6.730 Physics for Solid State Applications

Lecture 8: Lattice Waves in 1D Monatomic Crystals

Outline

- Overview of Lattice Vibrations so far
- Models for Vibrations in Discrete 1-D Lattice
- Example of Nearest Neighbor Coupling Only
- Relating Microscopic and Macroscopic Quantities

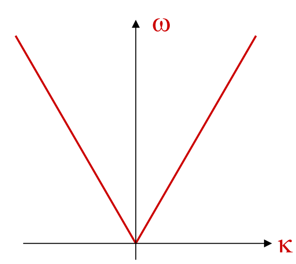
February 20, 2004

Continuum Models

1-D Wave Equation

$$\rho \frac{\partial^2 u_x}{\partial t^2} = E_Y \frac{\partial^2 u_x}{\partial x^2}$$

$$\frac{\partial^2 u_x}{\partial x^2} = \frac{1}{c^2} \frac{\partial^2 u_x}{\partial t^2} \qquad c = \sqrt{\frac{E_Y}{\rho}}$$



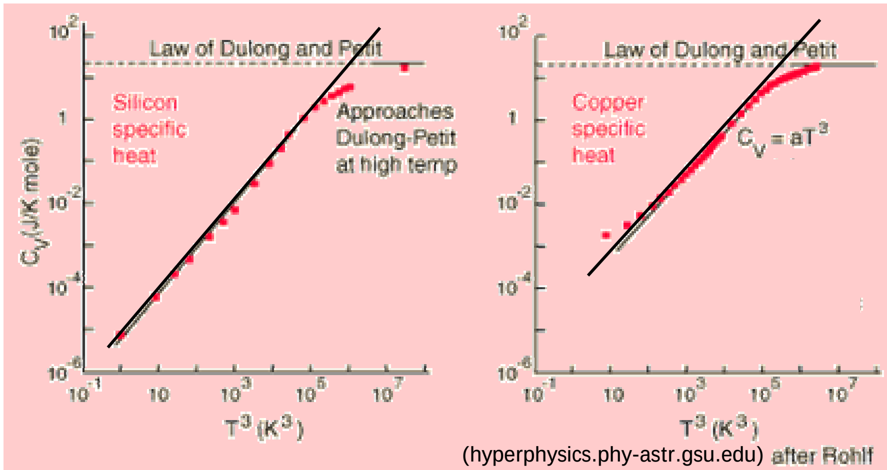
Velocity of sound, c, is proportional to stiffness and inverse prop. to inertia

Periodic Boundary Conditions: Traveling Waves

$$u_x(x,t) = A_{\pm} \exp(ikx) \exp(i\omega t) \qquad \omega = ck$$

Continuum Models

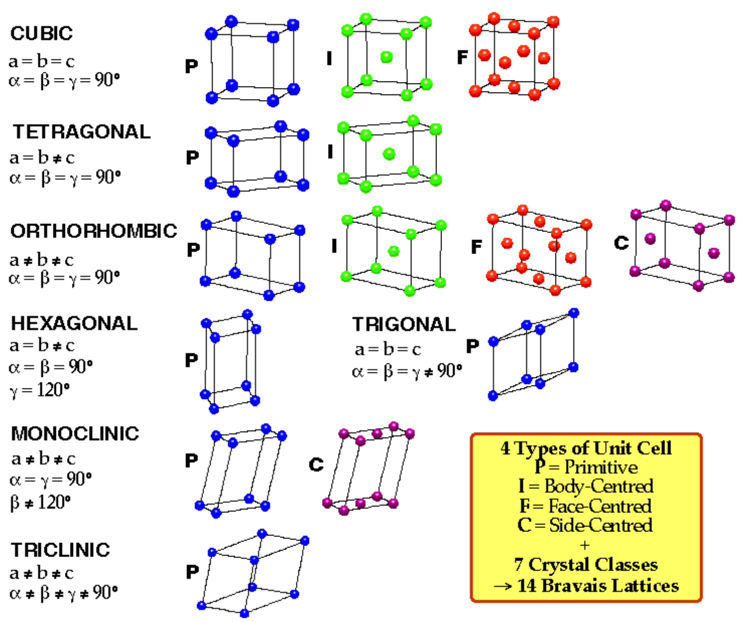
T^3 Specific Heat



$$C_v = C_{el} + C_{phonon} = \gamma T + AT^3$$

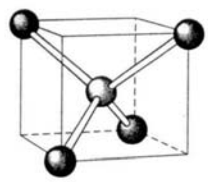
The Atomistic Perspective

Arrangement of Atoms and Bond Orientations

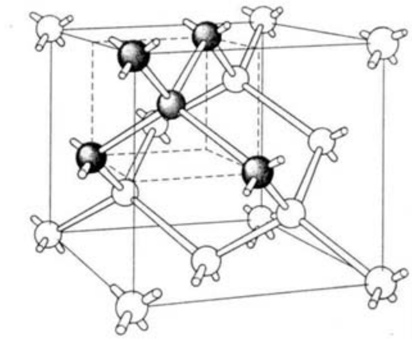


The Atomistic Perspective
Arrangement of Atoms and Bond Orientations

Diamond Crystal Structure:
Silicon



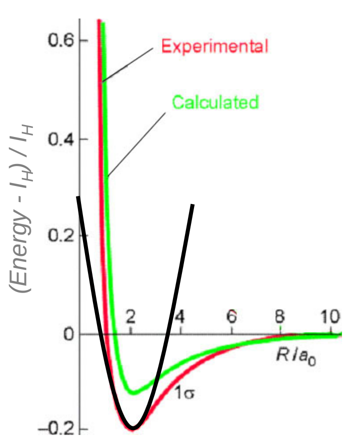
Bond angle = 109.5º



- Add 4 atoms to a FCC
- Tetrahedral bond arrangement
- Each atom has 4 nearest neighbors and 12 next nearest neighbors

The Atomistic Perspective
Vibrational Motion of Nuclei

$$E_{\mathbf{r}}^{n0} P_{n0}(r) = \left[-\frac{\hbar^2}{2\mu} \frac{d^2}{dr^2} + V_{\text{eff}}(r) \right] P_{n0}(r)$$

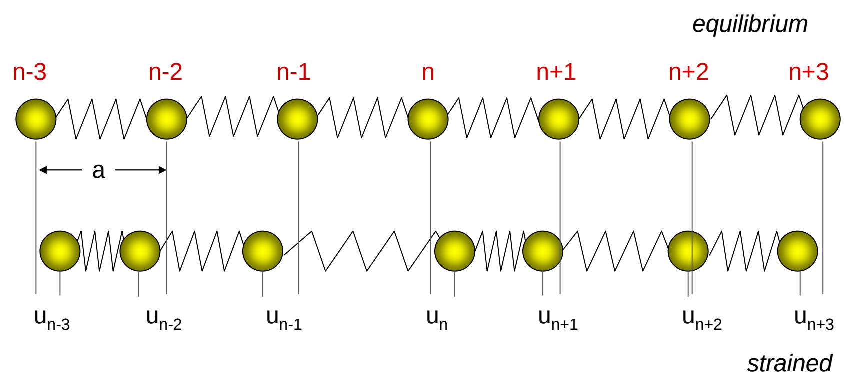


$$V_{\text{eff}}(r) = V_o + \frac{1}{2}(r - R_o)^2 \underbrace{\left(\frac{d^2V}{dr^2} \right)_{R_o}}$$

"spring constant"

$$E_{\mathbf{r}}^{n0} = V_o + \hbar\omega_o(n + \frac{1}{2})$$

Strain in a Discrete Lattice
Example of Nearest Neighbor Interactions



$u[n,t]$ is the discrete displacement of an atom from its equilibrium position

Strain in a Discrete Lattice
General Expansion

The potential energy associated with the strain is a complex function of the displacements. A Taylor series expansion in the displacements gives

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

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

where $V_0 = V(\{u[i,t]\})_{\text{eq}}$

and the force on each lattice atom

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

Harmonic Matrix

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

$\widetilde{D}(n,m) = \widetilde{D}(m,n)$ $\qquad$ $\widetilde{D}(n,m) = \widetilde{D}(n-m)$ $\qquad$ for infinite lattices

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

Dynamics of Lattice Atoms

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

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

$$M\frac{d^2}{dt^2}u[j] = -\frac{\partial}{\partial u[j]}V(\{u[i]\})$$

$$= -\frac{1}{2}\sum_{m=-\infty}^{\infty}\widetilde{D}(j,m)u[m] - \frac{1}{2}\sum_{n=-\infty}^{\infty}u[n]\widetilde{D}(n,j)$$

$$= -\sum_{m=-\infty}^{\infty}\widetilde{D}(j,m)u[m]$$

Solutions of Equations of Motion

Convert to Difference Equation

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

Time harmonic solutions...

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

Plugging in, converts equation of motion into coupled difference equations:

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

Solutions of Equations of Motion

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

We can guess solution of the form:

$\tilde{U}[p+1] = \tilde{U}[p]z^{-1}$ and $\tilde{U}[p] = \tilde{U}[0]z^{-p}$

This is equivalent to taking the z-transform...

$$M\omega^2\tilde{U}[0] = \left(\sum_{m=-\infty}^{\infty}\widetilde{D}(n,m)z^{n-m}\right)\tilde{U}[0]$$

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

Solutions of Equations of Motion

Consider Undamped Lattice Vibrations

$$M\omega^2 = \sum_{m=-\infty}^{\infty} \widetilde{D}(n,m) z^{n-m} \qquad \tilde{U}[p] = \tilde{U}[0] z^{-p}$$

We are going to consider the undamped vibrations of the lattice:

$$|U[m]| = |U[n]|$$

$$|z| = 1$$

$$z = e^{-ika}$$

$$\boxed{\tilde{u}[n,t] = \tilde{U}[0] e^{i(kna-\omega t)}}$$

Solutions of Equations of Motion

Dynamical Matrix

$$M\omega^2 = \sum_{m=-\infty}^{\infty} \widetilde{D}(n,m) z^{n-m} \qquad \tilde{u}[n,t] = \tilde{U}[0] e^{i(kna-\omega t)}$$

$$z = e^{-ika}$$

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

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

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

Solutions of Equations of Motion

Dynamical Matrix

$$M\omega^2 = D(k) = \underbrace{\sum_{p=-\infty}^{\infty} \widetilde{D}(p) e^{-ikap}}_{\text{Dynamical Matrix } D(k)}$$

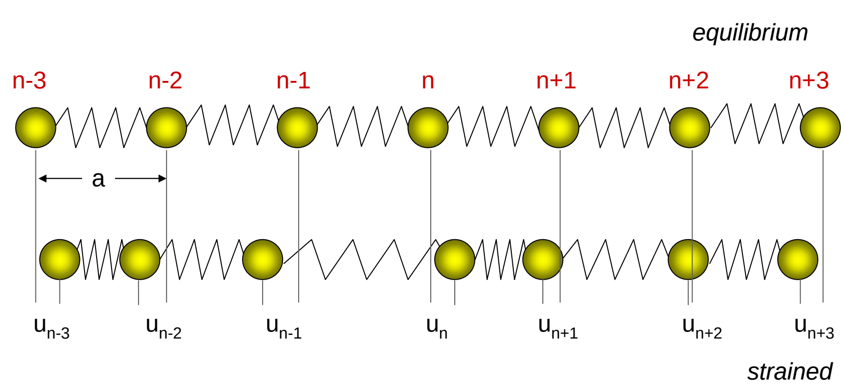
$$\widetilde{D}(n,m) = \left(\frac{\partial^2 V}{\partial u[n,t]\, \partial u[m,t]} \right)_{\text{eq}}$$

$$\widetilde{D}(n,m) = \widetilde{D}(n-m) = \widetilde{D}(p)$$

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

Strain in a Discrete Lattice

Example of Nearest Neighbor Interactions



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

Strain in a Discrete Lattice

Example of Nearest Neighbor Interactions

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

$$\begin{aligned}
\widetilde{D}(n,m) &= \left(\frac{\partial^2 V}{\partial u[n,t]\, \partial u[m,t]}\right)_{\text{eq}} \\
&= \frac{\partial}{\partial u[n,t]} \left(\sum_{p=-\infty}^{\infty} \alpha \left(u[p+1] - u[p]\right) \left(\delta_{m,p+1} - \delta_{m,p}\right) \right) \\
&= \frac{\partial}{\partial u[n,t]} \alpha \left(u[m] - u[m-1] - u[m+1] + u[m]\right) \\
&= \alpha \left(2\delta_{n,m} - \delta_{n-1,m} - \delta_{n+1,m}\right) \\
&= \alpha \left(2\delta_{n-m,0} - \delta_{n-m,1} - \delta_{n-m,-1}\right) \\
&= \widetilde{D}(n-m)
\end{aligned}$$

Strain in a Discrete Lattice

Example of Nearest Neighbor Interactions

Harmonic matrix:

$$\widetilde{D}(n,m) = \left(\frac{\partial^2 V}{\partial u[n,t]\, \partial u[m,t]}\right)_{\text{eq}} = \alpha \left(2\delta_{n-m,0} - \delta_{n-m,1} - \delta_{n-m,-1}\right)$$

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

Dynamical matrix:

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

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

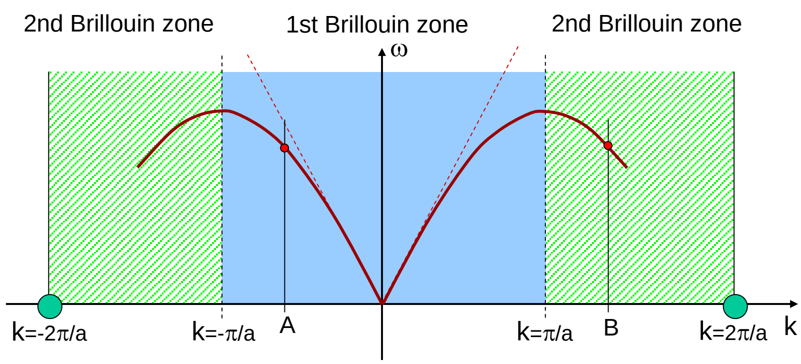
$$\omega = \sqrt{\frac{D(k)}{M}} = 2\sqrt{\frac{\alpha}{M}} \left|\sin\left(\frac{ka}{2}\right)\right|$$

Dispersion Relation

Strain in a Discrete Lattice

Example of Nearest Neighbor Interactions

$$\omega = 2\sqrt{\frac{\alpha}{M}}\left|\sin\left(\frac{ka}{2}\right)\right|$$



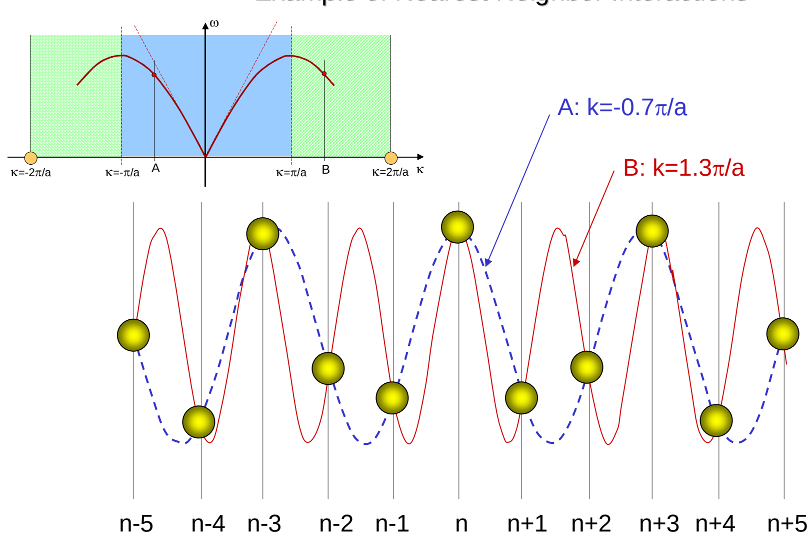
From what we know about Brillouin zones the points A and B (related by a reciprocal lattice vector) must be identical

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

This implies that the wave form of the vibrating atoms must also be identical.

Strain in a Discrete Lattice

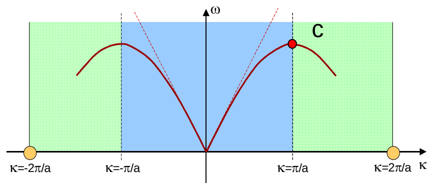
Example of Nearest Neighbor Interactions



But: note that point B represents a wave travelling right, and point A one travelling left

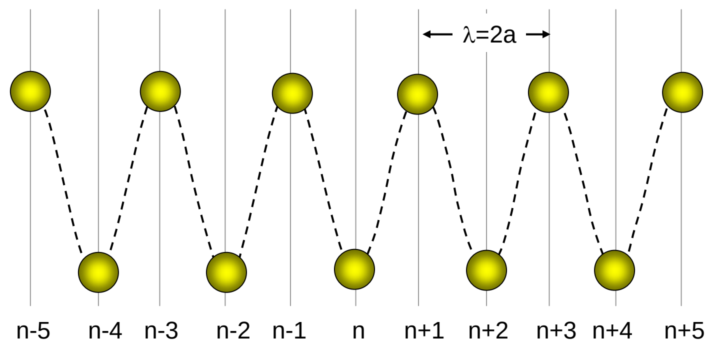
Strain in a Discrete Lattice

Example of Nearest Neighbor Interactions



Consider point C at the zone boundary

When k=π/a, λ=2a, and motion becomes that of a standing wave (the atoms are bouncing backward and forward against each other



Strain in a Discrete Lattice

Example of Nearest Neighbor Interactions

$$\omega = 2\sqrt{\frac{\alpha}{M}}\left|\sin\left(\frac{ka}{2}\right)\right|$$

In the limit of long-wavelength, we should recover the continuum model…

$$\omega \underset{k\to 0}{\longrightarrow} \left(\frac{4\alpha}{M}\right)^{1/2}\frac{a}{2}k$$

Linear dispersion, just like the sound waves for the continuum solid

$$\omega = c_s k \qquad \text{where} \qquad c_s = \sqrt{\frac{E_Y}{\rho}}$$

$$\left(\frac{4\alpha}{M}\right)^{1/2}\frac{a}{2} = \sqrt{\frac{E_Y}{\rho}}$$

$$\alpha = aE_Y$$

$$\omega_{MAX} = (4\alpha/M)^{1/2} = 2c_s/a$$

Connects the microscopic with the macroscopic