6.730 Physics for Solid State Applications

Lecture 10, 11: Specific Heat of Discrete Lattice

Outline

- 2-D Lattice Waves Solutions
- Review Continuum Specific Heat Calculation
- Density of Modes
- Quantum Theory of Lattice Vibrations
- Specific Heat for Lattice
- Approximate Models

Lattice Waves in 3-D Crystals

Second order Taylor series expansion for total potential energy:

$$V(\{u[\mathbf{R_s},\mathbf{t}]\}) = \mathbf{V_o} + \frac{1}{2}\sum_{\mathbf{i}}\sum_{\mathbf{j}}\sum_{\mathbf{R_p}}\sum_{\mathbf{R_m}} \mathbf{u_i}[\mathbf{R_p},\mathbf{t}]\,\widetilde{\mathbf{D}}_{\mathbf{i},\mathbf{j}}(\mathbf{R_p},\mathbf{R_m})\,\mathbf{u_j}[\mathbf{R_m},\mathbf{t}]$$

Harmonic Matrix:

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

Equation of motion for lattice atoms assuming ‘plane wave’ solutions:

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

Dynamical Matrix:

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

Lattice Waves in 3-D Crystals

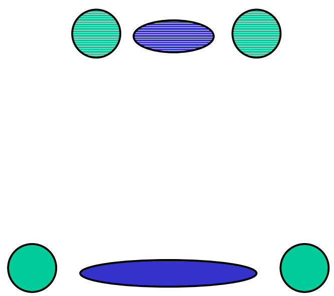
$$\left(\mathbf{M}^{-1}\mathbf{D}(\mathbf{k})\right)\vec{\epsilon} = \omega^2\vec{\epsilon}$$

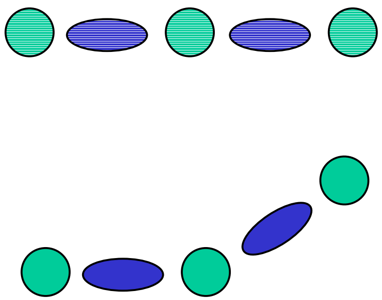
$$\epsilon[\mathbf{R_n}] = \begin{pmatrix} \epsilon_{1x}[\mathbf{R_n}] \\ \epsilon_{2x}[\mathbf{R_n}] \\ \vdots \\ \epsilon_{1y}[\mathbf{R_n}] \\ \epsilon_{2y}[\mathbf{R_n}] \\ \vdots \\ \epsilon_{1z}[\mathbf{R_n}] \\ \epsilon_{2z}[\mathbf{R_n}] \\ \vdots \end{pmatrix} \quad \mathbf{M} = \begin{pmatrix} M_1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \cdots \\ 0 & M_2 & 0 & 0 & 0 & 0 & 0 & 0 & \cdots \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & M_1 & 0 & 0 & 0 & 0 & \cdots \\ 0 & 0 & 0 & 0 & M_2 & 0 & 0 & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots\vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & 0 & M_1 & 0 & \cdots \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & M_2 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

Dimension of system is given by

(number of basis atoms) x (dimension of lattice)

Bond Stretching and Bending





$$E_s = \frac{1}{2}\alpha_s \left(\Delta L\right)^2$$

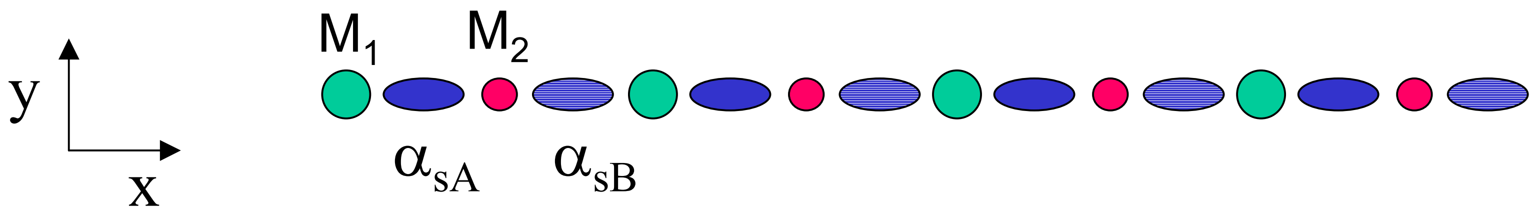
$$E_\phi = \frac{1}{2}\alpha_\phi L^2 (\Delta\phi)^2$$

$$E_s = \frac{1}{2}\alpha_s \left(\hat{\mathbf{b}}_{i,j} \cdot \left(\mathbf{u_j} - \mathbf{u_i}\right)\right)^2$$

$$E_\phi = \frac{1}{2}\alpha_\phi \left(\left|\mathbf{u_i} - \mathbf{u_j}\right|^2 - \left[\hat{\mathbf{b}}_{i,j} \cdot \left(\mathbf{u_i} - \mathbf{u_j}\right)\right]^2\right)$$

Example: 1-D Diatomic Lattice with Bond Stretching and Bending

Potential Energy



$$E_s = \frac{1}{2}\alpha_s\,(\Delta L)^2$$

$$E_\phi = \frac{1}{2}\alpha_\phi L^2(\Delta\phi)^2$$

$$E_s = \frac{1}{2}\alpha_s\left(\hat{\mathbf{b}}_{i,j}\cdot\left(\mathbf{u_j}-\mathbf{u_i}\right)\right)^2$$

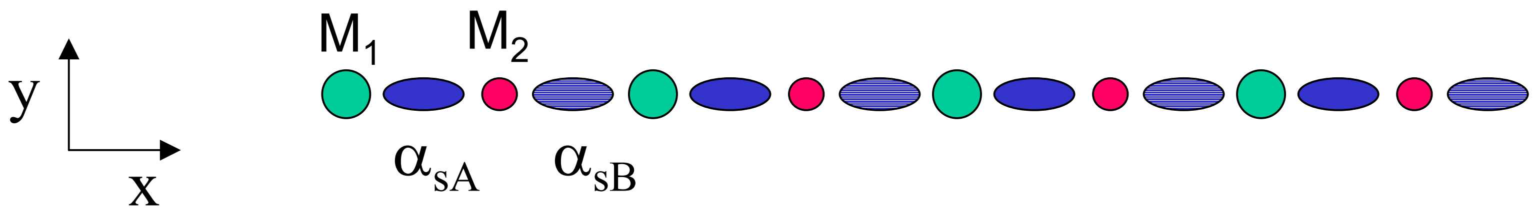
$$E_\phi = \frac{1}{2}\alpha_\phi\left(\left|\mathbf{u_i}-\mathbf{u_j}\right|^2-\left[\hat{\mathbf{b}}_{i,j}\cdot\left(\mathbf{u_i}-\mathbf{u_j}\right)\right]^2\right)$$

$$E_s = \frac{1}{2}\alpha_{sA}\left(\mathbf{u_{1x}[R]}-\mathbf{u_{2x}[R]}\right)^2$$

$$E_\phi = \frac{1}{2}\alpha_\phi\left|\mathbf{u_{1y}}-\mathbf{u_{2y}}\right|^2$$

Example: '1-D' Diatomic Lattice with Bond Stretching and Bending

Potential Energy



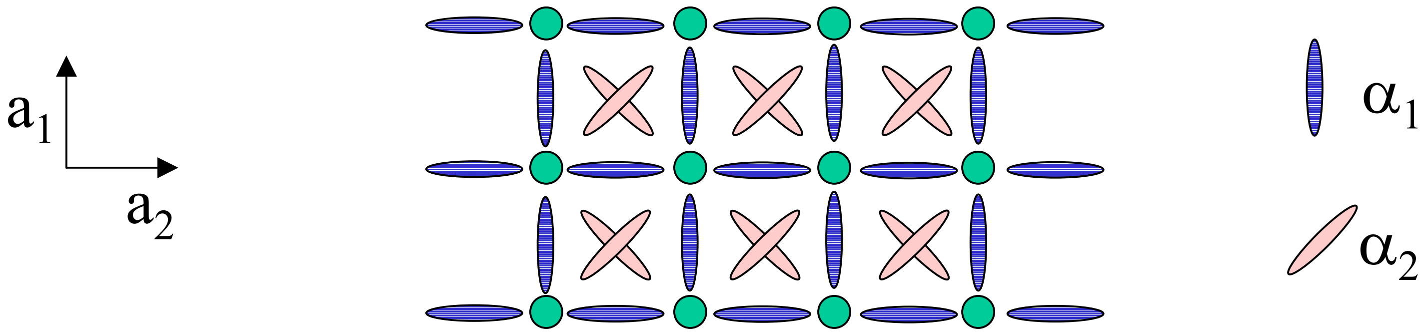
$$V = \ldots \frac{1}{2}\alpha_{sA}\left(\mathbf{u_{1x}}[\mathbf{R}] - \mathbf{u_{2x}}[\mathbf{R}]\right)^2 + \frac{1}{2}\alpha_{\phi A}\left(\mathbf{u_{1y}}[\mathbf{R}] - \mathbf{u_{2y}}[\mathbf{R}]\right)^2$$

$$+\frac{1}{2}\alpha_{sB}\left(\mathbf{u_{1x}}[\mathbf{R}] - \mathbf{u_{2x}}[\mathbf{R}-\mathbf{a}]\right)^2 + \frac{1}{2}\alpha_{\phi B}\left(\mathbf{u_{1y}}[\mathbf{R}] - \mathbf{u_{2y}}[\mathbf{R}-\mathbf{a}]\right)^2 + \ldots$$

$$\mathbf{D}(\mathbf{k}) = \begin{array}{c} \\ \mathbf{u_{1x}} \\ \mathbf{u_{2x}} \\ \mathbf{u_{1y}} \\ \mathbf{u_{2x}} \end{array} \begin{array}{cccc} \mathbf{u_{1x}} & \mathbf{u_{2x}} & \mathbf{u_{1y}} & \mathbf{u_{2y}} \\ \alpha_{sA}+\alpha_{sB} & -\alpha_{sA}-\alpha_{sB}e^{-ika} & 0 & 0 \\ -\alpha_{sA}-\alpha_{sB}e^{ika} & \alpha_{sA}+\alpha_{sB} & 0 & 0 \\ 0 & 0 & \alpha_{\phi A}+\alpha_{\phi B} & -\alpha_{\phi A}-\alpha_{\phi B}e^{-ika} \\ 0 & 0 & -\alpha_{\phi A}-\alpha_{\phi B}e^{ika} & \alpha_{\phi A}+\alpha_{\phi B} \end{array}$$

Example: 2-D Lattice with Bond Stretching

Potential Energy



$$V = \cdots + \frac{\alpha_1}{2}\left|\hat{\mathbf{a}}_1 \cdot (\mathbf{u}[\mathbf{R}+\mathbf{a}_1] - \mathbf{u}[\mathbf{R}])\right|^2 + \frac{\alpha_1}{2}\left|\hat{\mathbf{a}}_1 \cdot (\mathbf{u}[\mathbf{R}-\mathbf{a}_1] - \mathbf{u}[\mathbf{R}])\right|^2$$

$$+\frac{\alpha_1}{2}\left|\hat{\mathbf{a}}_2 \cdot (\mathbf{u}[\mathbf{R}+\mathbf{a}_2] - \mathbf{u}[\mathbf{R}])\right|^2 + \frac{\alpha_1}{2}\left|\hat{\mathbf{a}}_2 \cdot (\mathbf{u}[\mathbf{R}-\mathbf{a}_2] - \mathbf{u}[\mathbf{R}])\right|^2$$

$$+\frac{\alpha_2}{2}\left|\frac{\hat{\mathbf{a}}_1 + \hat{\mathbf{a}}_2}{\sqrt{2}} \cdot (\mathbf{u}[\mathbf{R}+\mathbf{a}_1+\mathbf{a}_2] - \mathbf{u}[\mathbf{R}])\right|^2$$

$$+\frac{\alpha_2}{2}\left|\frac{-\hat{\mathbf{a}}_1 + \hat{\mathbf{a}}_2}{\sqrt{2}} \cdot (\mathbf{u}[\mathbf{R}-\mathbf{a}_1+\mathbf{a}_2] - \mathbf{u}[\mathbf{R}])\right|^2$$

Example: 2-D Lattice with Bond Stretching

Elements of the Dynamical Matrix

$$\mathbf{D}_{\mathbf{xx}}(\mathbf{k}) = \alpha_1\left(\mathbf{1} - \mathbf{e}^{-\mathbf{ik}\cdot\mathbf{a}_1}\right) + \alpha_1\left(\mathbf{1} - \mathbf{e}^{\mathbf{ik}\cdot\mathbf{a}_1}\right) + \mathbf{0} + \mathbf{0}$$

$$+\frac{\alpha_2}{2}\left(1 - e^{-i\mathbf{k}\cdot(\mathbf{a}_1+\mathbf{a}_2)}\right) + \frac{\alpha_2}{2}\left(1 - e^{-i\mathbf{k}\cdot(-\mathbf{a}_1-\mathbf{a}_2)}\right)$$

$$+\frac{\alpha_2}{2}\left(1 - e^{-i\mathbf{k}\cdot(-\mathbf{a}_1+\mathbf{a}_2)}\right) + \frac{\alpha_2}{2}\left(1 - e^{-i\mathbf{k}\cdot(\mathbf{a}_1-\mathbf{a}_2)}\right)$$

Example: 2-D Lattice with Bond Stretching

Dynamical Matrix

$$\mathbf{D}(\mathbf{k}) = \begin{pmatrix} 2\alpha_1(1-\cos k_x a) + 2\alpha_2(1-\cos k_x a \cos k_y a) & 2\alpha_2 \sin k_x a \sin k_y a \\ 2\alpha_2 \sin k_x a \sin k_y a & 2\alpha_1(1-\cos k_y a) + 2\alpha_2(1-\cos k_x a \cos k_y a) \end{pmatrix}$$

$$\mathbf{M} = \mathsf{M}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

$$\frac{1}{M}\mathbf{D}(\mathbf{k})\tilde{\epsilon} = \omega^{\mathbf{2}}\tilde{\epsilon}$$

Example: 2-D Lattice with Bond Stretching

Dispersion Relation

$$\mathbf{D}(k_x,0) = \begin{pmatrix} 2(\alpha_1+\alpha_2)(1-\cos k_x a) & 0 \\ 0 & 2\alpha_2(1-\cos k_x a) \end{pmatrix}$$

Longitudinal Waves:

$$\omega_1(k_x,0) = \sqrt{\frac{4(\alpha_1+\alpha_2)}{M}}\sin\frac{k_x a}{2} \qquad \vec{\epsilon}_1(k_x,0) = \begin{matrix} 1 \\ 0 \end{matrix}$$

Transverse Waves:

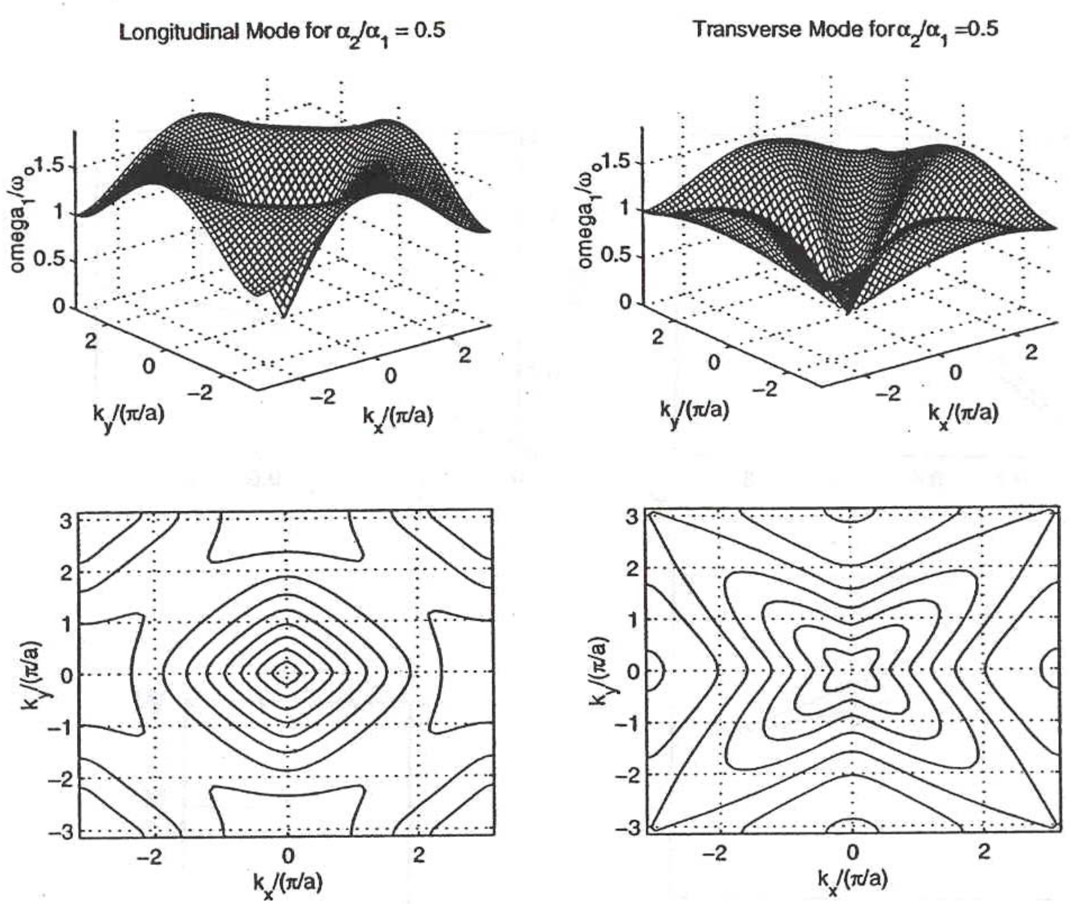
$$\omega_2(k_x,0) = \sqrt{\frac{4\alpha_2}{M}}\sin\frac{k_x a}{2} \qquad \vec{\epsilon}_2(k_x,0) = \begin{matrix} 0 \\ 1 \end{matrix}$$

$$\tilde{u}_i[\mathbf{R_n},\mathbf{t}] = \mathbf{e}^{\mathbf{i}(\mathbf{k}\cdot\mathbf{R_n}-\omega_\mathbf{i}(\mathbf{k})\mathbf{t})}\,\tilde{\epsilon}_\mathbf{i}(\mathbf{k})$$

Example: 2-D Lattice with Bond Stretching

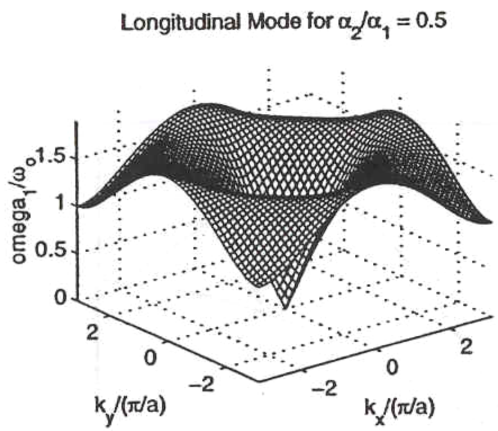
Dispersion Relations

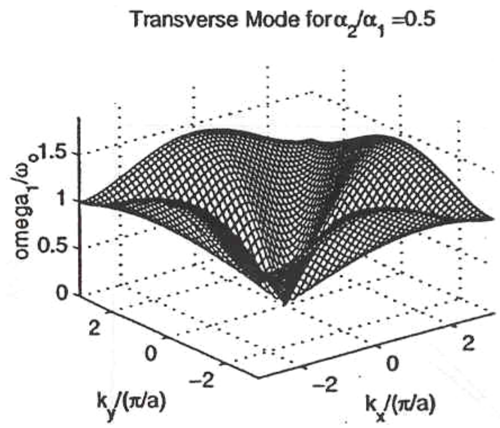
$$\mathrm{D}(\mathbf{k}) = \begin{pmatrix} 2\alpha_1(1-\cos k_x a) + 2\alpha_2(1-\cos k_x a \cos k_y a) & 2\alpha_2 \sin k_x a \sin k_y a \\ 2\alpha_2 \sin k_x a \sin k_y a & 2\alpha_1(1-\cos k_y a) + 2\alpha_2(1-\cos k_x a \cos k_y a) \end{pmatrix}$$

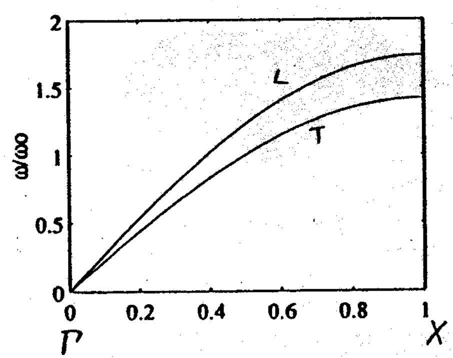


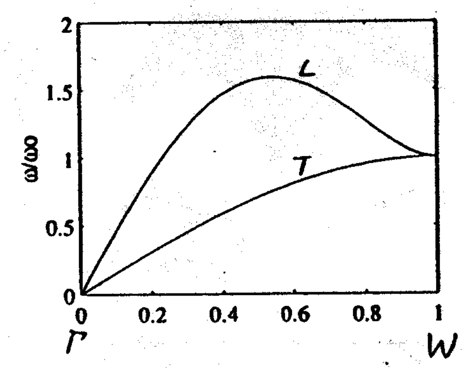
Example: 2-D Lattice with Bond Stretching

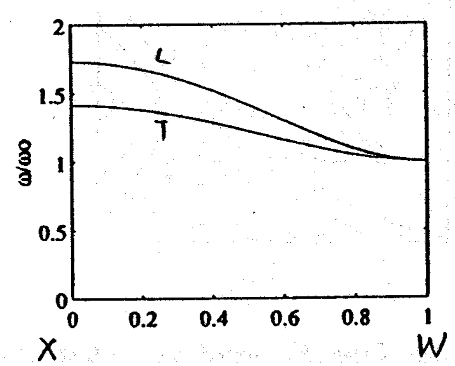
Dispersion Relations

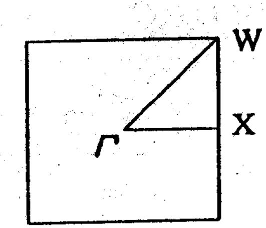












Specific Heat of Solid
How much energy is in each mode ?

Approach:

- Quantize the amplitude of vibration for each mode

- Treat each quanta of vibrational excitation as a bosonic particle, *the phonon*

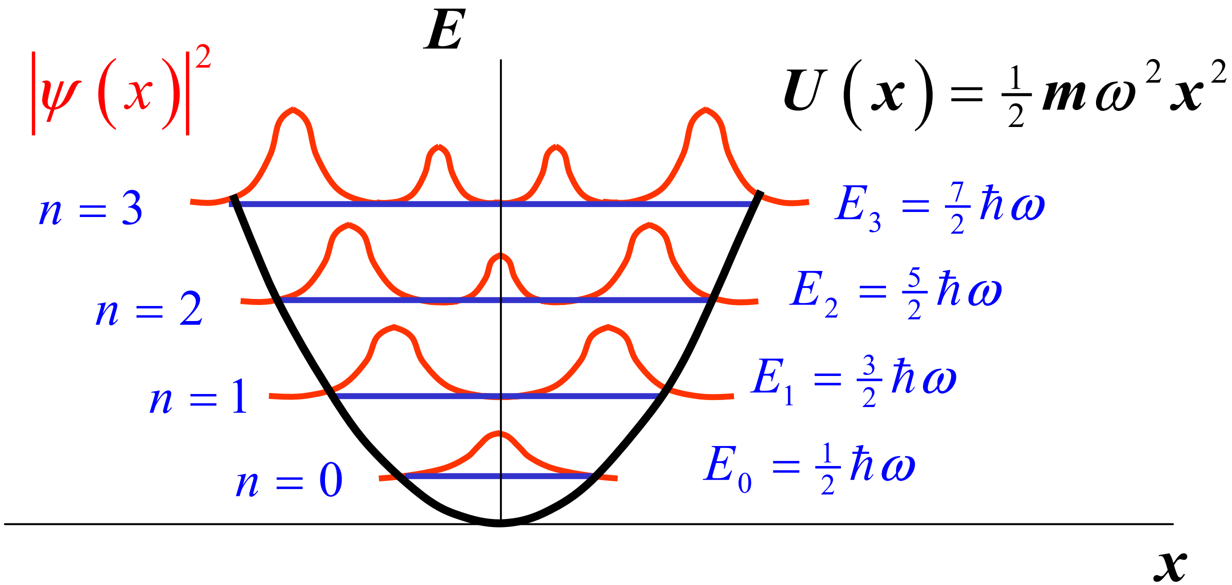
$$E = \sum_{\mathbf{k},\sigma} \hbar\omega_{\mathbf{k},\sigma} \left[\langle n_{\mathbf{k},\sigma} \rangle + \frac{1}{2} \right]$$

- Use Bose-Einstein statistics to determine the number of phonons in each mode

$$\langle n_{\mathbf{k},\sigma} \rangle = \frac{1}{e^{\hbar\omega_{\mathbf{k},\sigma}/k_B T} - 1}$$

$$\frac{E}{V} = \sum_{\sigma} \int \frac{\hbar\omega}{e^{\hbar\omega/k_B T} - 1} g_\sigma(\omega)\, d\omega$$

Simple Harmonic Oscillator



$$\hat{a} = \sqrt{\frac{M\omega^2}{2\hbar}}\hat{x} + i\sqrt{\frac{1}{2M\hbar\omega}}\hat{p} \qquad \hat{a}^\dagger = \sqrt{\frac{M\omega^2}{2\hbar}}\hat{x} - i\sqrt{\frac{1}{2M\hbar\omega}}\hat{p}$$

$$[\hat{x}, \hat{p}] = i\hbar \quad \Rightarrow \quad \left[\hat{a}, \hat{a}^\dagger\right] = 1$$

$$H = \hbar\omega\left[a^\dagger a + \frac{1}{2}\right]$$

Hamiltonian for Discrete Lattice

Potential energy of bonds in 3-D lattice with basis:

$$V(\{u[\mathbf{R_s},\mathbf{t}]\}) = \mathbf{V_o} + \frac{\mathbf{1}}{\mathbf{2}} \sum_{\mathbf{i}} \sum_{\mathbf{j}} \sum_{\mathbf{R_p}} \sum_{\mathbf{R_m}} \mathbf{u_i}[\mathbf{R_p},\mathbf{t}]\, \widetilde{\mathbf{D}}_{\mathbf{i},\mathbf{j}}(\mathbf{R_p},\mathbf{R_m})\, \mathbf{u_j}[\mathbf{R_m},\mathbf{t}]$$

For single atom basis in 3-D, μ & ν denote x,y, or z direction:

$$H = \frac{M}{2} \sum_{\mathbf{R_j}} \sum_{\mu} \dot{\mathbf{u}}_\mu[\mathbf{R_j},\mathbf{t}]\, \dot{\mathbf{u}}_\mu[\mathbf{R_j},\mathbf{t}] + \sum_{\mathbf{R_j}} \sum_{\mathbf{R_k}} \sum_{\mu} \sum_{\nu} \mathbf{u}_\mu[\mathbf{R_j},\mathbf{t}]\, \widetilde{\mathbf{D}}_{\mu\nu}(\mathbf{R_j}-\mathbf{R_k})\, \mathbf{u}_\nu[\mathbf{R_k},\mathbf{t}]$$

$$[\widehat{x},\widehat{p}] = i\hbar \quad \Longrightarrow \quad M\left[\mathbf{u}_\mu[\mathbf{R_j},\mathbf{t}],\dot{\mathbf{u}}_\nu[\mathbf{R_k},\mathbf{t}]\right] = i\hbar\delta_{\mu,\nu}\,\delta_{R_j,R_k}$$

Hamiltonian for Discrete Lattice
Plane Wave Expansion

$$H = \frac{M}{2}\sum_{\mathbf{R_j}}\sum_{\mu}\dot{\mathbf{u}}_{\mu}[\mathbf{R_j},\mathbf{t}]\,\dot{\mathbf{u}}_{\mu}[\mathbf{R_j},\mathbf{t}] + \sum_{\mathbf{R_j}}\sum_{\mathbf{R_k}}\sum_{\mu}\sum_{\nu}\mathbf{u}_{\mu}[\mathbf{R_j},\mathbf{t}]\,\widetilde{\mathbf{D}}_{\mu\nu}(\mathbf{R_j}-\mathbf{R_k})\,\mathbf{u}_{\nu}[\mathbf{R_k},\mathbf{t}]$$

The lattice wave can be represented as a superposition of plane waves (eigenmodes) with a known dispersion relation (eigenvalues)….

$$\mathbf{u}[\mathbf{R_j},\mathbf{t}] = \sum_{\mathbf{k}}\sum_{\sigma}\mathbf{b}_{\mathbf{k}\sigma}\,\mathbf{e}^{\mathbf{ikR_j}}\,\tilde{\epsilon}_{\mathbf{k}\sigma}$$

$$\sum_{\nu}\widetilde{\mathbf{D}}_{\mu\nu}\vec{\epsilon}_{\mathbf{k}\sigma\nu} = M\omega^2_{\mathbf{k}\sigma}\vec{\epsilon}_{\mathbf{k}\sigma\mu}$$

σ denotes polarization

$$H = \frac{MN}{2}\sum_{\mathbf{k}}\sum_{\sigma}\dot{\mathbf{b}}_{-\mathbf{k}\sigma}\,\dot{\mathbf{b}}_{\mathbf{k}\sigma} + \frac{MN}{2}\sum_{\mathbf{k}}\sum_{\sigma}\omega^2_{\mathbf{k}\sigma}\mathbf{b}_{-\mathbf{k}\sigma}\,\mathbf{b}_{\mathbf{k}\sigma}$$

Commutation Relation for Plane Wave Displacement

$$M\left[\mathbf{u}_\mu[\mathbf{R_j},\mathbf{t}],\dot{\mathbf{u}}_\nu[\mathbf{R_k},\mathbf{t}]\right]=i\hbar\delta_{\mu,\nu}\,\delta_{R_j,R_k}$$

$$\mathbf{u}[\mathbf{R_j},\mathbf{t}]=\sum_{\mathbf{k}}\sum_{\sigma}\mathrm{b}_{\mathbf{k}\sigma}\,\mathbf{e}^{\mathbf{ikR_j}}\,\tilde{\epsilon}_{\mathbf{k}\sigma}$$

$$M\sum_{\mathbf{k}}\sum_{\mathbf{k}'}\sum_{\sigma}\sum_{\sigma'}\left[\mathrm{b}_{\mathbf{k}\sigma},\dot{\mathrm{b}}_{\mathbf{k}'\sigma'}\right]\,e^{i\mathbf{kR_j}+\mathbf{ik}'\mathbf{R_k}}\,\epsilon_{\mu,\mathbf{k}\sigma}\epsilon_{\nu,\mathbf{k}'\sigma'}=i\hbar\,\delta_{\mu,\nu}\,\delta_{R_j,R_k}$$

$$\sum_{\mu}\epsilon_{\mu,\mathbf{k}\sigma}\epsilon_{\mu,\mathbf{k}\sigma'}=\delta_{\sigma,\sigma'}$$

$$\sum_{\sigma}\epsilon_{\mu,\mathbf{k}\sigma}\epsilon_{\nu,\mathbf{k}\sigma}=\delta_{\mu,\nu}$$

$$\boxed{M\left[\mathrm{b}_{\mathbf{k}\sigma},\dot{\mathrm{b}}_{\mathbf{k}'\sigma'}\right]=i\hbar\,\delta_{\sigma\sigma'}\,\delta_{\mathbf{k},-\mathbf{k}'}}$$

…commute unless we have same polarization and k-vector

Creation and Annhilation Operators for Lattice Waves

$$\hat{a}_{\mathbf{k}\sigma} = \sqrt{\frac{MN\omega_{\mathbf{k}\sigma}}{2\hbar}}\,\mathbf{b}_{\mathbf{k}\sigma} + \mathbf{i}\sqrt{\frac{MN}{2\hbar\omega_{\mathbf{k},\sigma}}}\,\dot{\mathbf{b}}_{\mathbf{k}\sigma}$$

$$\hat{a}^{\dagger}_{\mathbf{k}\sigma} = \sqrt{\frac{MN\omega_{\mathbf{k}\sigma}}{2\hbar}}\,\mathbf{b}_{-\mathbf{k}\sigma} - \mathbf{i}\sqrt{\frac{MN}{2\hbar\omega_{\mathbf{k},\sigma}}}\,\dot{\mathbf{b}}_{-\mathbf{k}\sigma}$$

$$\left[\hat{a}_{\mathbf{k},\sigma}, \hat{a}^{\dagger}_{\mathbf{k}',\sigma'}\right] = \delta_{\mathbf{k},\mathbf{k}'}\delta_{\sigma,\sigma'}$$

$$H = \sum_{\mathbf{k}}\sum_{\sigma}\frac{\hbar\omega_{\mathbf{k}\sigma}}{2}\left[a^{\dagger}_{\mathbf{k}\sigma}a_{\mathbf{k}\sigma} + a_{-\mathbf{k}\sigma}a^{\dagger}_{-\mathbf{k}\sigma}\right]$$

$$H = \sum_{\mathbf{k}}\sum_{\sigma}\hbar\omega_{\mathbf{k}\sigma}\left[a^{\dagger}_{\mathbf{k}\sigma}a_{\mathbf{k}\sigma} + \frac{1}{2}\right]$$

Operators for the Lattice Displacement

$$\hat{a}_{\mathbf{k}\sigma} = \sum_{\mathbf{R_j}} \frac{e^{-i\mathbf{k}\mathbf{R_j}}}{\sqrt{N}} \vec{\epsilon}_{\mathbf{k}\sigma} \left(\sqrt{\frac{M\omega_{\mathbf{k}\sigma}}{2\hbar}} \mathbf{u}[\mathbf{R_j}, \mathbf{t}] + \mathbf{i} \sqrt{\frac{1}{2M\hbar\omega_{\mathbf{k}\sigma}}} \mathbf{M}\dot{\mathbf{u}}[\mathbf{R_j}, \mathbf{t}] \right)$$

$$\hat{a}^{\dagger}_{\mathbf{k}\sigma} = \sum_{\mathbf{R_j}} \frac{e^{i\mathbf{k}\mathbf{R_j}}}{\sqrt{N}} \vec{\epsilon}_{\mathbf{k}\sigma} \left(\sqrt{\frac{M\omega_{\mathbf{k}\sigma}}{2\hbar}} \mathbf{u}[\mathbf{R_j}, \mathbf{t}] - \mathbf{i} \sqrt{\frac{1}{2M\hbar\omega_{\mathbf{k}\sigma}}} \mathbf{M}\dot{\mathbf{u}}[\mathbf{R_j}, \mathbf{t}] \right)$$

$$\mathbf{u}[\mathbf{R_j}, \mathbf{t}] = \sum_{\mathbf{k}} \sum_{\mu} \mathbf{b}_{\mathbf{k}\mu} \, \mathbf{e}^{\mathbf{ikR_j}} \, \tilde{\epsilon}_{\mathbf{k}\mu}$$

$$\mathbf{u}[\mathbf{R_j}, \mathbf{t}] = \sum_{\mathbf{k}\sigma} \sqrt{\frac{\hbar}{2MN\omega_{\mathbf{k}\sigma}}} \left(\hat{\mathbf{a}}_{\mathbf{k}\sigma} \mathbf{e}^{\mathbf{ikR_j}} + \hat{\mathbf{a}}_{\mathbf{k}^{\dagger}\sigma} \mathbf{e}^{-\mathbf{ikR_j}} \right) \tilde{\epsilon}_{\mathbf{k}\sigma}$$

We will use this for electron-phonon scattering…

Specific Heat with Continuum Model for Solid

$$\frac{E}{V} = \sum_\sigma \int \frac{\hbar\omega}{e^{\hbar\omega/k_BT} - 1} g_\sigma(\omega)\, d\omega$$

3-D continuum density of modes in $d\omega$: $g_\sigma(\omega) = \frac{\omega^2}{2\pi^2 c_\sigma^3}$

$$\frac{E}{V} = \sum_\sigma \int \frac{\hbar\omega^3}{2\pi^2 c_\sigma^3 (e^{\hbar\omega/k_BT} - 1)}\, d\omega$$

$$= \sum_\sigma \frac{\pi^2 k_B^4 T^4}{30 c_\sigma^3 \hbar^3}$$

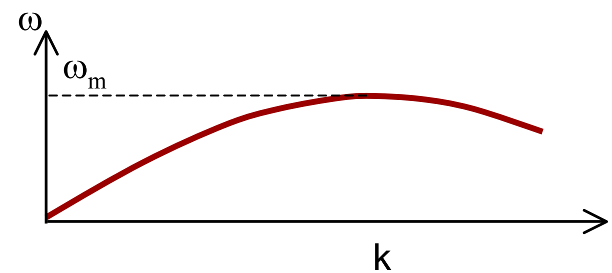
$$C_V = \frac{\partial(E/V)}{\partial T} = AT^3$$

Specific Heat with Discrete Lattice
Density of Modes from Dispersion

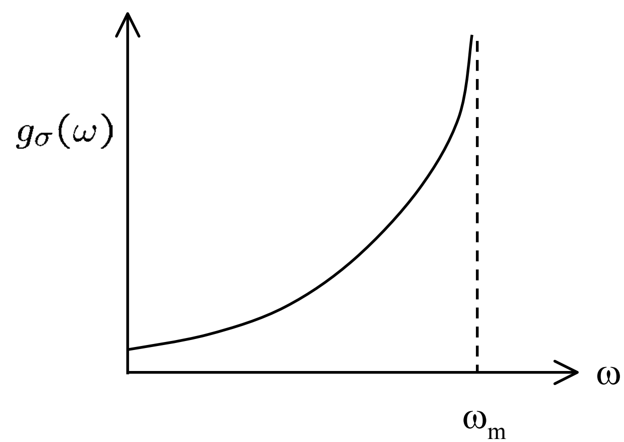
1-D continuum density of modes in $d\omega$: $g_\sigma(\omega)$

$$\frac{dk}{2\pi} = g(\omega)\, d\omega \quad \Rightarrow \quad g_{1D}(\omega) = 2\frac{1}{2\pi}\frac{1}{|\partial\omega/\partial k|}$$

$$\omega = \omega_m \left|\sin\left(\frac{ka}{2}\right)\right| \qquad \text{for} \qquad \omega_m = 2\sqrt{\alpha/M}$$



$$g_{1D}(\omega) = \frac{2}{a\pi}\frac{1}{\omega_m \cos\left(\frac{ka}{2}\right)} = \frac{2}{\pi a}\frac{1}{\sqrt{\omega_m^2 - \omega^2}}$$

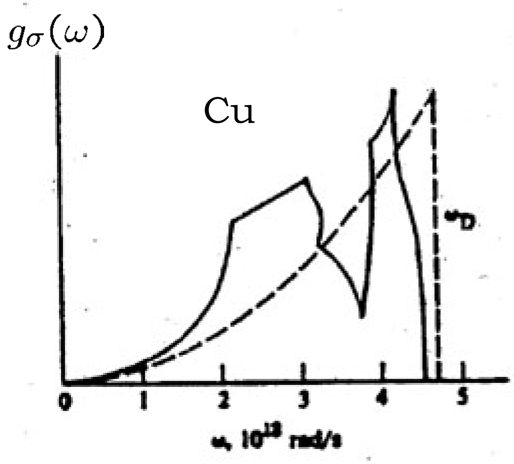


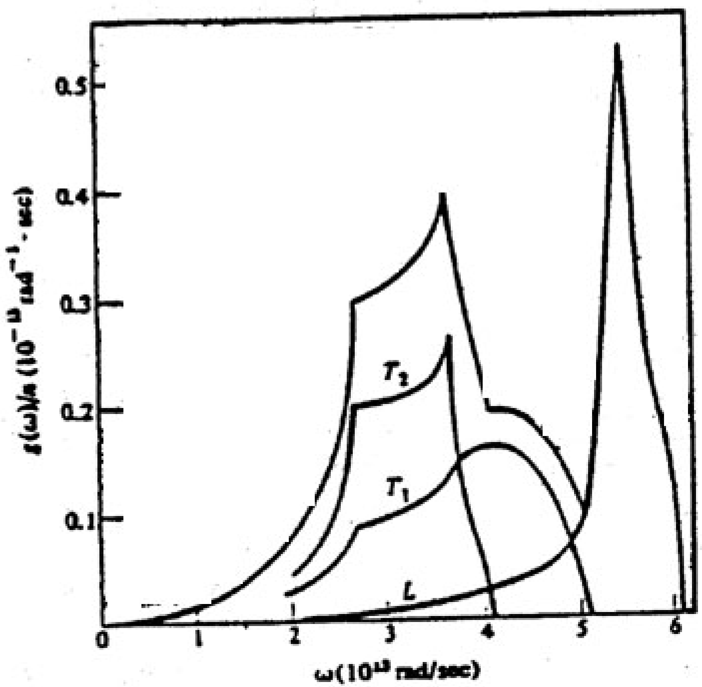
Specific Heat with Discrete Lattice

Density of Modes from Dispersion

$$\frac{E}{V} = \sum_{\sigma} \int \frac{\hbar\omega}{e^{\hbar\omega/k_B T} - 1} g_\sigma(\omega)\, d\omega$$

3-D continuum density of modes in $d\omega$: $g_\sigma(\omega)$





Specific Heat of Solid
How much energy is in each mode ?

Approach:

- Quantize the amplitude of vibration for each mode
- Treat each quanta of vibrational excitation as a bosonic particle, *the phonon*

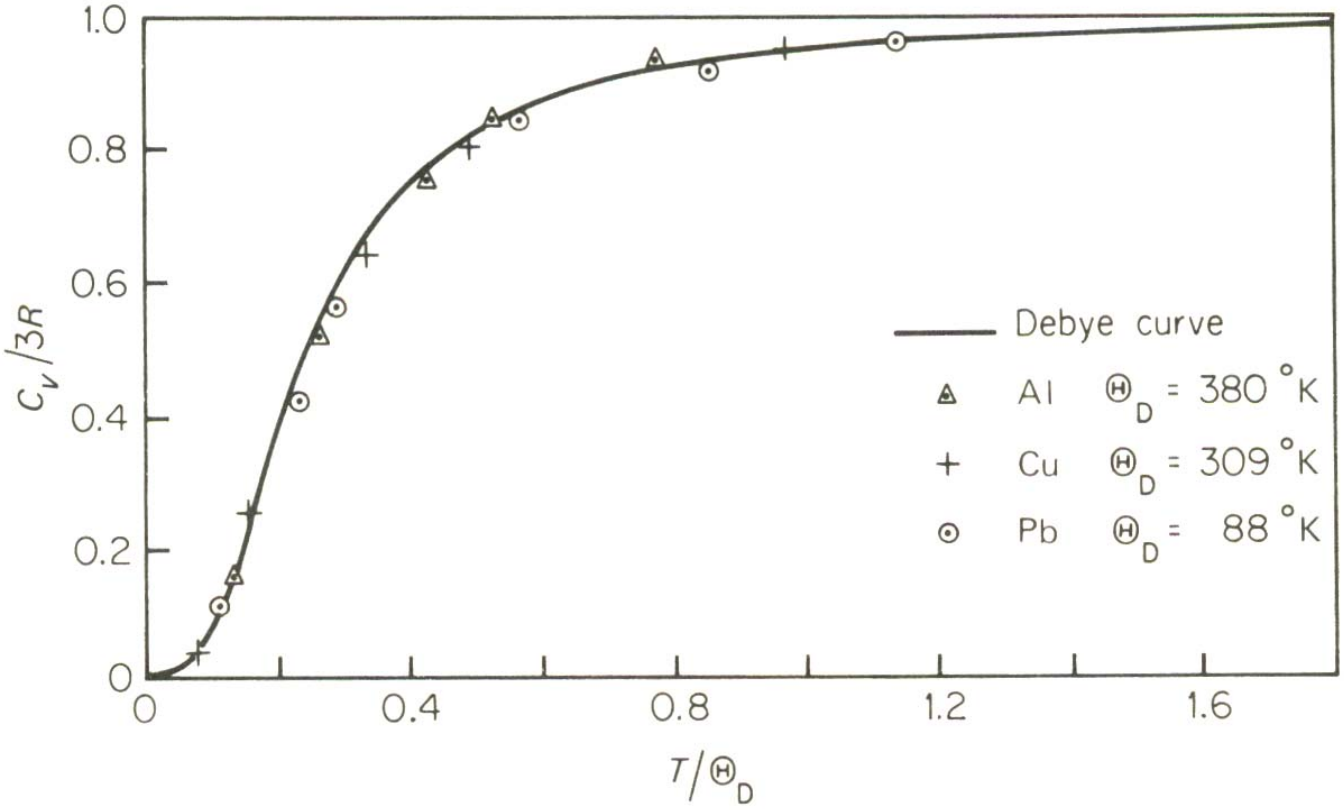
$$H = \sum_{\mathbf{k}} \sum_{\sigma} \hbar\omega_{\mathbf{k}\sigma} \left[a^{\dagger}_{\mathbf{k}\sigma} a_{\mathbf{k}\sigma} + \frac{1}{2} \right]$$

$$E = \sum_{\mathbf{k},\sigma} \hbar\omega_{\mathbf{k},\sigma} \left[\langle n_{\mathbf{k},\sigma} \rangle + \frac{1}{2} \right]$$

- Use Bose-Einstein statistics to determine the number of phonons in each mode

$$\langle n_{\mathbf{k},\sigma} \rangle = \frac{1}{e^{\hbar\omega_{\mathbf{k},\sigma}/k_B T} - 1} \qquad \frac{E}{V} = \sum_{\sigma} \int \frac{\hbar\omega}{e^{\hbar\omega/k_B T} - 1} g_{\sigma}(\omega)\, d\omega$$

Specific Heat of Solid
How much energy is in each mode ?



And we are done…