Lecture 6
Phonon Dynamics

It's a little like photons.

Questions

Generalize to three dimensions, but consider <u>simple cubic</u> lattice for simplicity and <u>two</u> atoms per unit cell

- How many phonon branches do you think will exist?
- How many of them are acoustic (i.e. $\omega \to 0$ as $k \to 0$)?
- Describe possible polarizations of acoustic phonon branches. Which do you think will have lower energies?

Acoustic and Optical Branches

- # of branches = Dh

  D = spatial dimension

  h = # of atoms in the <u>primitive</u> basis

  (Consider k=0 only, as the number of branches should be indep. of k. Number of possible branches = number of possible normal modes for each primitive basis = Dh.)
- # of acoustic branches = D

  i.e. 1 in 1d, 2 in 2d, 3 in 3d

  1 LA – longitudinal acoustic,

  and the rest are TA – transverse
- # of optical branches = Dh – D

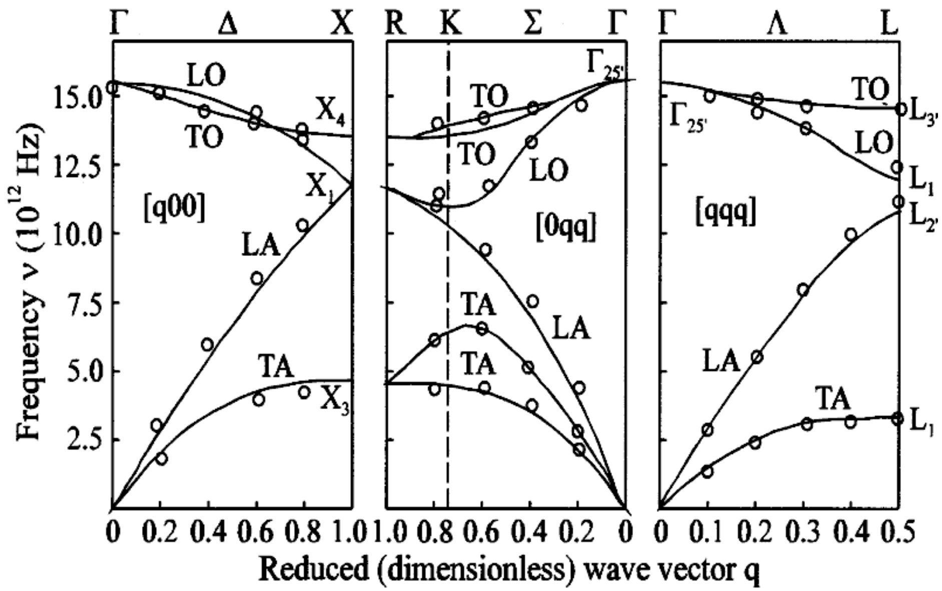
A and O Branches – example

Material = Si

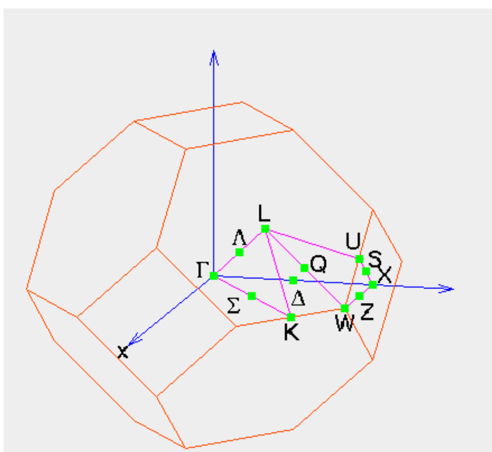
(note: 10^{12} Hz = THz = 4.1 meV)

Diamond structure

2 atom basis in fcc



http://www.ioffe.rssi.ru/SVA/NSM/Semicond/SiGe/mechanic.html



http://cst-www.nrl.navy.mil/~mehl/phonons/fcczone.png

Generally, TA has lower energy than LA, and tends to be degenerate.

Phonons

- Quantize normal mode equation. This is just a Harmonic Oscillator Problem.
- Energy levels for each normal mode is then given by

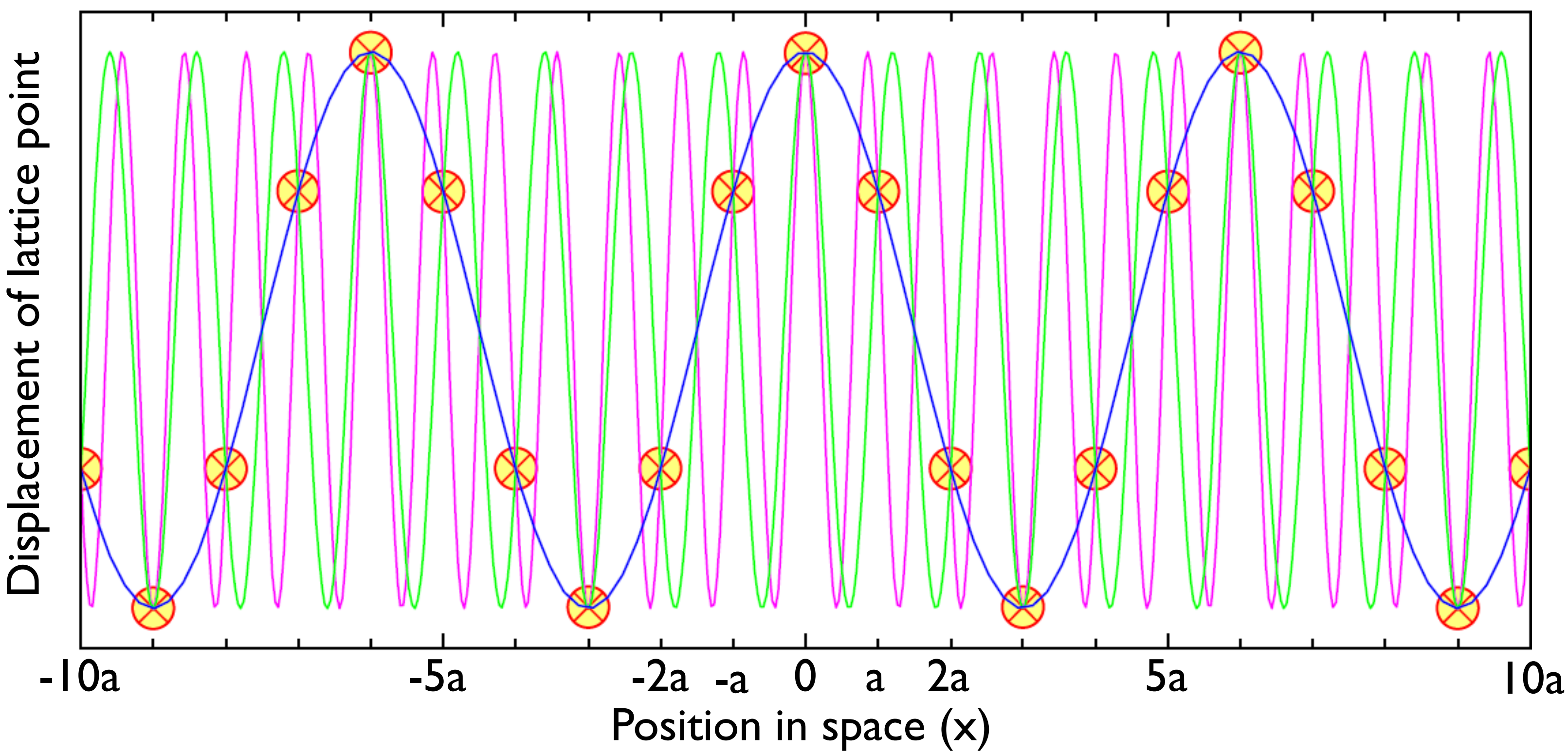
  $$(n + \tfrac{1}{2})\, \hbar\omega$$

  where $\omega=\omega(k, \text{other quantum numbers})$, and

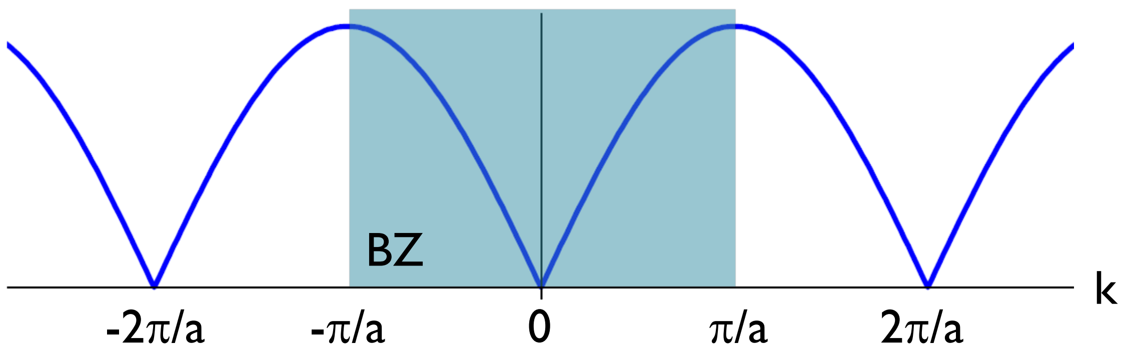
  $n = 0, 1, 2, \ldots$
- Quantum of these (vibrational) normal modes is called **phonon**, i.e. n describes the number of phonons.
- As we have seen, k is a good quantum number for describing phonons. Other good quantum numbers are polarizations, i.e. T or L – transverse or longitudinal.

Crystal Momentum

cos(kx) with k = $\pi/(3a)$ (blue), $\pi/(3a)-2\pi/a$ (green), $\pi/(3a)+2\pi/a$ (magenta).
Crystal (yellow circles) is defined by lattice constant a.
There is no difference between all these waves if they represent lattice displacment, i.e. phonon amplitude, in the crystal.

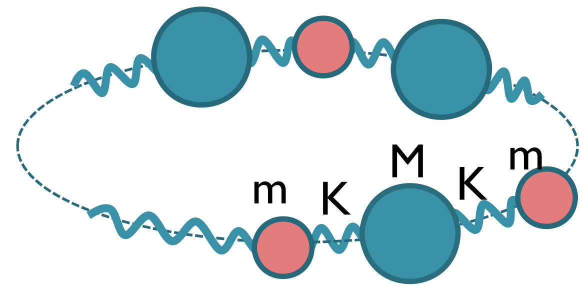


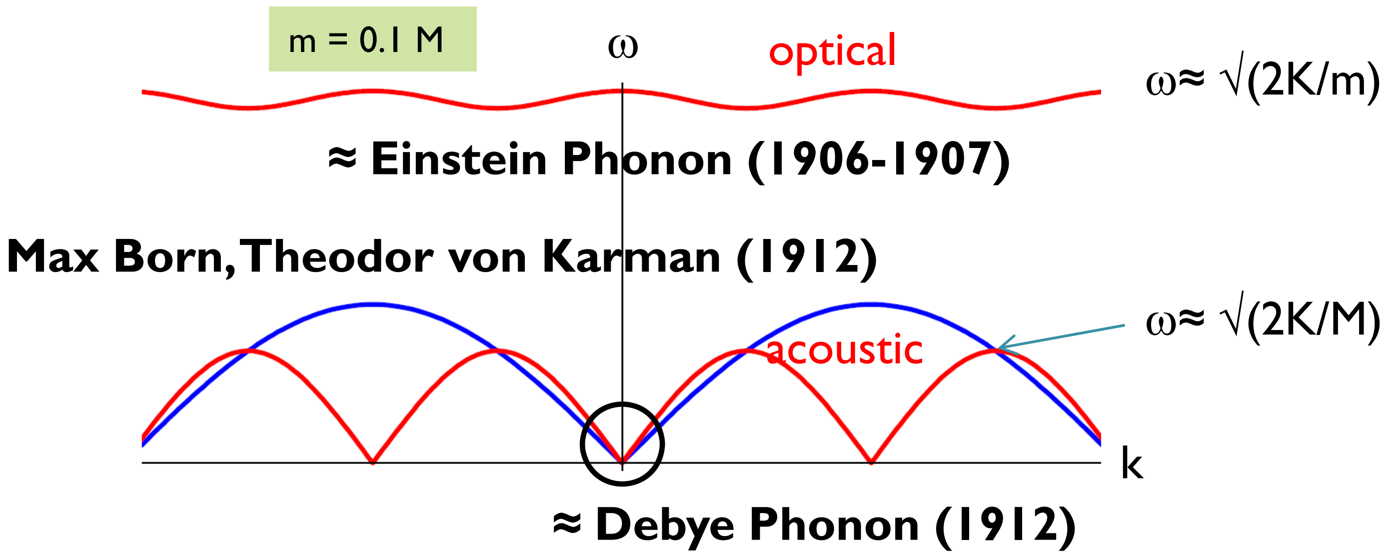
Crystal Momentum Conservation



- k is a good quantum number (i.e. eigenvalue $\omega=\omega(k)$), but is ambiguous up to wave vector $2\pi/a$, or **G** (R.L. vector) in general.
- $\hbar k$ (or sloppily just k) is called "**crystal momentum**"
- A continuous translational symmetry is broken but there is a discrete translational symmetry. Symmetry implies a conserved quantity, which in this case is the crystal momentum.
- It is as though the "new vacuum," i.e. the lattice, is able to impart momentum $\hbar\mathbf{G}$ to any wave (phonon, electron, neutron, photon, …) that exist in it (remember Bragg's diffraction $\mathbf{q}=\mathbf{G}$).

How phonons came to be

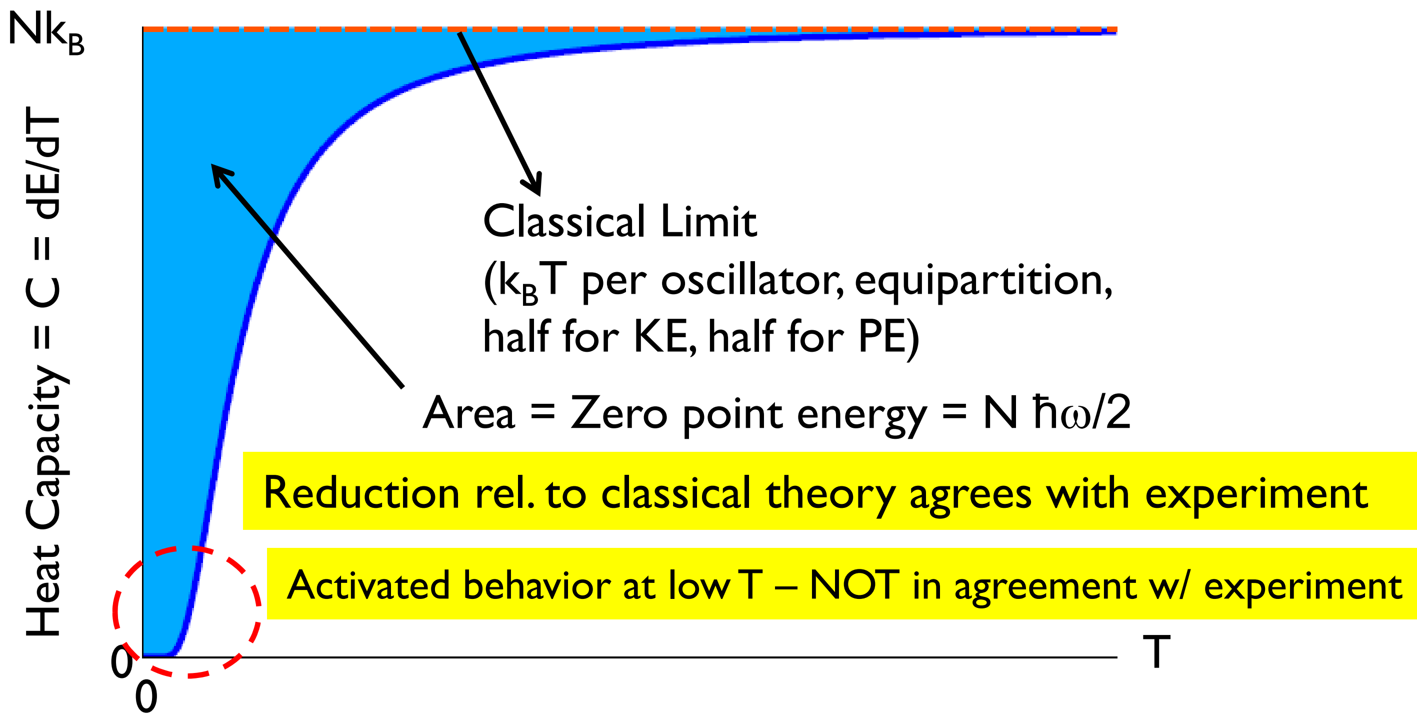




- Einstein Phonon: **$\omega = \omega_0$ = constant**
  Independent single oscillator at each atom
- Debye Phonon: **ω = vk**
  Sound wave

Thermodynamics of Einstein Phonon

- Single frequency mode per lattice point and no coupling between neighboring mode → ω is independent of k ("dispersion-less")
- Just treat like N independent oscillators.



Einstein Phonon Problem (N=1)

Stat. Mech. $$E = \frac{\sum_{n=0}^{\infty}\left(n+\frac{1}{2}\right)\hbar\omega\exp\left[-\frac{\left(n+\frac{1}{2}\right)\hbar\omega}{k_B T}\right]}{\sum_{n=0}^{\infty}\exp\left[-\frac{\left(n+\frac{1}{2}\right)\hbar\omega}{k_B T}\right]} = \frac{1}{Z}\frac{\partial Z}{\partial(-\beta)} = -\frac{\partial(\ln Z)}{\partial\beta} \qquad \beta = \frac{1}{k_B T}$$

$$Z = \sum_{n=0}^{\infty}\exp\left[-\left(n+\frac{1}{2}\right)\beta\hbar\omega\right] = \exp\left(-\frac{1}{2}\beta\hbar\omega\right)\frac{1}{1-\exp(-\beta\hbar\omega)} \qquad -\ln(Z) = \frac{1}{2}\beta\hbar\omega + \ln[1-\exp(-\beta\hbar\omega)]$$

n(ω): Bose Einstein Func

$$E = \frac{1}{2}\hbar\omega + \hbar\omega\frac{\exp(-\beta\hbar\omega)}{1-\exp(-\beta\hbar\omega)} = \frac{1}{2}\hbar\omega + \frac{\hbar\omega}{\exp(\beta\hbar\omega)-1} = \boxed{\frac{1}{2}\hbar\omega + \hbar\omega\cdot n(\omega)}$$

Gapped, or Activated behavior

Heat Capacity

$$C = \frac{\partial E}{\partial T}$$

Low Temperature $\beta\hbar\omega \to \infty$

$$n(\omega) \approx \exp(-\beta\hbar\omega)$$

$$E \approx \frac{1}{2}\hbar\omega + \hbar\omega\exp\left(-\frac{\hbar\omega}{k_B T}\right)$$

$$C \approx k_B\left(\frac{\hbar\omega}{k_B T}\right)^2\exp\left(-\frac{\hbar\omega}{k_B T}\right)$$

High Temperature $\beta\hbar\omega \to 0$

$$n(\omega) \approx (\beta\hbar\omega)^{-1}\cdot\left(1-\frac{1}{2}\beta\hbar\omega\right)$$

$$E \approx k_B T\left(1 + O\left(\frac{\omega}{T}\right)^2\right)$$

$$C \approx k_B$$

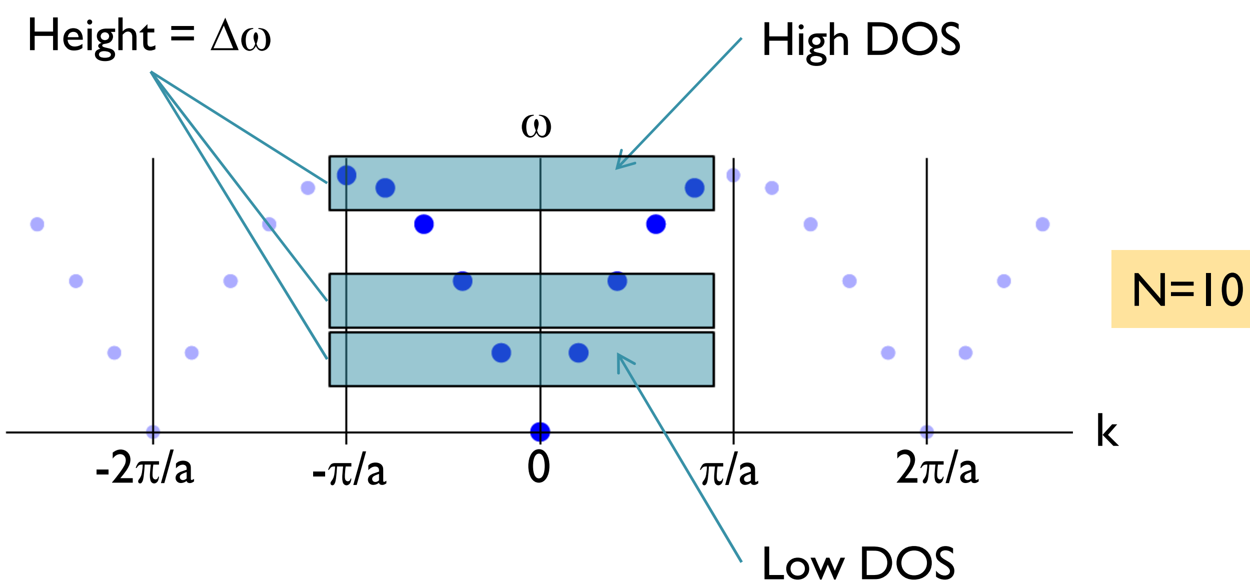
Classical Mech

$$\int_0^{k_B T} dT\, C = \int_0^{k_B T} dT\,\hbar\omega\frac{\partial n(\omega,T)}{\partial T} = \hbar\omega[n(\omega,T) - n(\omega,T=0)] \to k_B T - \frac{1}{2}\hbar\omega = \text{classical energy} - \frac{1}{2}\hbar\omega$$ as $\frac{k_B T}{\hbar\omega} \to \infty$

Thus, $$\int_0^{\infty} dT\, C_{classical} - \int_0^{\infty} dT\, C_{quantum} = \frac{1}{2}\hbar\omega$$

Density of States (DOS)

- For a given constant $\Delta\omega$, the number of available quantum states = number of blue dots = Density of States

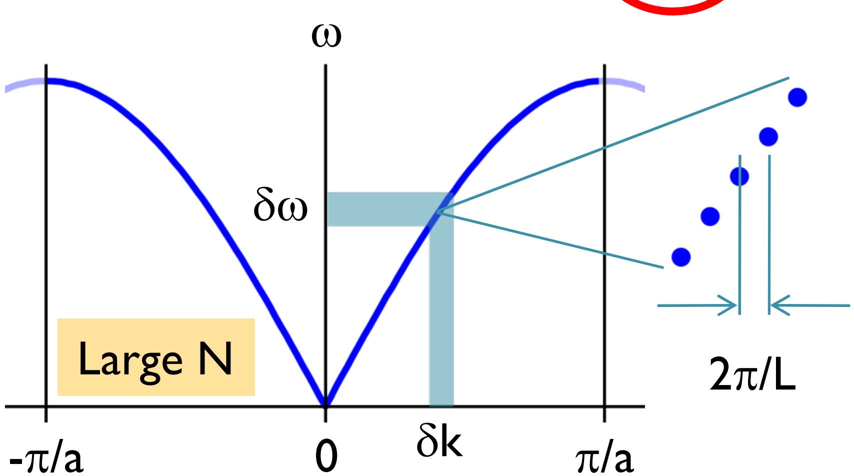


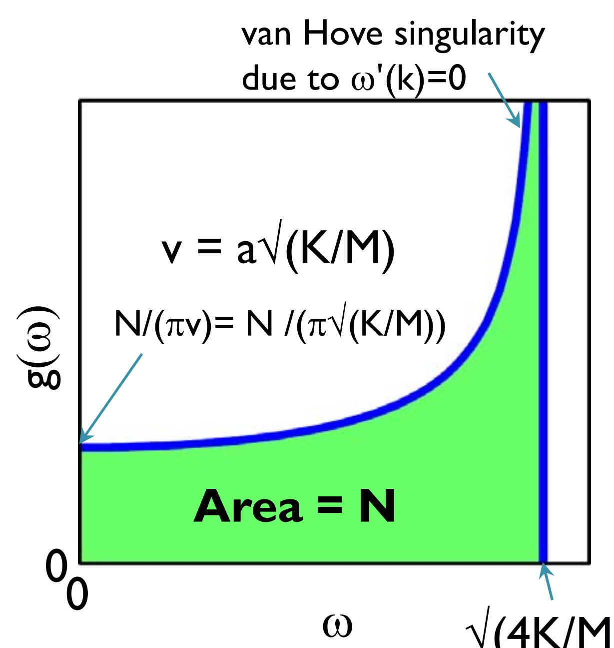
Density of States (DOS)

- Given $\omega=\omega(k)$, # of quantum states for $\delta\omega$

  $= \delta k \cdot 2 /(2\pi/L)$

  $= (\delta k/\delta\omega) \cdot \delta\omega \cdot L/\pi \equiv g(\omega)\ \delta\omega$
- $g(\omega) \equiv$ DOS per unit energy and unit system "volume" $= L/(\pi\omega'(k))$





DOS in 3D

- Special case of $\omega = vk$ where $k = |\mathbf{k}|$ (Easily generalized to $\omega = \omega(k)$)
- Number of states in small volume element in **k** space = $\delta k_x \delta k_y \delta k_z/(2\pi/L)^3 = \delta(\cos\theta)\delta\phi\delta k/(2\pi/L)^3 = \delta(\cos\theta)\delta\phi k^2\delta k\, V/(2\pi)^3$ $(V=L^3)$
- To calculate DOS, note that ω depends only on k, $\delta\omega = v\delta k$. I.e., integrate over θ, ϕ.

  $g(\omega)\delta\omega = 4\pi k^2 \delta k\, V/(2\pi)^3 = \omega^2\delta\omega V/(2\pi^2 v^3)$
- Now consider 1 longitudinal and 2 transverse:

  $g(\omega) = V\omega^2(1/v_L^3 + 2/v_T^3)/(2\pi^2)$
- Debye Model: Determine ω_D from $\int_0^{\omega_D} d\omega\, g(\omega) = 3N$

  (N = # of primitive lattice points)