Physics 489 S 04 Lecture 10
Quantized Lattice Vibrations, Thermal Properties (A & M chapter 23)

1. Review of classical theory:
   Within harmonic approximation, the exact solution of lattice vibrations is a set of *independent harmonic oscillators*, labelled by wavevector $\mathbf{k}$
   For each $\mathbf{k}$ there are $s = D * S$ modes (D = dimension; S = # atoms per cell) with frequency $\omega_s(\mathbf{k})$
   There are D acoustic modes with $\omega \to 0$ as $\mathbf{k} \to 0$

2. Quantum Theory (Using results stated in Review of Statistics, Lecture 1)
   Each oscillator of frequency ω has quantized energies $E_n = (n + 1/2)\hbar\omega$
   Quantum particles (phonons) obeying Bose statistics
   Average occupation: Planck distribution, $< n >= (e^{\beta\hbar\omega} - 1)^{-1}$, $\beta = 1/k_B T$
   Total energy density: $(1/V)E_{tot} = (1/V)\sum_{s,\mathbf{k}} \hbar\omega_s(\mathbf{k}) \left(< n_s(\mathbf{k}) > +\frac{1}{2}\right)$

3. Specific Heat $C_V = (1/V)dE_{tot}/dT = (1/V)\sum_{s,\mathbf{k}} \hbar\omega_s(\mathbf{k}) \frac{d< n_s(\mathbf{k})>}{dT}$
   For $k_B T >> \hbar\omega$, $< n >= k_B T/\hbar\omega$, and C_V approaches the classical value Dk_B per nucleus, D = dimension
   For low T only vibrations with $\omega_s(\mathbf{k})$ of order $k_B T$ contribute to C_V
   For sufficiently low T in all solids, only acoustic modes with $\omega = v_{sound}k$ contribute and $C_V \propto T^D$, where D = dimension

4. Debye model (correct for acoustic modes, qualitatively correct for other modes)
   Approximate all frequencies by $\omega = v_{sound}k$, v_{sound} = spherical average
   $k_{max} = k_D$ defined to sum to the right number of modes
   In 3 dimensions, k is in a sphere with volume $(4\pi/3)k_D^3 = (2\pi)^3/V_{atom}$
   Debye Temperature Θ_D defined by $k_B\Theta_D = \omega_{max} = v_{sound}k_D$
   At low T, $C_V = 3(N/V)k_B(4\pi^4/5)(T/\Theta_D)^3$ (in 3D)
   Can consider C_V at low T to define Θ_D for a given material

5. Einstein Model: $\omega_s(\mathbf{k})$ modelled as constant ω_s independent of k
   (Appropriate for optic modes only)
   Gives $C_V \propto exp(-\beta\hbar\omega_s)$ for low T

6. Typical magnitudes
   Phonon energy $\hbar\omega = 0$ to a maximum value of $\approx 10^{-2}$ to $\approx 10^{-1}$ eV
   Debye energy - $\approx 10^{-2}$ to $\approx 10^{-1}$ eV, Debye Temperature - ≈ 100 to ≈ 1000 K

7. Density of states = number of states per unit energy per unit volume
   Determines all quantities that depend only on energy, e.g., C_V
   $g(\omega) = (1/V)\sum_{s,\mathbf{k}} \delta(\omega - \omega_{s,\mathbf{k}})$
   For vibrations at low ω, $g(\omega) \propto \omega^{D-1}$, where D is the dimension.

Figure 1: Phonon dispersion and density of states in 1 and 3 dimensions

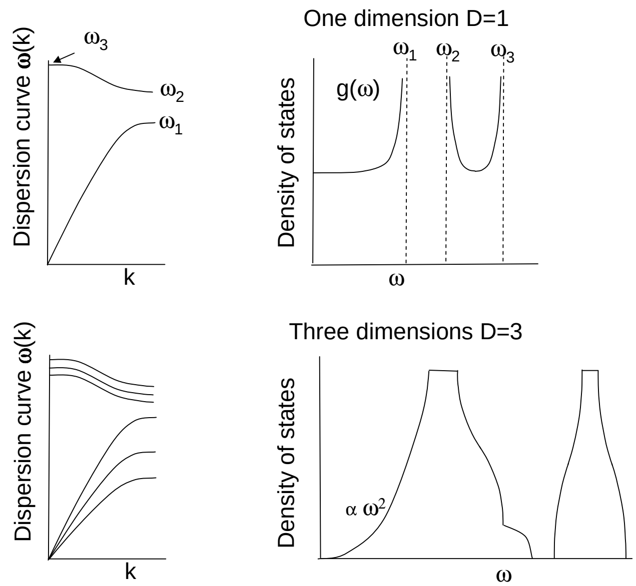

Figure 2: Debye approximation to the dispersion and density of states in 3 dimensions. Typical specific heat which is reasonably approximated by Debye model.