{n\beta w}$ , is positive definite (Sect. 2.2), then the matrix of entries  $Q_{mu}^{nw}$  defined in (2.91) is positive definite as well (Prob. 2.6). Note that due to the coordinate-inversion invariance it is

$$Q_{nu}^{nw} = Q_{mu}^{nw}, \quad Q_{nu}^{0w} = Q_{0u}^{nw}, \quad Q_u^w(-\mathbf{l}_n) = Q_u^w(\mathbf{l}_n). \quad (2.92)$$

In the above it is  $\psi_{mu} = \psi_u(\mathbf{l}_m)$ ,  $\psi_{nw} = \psi_w(\mathbf{l}_n)$ . When the long-wavelength modes are considered, the crystal may be treated as a continuous medium; for this reason,

<sup>15</sup> In contrast, in the case of optical branches the nuclei belonging to the same elementary cell have also a motion relative to each other.

the translational vectors  $\mathbf{l}_m$ ,  $\mathbf{l}_n$  are replaced when necessary with the continuous position variable  $\mathbf{r}$ . In the same order of approximation, one may assume that the displacement at the  $m$ th or  $n$ th cell varies little with respect to that in the origin: this allows one to expand  $\psi_w(\mathbf{l}_n)$  around  $\mathbf{l}_0 = 0$  at the right hand side of (2.90); truncating the expansion to second order yields

$$\psi_w(\mathbf{l}_n) \simeq \psi_w(0) + \sum_{i=1}^3 \left( \frac{\partial \psi_w}{\partial x_i} \right)_0 l_{ni} + \frac{1}{2} \sum_{i,j=1}^3 \left( \frac{\partial^2 \psi_w}{\partial x_i \partial x_j} \right)_0 l_{ni} l_{nj}, \quad (2.93)$$

so that (2.90) becomes

$$M \ddot{\psi}_u(\mathbf{l}_m) = - \sum_{n=1}^{N_c} \sum_{w=1}^3 Q_{mu}^{nw} \left[ \psi_w(0) + \sum_{i=1}^3 (\dots) l_{ni} + \frac{1}{2} \sum_{i,j=1}^3 (\dots) l_{ni} l_{nj} \right], \quad (2.94)$$

where the dots stand for the coefficients of (2.93). The right hand side of (2.94) simplifies greatly thanks to some of the invariance properties demonstrated in Sect. 2.10. The first term at the right hand side vanishes due to translational invariance (2.77):

$$\sum_{n=1}^{N_c} \sum_{w=1}^3 Q_{mu}^{nw} \psi_w(0) = \sum_{\alpha=1}^{N_b} \sum_{w=1}^3 \left( \sum_{n=1}^{N_c} \sum_{\beta=1}^{N_b} c_m^n \beta_w^\alpha \right) \psi_w(0) = 0. \quad (2.95)$$

As for the second term at the right hand side of (2.94) one finds

$$\sum_{n=1}^{N_c} \sum_{w=1}^3 Q_{mu}^{nw} \sum_{i=1}^3 \left( \frac{\partial \psi_w}{\partial x_i} \right)_0 l_{ni} = \sum_{w,i=1}^3 \left( \frac{\partial \psi_w}{\partial x_i} \right)_0 \sum_{n=1}^{N_c} Q_{mu}^{nw} l_{ni}, \quad (2.96)$$

where one may replace index  $m$  with 0 by choosing the  $m$ th node as the coordinate origin. In addition, due to the crystal periodicity one may also make the coordinate origin to coincide with the center of the crystal. As a consequence, the sum over  $n$  in (2.96) splits into terms of the form

$$Q_u^w(\mathbf{l}_n) l_{ni} + Q_u^w(-\mathbf{l}_n) (-l_{ni}) = 0, \quad (2.97)$$

whose vanishing is due to the coordinate-inversion invariance (2.92). In conclusion, the dynamical relation (2.94) reduces to

$$M \ddot{\psi}_u(\mathbf{l}_m) = - \sum_{n=1}^{N_c} \sum_{w=1}^3 Q_{0u}^{nw} \frac{1}{2} \sum_{i,j=1}^3 \left( \frac{\partial^2 \psi_w}{\partial x_i \partial x_j} \right)_0 l_{ni} l_{nj}. \quad (2.98)$$

Revanth Reddy Pannala  
EBIT, Unibo  
టెక్నాలజీస్ ఎస్ఎల్

