6.730 Physics for Solid State Applications

Lecture 9: Lattice Waves in 1D with Diatomic Basis

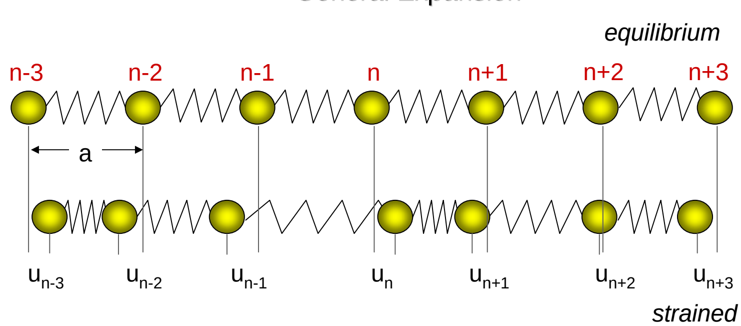
Outline

- Review Lecture 8
- 1-D Lattice with Basis
- Example of Nearest Neighbor Coupling
- Optical and Acoustic Phonon Branches

February 23, 2004

Strain in a Discrete 1-D Monatomic Lattice

General Expansion



$$F[n,t] = -\left(\frac{\partial V}{\partial u[n,t]}\right)_{eq} = 0$$

$$V(\{u[i,t]\}) = V_o + \sum_{m=-\infty}^{\infty} \left(\frac{\partial V}{\partial u[m,t]}\right)_{\text{eq}} u[m,t]$$

$$+\frac{1}{2} \sum_{n=-\infty}^{\infty} \sum_{m=-\infty}^{\infty} u[n,t] \left(\frac{\partial^2 V}{\partial u[n,t]\, \partial u[m,t]}\right)_{\text{eq}} u[m,t] + \cdots$$

Equations of Motion for Lattice Atoms

$$V(\{u[i,t]\}) = V_o + \frac{1}{2}\sum_{n=-\infty}^{\infty}\sum_{m=-\infty}^{\infty} u[n,t]\left(\frac{\partial^2 V}{\partial u[n,t]\,\partial u[m,t]}\right)_{\text{eq}} u[m,t] + \cdots$$

Harmonic Matrix: $\widetilde{D}(n,m) = \left(\frac{\partial^2 V}{\partial u[n,t]\,\partial u[m,t]}\right)_{\text{eq}}$

$$V(\{u[i,t]\}) = V_o + \frac{1}{2}\sum_{n=-\infty}^{\infty}\sum_{m=-\infty}^{\infty} u[n,t]\widetilde{D}(n,m)u[m,t]$$

Force on the j^{th} atom (away from equilibrium)...

$$M\frac{d^2}{dt^2}u[j] = -\frac{\partial}{\partial u[j]}V(\{u[i]\}) = -\sum_{m=-\infty}^{\infty}\widetilde{D}(j,m)u[m]$$

Solutions of Equations of Motion

$$M\frac{d^2}{dt^2}u[n,t] = -\sum_{m=-\infty}^{\infty}\widetilde{D}(n,m)u[m,t]$$

Assuming time-harmonic solutions, converts into coupled difference equations:

$$M\omega^2\tilde{U}[n] = \sum_{m=-\infty}^{\infty}\widetilde{D}(n,m)\tilde{U}[m]$$

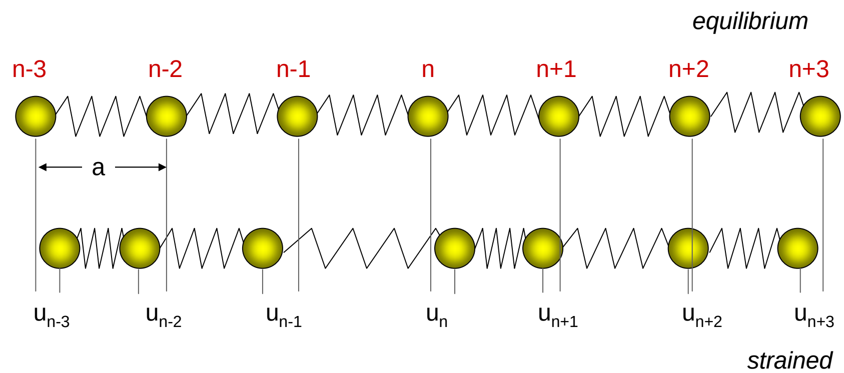
$$M\omega^2 = \sum_{m=-\infty}^{\infty}\widetilde{D}(n,m)e^{ika(m-n)}$$

$$= \underbrace{\sum_{p=-\infty}^{\infty}\widetilde{D}(p)e^{-ikap}}_{\text{Dynamical Matrix } D(k)}$$

$$\boxed{\omega = \sqrt{\frac{D(k)}{M}}}$$

Strain in a Discrete Lattice

Example of Nearest Neighbor Interactions



$$V = \sum_{p=-\infty}^{\infty} \frac{\alpha}{2} (u[p+1] - u[p])^2$$

Strain in a Discrete Lattice

Example of Nearest Neighbor Interactions

$$V = \sum_{p=-\infty}^{\infty} \frac{\alpha}{2} (u[p+1] - u[p])^2$$

$$\widetilde{D}(n,m) = \left(\frac{\partial^2 V}{\partial u[n,t]\, \partial u[m,t]} \right)_{\text{eq}} = \widetilde{D}(n-m)$$

$$= \frac{\partial}{\partial u[n,t]} \alpha \left(u[m] - u[m-1] - u[m+1] + u[m] \right)$$

$$\widetilde{D}(0) = 2\alpha \qquad \text{and} \qquad \widetilde{D}(\pm 1) = -\alpha$$

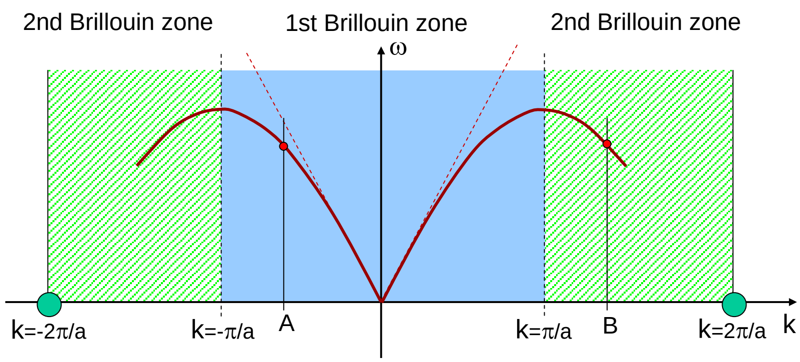
$$D(k) = \sum_{p=-\infty}^{\infty} \widetilde{D}(p) e^{-ikap}$$

$$D(k) = 2\alpha - \alpha e^{-ika} - \alpha e^{ika} = 2\alpha(1 - \cos ka) = 4\alpha \sin^2 (\frac{ka}{2})$$

Strain in a Discrete Lattice

Example of Nearest Neighbor Interactions

$$M\omega^2 = D(k) = 4\alpha \sin^2\left(\frac{ka}{2}\right) \Rightarrow \omega = 2\sqrt{\frac{\alpha}{M}}\left|\sin\left(\frac{ka}{2}\right)\right|$$

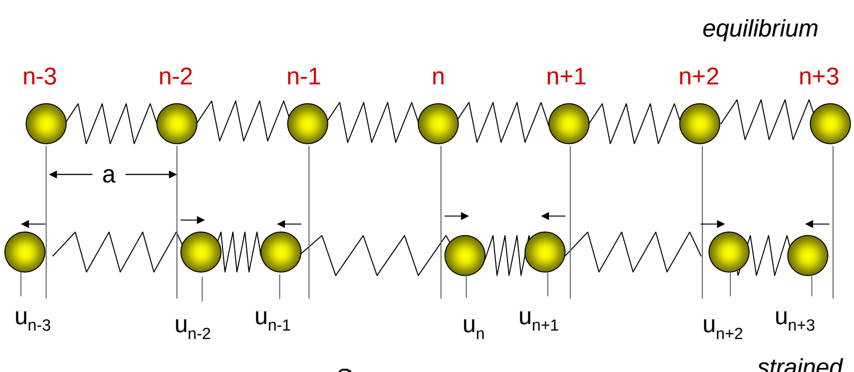


From what we know about Brillouin zones the points A and B (related by a reciprocal lattice vector) must be identical

$$\omega(k) = \omega(k + n2\pi/a)$$

ω_{max}

ω at the Brillouin Zone Edge k =π/a



$$M\frac{d^2}{dt^2}u_n = \alpha\, 4\, u_n$$

Therefore,

$$\omega(k = \pi/a) = \sqrt{\frac{4\alpha}{M}}$$

Summary of Phonon Dispersion Calculation

- Taylor series expansion for total potential stored in all bonds
  - Neglect first order since in equilibrium F=0
  - Truncate expansion at second order, assume small amplitudes
- Determine harmonic matrix from potential energy
  - Represents bond stiffness

$$\widetilde{D}(n,m) = \left(\frac{\partial^2 V}{\partial u[n,t]\,\partial u[m,t]}\right)_{\text{eq}}$$

- Assume time harmonic and discrete ‘plane wave’ solutions
- Determine dynamical matrix from harmonic matrix plus phase progression

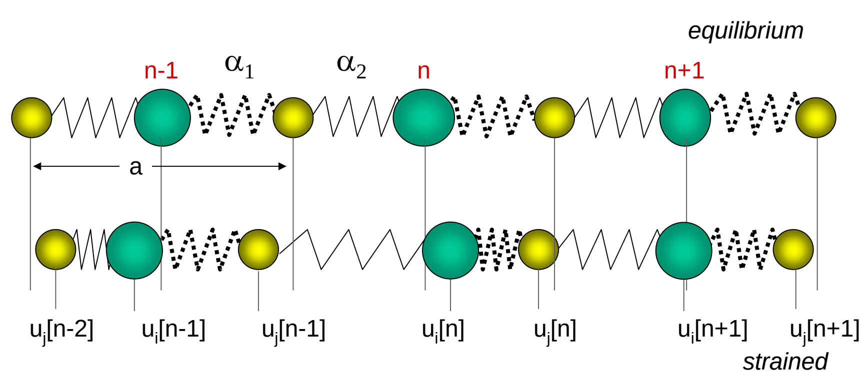
$$D(k) = \sum_{p=-\infty}^{\infty} \widetilde{D}(p) e^{-ikap}$$

- Determine dispersion relation

$$\omega = \sqrt{\frac{D(k)}{M}}$$

Strain in a Discrete Lattice with Basis

Example of Nearest Neighbor Interactions



$$V(\{u[s,t]\}) = V_o + \sum_{i=1}^{2} \sum_{m=-\infty}^{\infty} \left(\frac{\partial V}{\partial u_i[m,t]}\right)_{\text{eq}} u_i[m,t]$$

$$+\frac{1}{2} \sum_{i=1}^{2} \sum_{j=1}^{2} \sum_{p=-\infty}^{\infty} \sum_{m=-\infty}^{\infty} u_i[p,t] \left(\frac{\partial^2 V}{\partial u_i[p,t]\,\partial u_j[m,t]}\right)_{\text{eq}} u_j[m,t] + \cdots$$

Harmonic Matrix for 1-D Lattice with Basis

$$V(\{u[s,t]\}) = V_o + \frac{1}{2}\sum_{i=1}^{2}\sum_{j=1}^{2}\sum_{p=-\infty}^{\infty}\sum_{m=-\infty}^{\infty} u_i[p,t]\left(\frac{\partial^2 V}{\partial u_i[p,t]\,\partial u_j[m,t]}\right)_{\text{eq}} u_j[m,t]$$

$$\widetilde{\mathbf{D}}_{i,j}(p,m) = \left(\frac{\partial^2 V}{\partial u_i[p,t]\,\partial u_j[m,t]}\right)_{\text{eq}}$$

$$V(\{u[s,t]\}) = V_o + \frac{1}{2}\sum_{i=1}^{2}\sum_{j=1}^{2}\sum_{p=-\infty}^{\infty}\sum_{m=-\infty}^{\infty} u_i[p,t]\,\widetilde{\mathbf{D}}_{i,j}(p,m)\,u_j[m,t]$$

Equations of Motion

$$V(\{u[s,t]\}) = V_o + \frac{1}{2}\sum_{i=1}^{2}\sum_{j=1}^{2}\sum_{p=-\infty}^{\infty}\sum_{m=-\infty}^{\infty} u_i[p,t]\,\widetilde{\mathbf{D}}_{i,j}(p,m)\,u_j[m,t]$$

The force on the ℓ^{th} basis atom in the n^{th} unit cell...

$$F_\ell[n,t] = -\frac{\partial V}{\partial u_\ell[n,t]}$$

$$M_\ell \frac{d^2}{dt^2} u_\ell[n] = -\frac{\partial}{\partial u_\ell[n]} V(\{u_i[s]\})$$

$$M_i \frac{d^2}{dt^2} u_i[n] = -\sum_{j=1}^{2}\sum_{m=-\infty}^{\infty} \widetilde{\mathbf{D}}_{i,j}(n,m)\,u_j[m]$$

$$\tilde{u}_i[n,t] = U_i[n,\omega]e^{-i\omega t}$$

Matrix Representation of Equations of Motion

$$M_i\omega^2 U_i[n] = \sum_{j=1}^{2}\sum_{m=-\infty}^{\infty} \widetilde{\mathrm{D}}_{i,j}(n,m)U_j[m]$$

Can collect system of equations for each atom in the basis as a matrix...

$$\mathbf{U}[\mathbf{n}] = \begin{pmatrix} U_1[n] \\ U_2[n] \end{pmatrix} \qquad \mathbf{M} = \begin{pmatrix} M_1 & 0 \\ 0 & M_2 \end{pmatrix}$$

$$\omega^2\mathbf{M}\mathbf{U}[\mathbf{n}] = \sum_{\mathbf{m}=-\infty}^{\infty} \widetilde{\mathbf{D}}(\mathbf{n},\mathbf{m})\mathbf{U}[\mathbf{m}]$$

Plane Wave Solutions & the Dynamical Matrix

$$\mathbf{U}[\mathbf{n}+1] = \mathbf{e}^{\mathbf{ika}}\mathbf{U}[\mathbf{n}]$$

$$\mathbf{U}[\mathbf{n}] = \mathbf{e}^{\mathbf{ikna}}\mathbf{U}[0] = \mathbf{e}^{\mathbf{ikna}}\tilde{\epsilon}$$

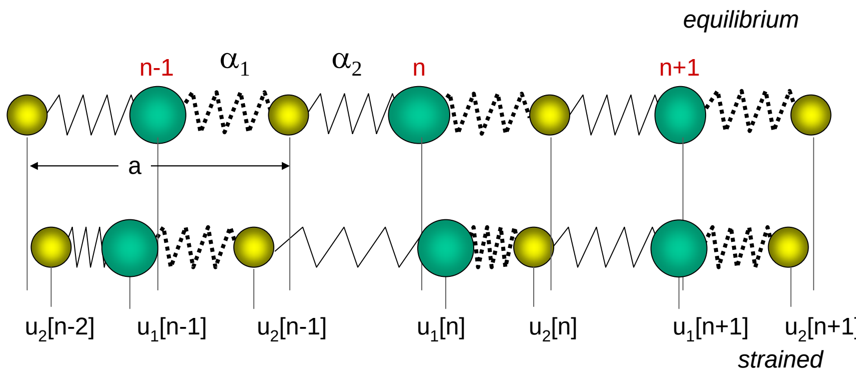
$$\omega^2\mathbf{M}\tilde{\epsilon} = \mathbf{D}(\mathbf{k})\tilde{\epsilon}$$

$$\mathbf{D}(\mathbf{k}) = \sum_{\mathbf{m}=-\infty}^{\infty} \widetilde{\mathbf{D}}(\mathbf{n}-\mathbf{m})\mathbf{e}^{\mathbf{ika}(\mathbf{m}-\mathbf{n})} = \sum_{\mathbf{p}=-\infty}^{\infty} \widetilde{\mathbf{D}}(\mathbf{p})\mathbf{e}^{-\mathbf{ikpa}}$$

$$\left(\mathbf{M}^{-1}\mathbf{D}(\mathbf{k})\right)\vec{\epsilon} = \omega^2\vec{\epsilon}$$

Strain in a Discrete Lattice

Example of Nearest Neighbor Interactions



$$V = \cdots + \frac{\alpha_1}{2}(u_1[s] - u_2[s])^2 + \frac{\alpha_2}{2}(u_1[s] - u_2[s-1])^2$$

$$+ \frac{\alpha_2}{2}(u_1[s+1] - u_2[s])^2 + \ldots$$

Dynamical Matrix for 1-D Lattice with Basis

Example of Nearest Neighbor Coupling

$$V = \cdots + \frac{\alpha_1}{2}(u_1[s] - u_2[s])^2 + \frac{\alpha_2}{2}(u_1[s] - u_2[s-1])^2$$

$$+ \frac{\alpha_2}{2}(u_1[s+1] - u_2[s])^2 + \ldots$$

$$\mathbf{D_{i,j}(k)} = \sum_{\mathbf{R_p}} \left(\frac{\partial^2 \mathbf{V}}{\partial \mathbf{u_i}[\mathbf{R_s} + \mathbf{R_p}, \mathbf{t}]\, \partial \mathbf{u_j}[\mathbf{R_s}, \mathbf{t}]} \right)_{eq} \mathbf{e^{-ik \cdot R_p}}$$

$$\mathbf{D(k)} = \begin{array}{c} \\ u_1 \\ u_2 \end{array} \begin{array}{c} \begin{array}{cc} u_1 & u_2 \end{array} \\ \begin{pmatrix} \alpha_1 + \alpha_2 & -\alpha_1 - \alpha_2 e^{-ika} \\ -\alpha_1 - \alpha_2 e^{ika} & \alpha_1 + \alpha_2 \end{pmatrix} \end{array}$$

Dispersion Relation for 1-D Lattice with Basis

Example of Nearest Neighbor Coupling

$$\left(\mathbf{M}^{-1}\mathbf{D}(\mathbf{k})\right)\vec{\epsilon} = \omega^2\vec{\epsilon}$$

$$\mathbf{M}^{-1} = \begin{pmatrix} \frac{1}{M_1} & 0 \\ 0 & \frac{1}{M_2} \end{pmatrix} \qquad \mathbf{D}(\mathbf{k}) = \begin{pmatrix} \alpha_1+\alpha_2 & -\alpha_1-\alpha_2 e^{-ika} \\ -\alpha_1-\alpha_2 e^{ika} & \alpha_1+\alpha_2 \end{pmatrix}$$

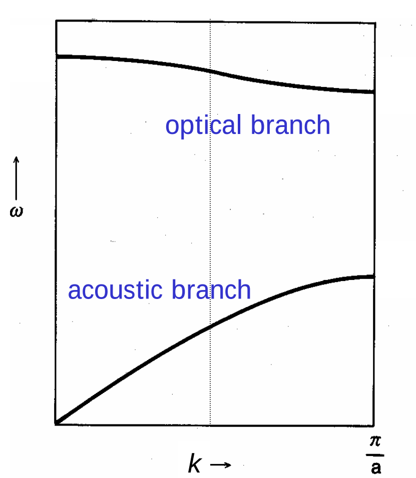
$$\begin{pmatrix} \frac{\alpha_1+\alpha_2}{M_1} & -\frac{\alpha_1+\alpha_2 e^{-ika}}{M_1} \\ -\frac{\alpha_1+\alpha_2 e^{ika}}{M_2} & \frac{\alpha_1+\alpha_2}{M_2} \end{pmatrix} \begin{pmatrix} \epsilon_1 \\ \epsilon_2 \end{pmatrix} = \omega^2 \begin{pmatrix} \epsilon_1 \\ \epsilon_2 \end{pmatrix}$$

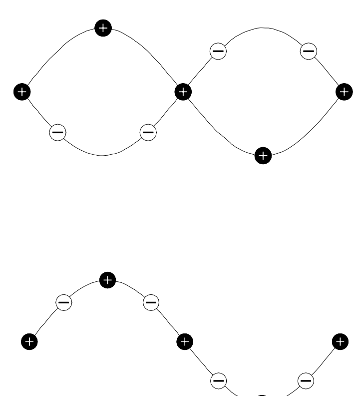
$$\omega^2 = \frac{\alpha_1+\alpha_2}{2}\left(\frac{1}{M_1}+\frac{1}{M_2}\right) \pm \left\{ \frac{(\alpha_1+\alpha_2)^2\left(\frac{1}{M_1}+\frac{1}{M_2}\right)^2}{4} - \frac{2\alpha_1\alpha_2(1-\cos ka)}{M_1 M_2} \right\}^{1/2}$$

Dispersion Relation for 1-D Lattice with Basis

Example of Nearest Neighbor Coupling

$$\omega^2 = \frac{\alpha_1+\alpha_2}{2}\left(\frac{1}{M_1}+\frac{1}{M_2}\right) \pm \left\{ \frac{(\alpha_1+\alpha_2)^2\left(\frac{1}{M_1}+\frac{1}{M_2}\right)^2}{4} - \frac{2\alpha_1\alpha_2(1-\cos ka)}{M_1 M_2} \right\}^{1/2}$$





Lattice Waves at k=0

Example of Nearest Neighbor Coupling

$$\begin{pmatrix} \dfrac{\alpha_1+\alpha_2}{M_1} & -\dfrac{\alpha_1+\alpha_2}{M_1} \\ -\dfrac{\alpha_1+\alpha_2}{M_2} & \dfrac{\alpha_1+\alpha_2}{M_2} \end{pmatrix} \begin{pmatrix} \epsilon_1(0) \\ \epsilon_2(0) \end{pmatrix} = \omega_\sigma^2 \begin{pmatrix} \epsilon_1(0) \\ \epsilon_2(0) \end{pmatrix}$$

$$\omega_1 = 0 \qquad \omega_2 = \sqrt{(\alpha_1+\alpha_2)\left(\frac{1}{M_1}+\frac{1}{M_2}\right)}$$

$$\begin{pmatrix} \epsilon_1^{(1)}(0) \\ \epsilon_2^{(1)}(0) \end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix} \qquad \begin{pmatrix} \epsilon_1^{(2)}(0) \\ \epsilon_2^{(2)}(0) \end{pmatrix} = \frac{1}{\sqrt{1+(M_2/M_1)^2}}\begin{pmatrix} M_2/M_1 \\ -1 \end{pmatrix}$$

Lattice Waves at Small k

Example of Nearest Neighbor Coupling

$$\omega_1 = \left(\frac{\alpha_1\alpha_2 a^2}{(\alpha_1+\alpha_2)(M_1+M_2)}\right)^{1/2} k \qquad \omega_2 \approx \sqrt{(\alpha_1+\alpha_2)\left(\frac{1}{M_1}+\frac{1}{M_2}\right)}$$

$$c_s = \left(\frac{\alpha_1\alpha_2}{(\alpha_1+\alpha_2)(M_1+M_2)}\right)^{1/2}$$

$$\begin{pmatrix} \epsilon_1^{(1)}(0) \\ \epsilon_2^{(1)}(0) \end{pmatrix} \approx \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix} \quad \text{for} \quad \omega_1 \approx c_s k$$

$$U_1[n+1] = e^{ika}U_1[n] \qquad U_2[n+1] = e^{ika}U_2[n]$$

Lattice Waves Near Zone Boundary

Example of Nearest Neighbor Coupling with M_1=M_2

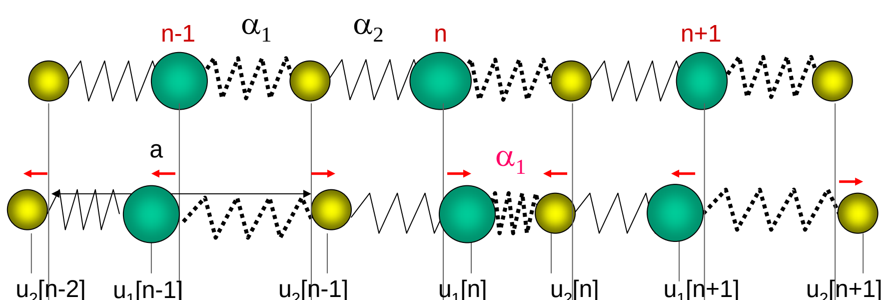
$$\begin{pmatrix} \frac{\alpha_1+\alpha_2}{M} & \frac{\alpha_2-\alpha_1}{M} \\ \frac{\alpha_2-\alpha_1}{M} & \frac{\alpha_1+\alpha_2}{M} \end{pmatrix} \begin{pmatrix} \epsilon_1^{(i)}(\frac{\pi}{a}) \\ \epsilon_2^{(i)}(\frac{\pi}{a}) \end{pmatrix} = \omega_i^2 \begin{pmatrix} \epsilon_1^{(i)}(\frac{\pi}{a}) \\ \epsilon_2^{(i)}(\frac{\pi}{a}) \end{pmatrix}$$

$$\omega_1 = \sqrt{\frac{2\alpha_1}{M}} \quad \text{and} \quad \omega_2 = \sqrt{\frac{2\alpha_2}{M}}$$

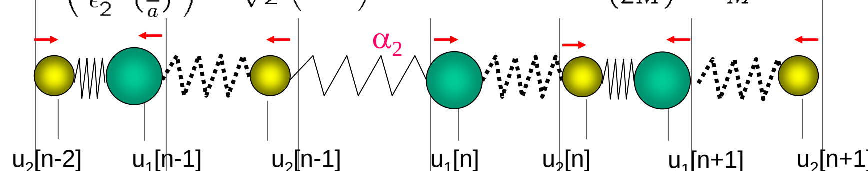
$$\begin{pmatrix} \epsilon_1^{(1)}(\frac{\pi}{a}) \\ \epsilon_2^{(1)}(\frac{\pi}{a}) \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix} \quad \text{for} \quad \omega_1^2 = \frac{2\alpha_1}{M}$$

$$\begin{pmatrix} \epsilon_1^{(2)}(\frac{\pi}{a}) \\ \epsilon_2^{(2)}(\frac{\pi}{a}) \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \quad \text{for} \quad \omega_1^2 = \frac{2\alpha_2}{M}$$

At the Brillion Zone Edge k = π/a



$$\begin{pmatrix} \epsilon_1^{(1)}(\frac{\pi}{a}) \\ \epsilon_2^{(1)}(\frac{\pi}{a}) \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix} \quad \text{for} \quad \omega_1^2 = \frac{4\alpha_1}{(2M)} = \frac{2\alpha_1}{M}$$



$$\begin{pmatrix} \epsilon_1^{(1)}(\frac{\pi}{a}) \\ \epsilon_2^{(1)}(\frac{\pi}{a}) \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \quad \text{for} \quad \omega_1^2 = \frac{4\alpha_2}{(2M)} = \frac{2\alpha_2}{M}$$

Dispersion Relation for 3-D Lattices