Physics 489 S 04 Lecture 8
Lattice Vibrations I (Ashcroft and Mermin, chapter 21, 22)

1. Failure of the Static Lattice Model. Vibrations of nuclei needed to explain:
   i) Specific heat, thermal expansion, melting
   ii) Lattice contribution to thermal conductivity
   iii) Scattering of electrons: origin of electronic relaxation; resistivity
   iv) Sound waves
   v) Scattering of light, x-rays, neutrons, ...
   vi) Quantum effects: Specific heat at low T not given by classical equipartition; zero point motion; superconductivity.

2. Adiabatic (Born-Oppenheimer) approximation.
   Electrons follow the nuclei instantaneously
   Electrons always in their ground state which is a function of nuclear positions
   Energy of system = function of coordinates of nuclei, $E(\{\mathbf{R}_i\})$

3. Harmonic approximation.
   Define nuclear coordinates $\mathbf{R}_i = \mathbf{R}_i^0 + \mathbf{u}_i$, $\mathbf{u}_i$ is displacement from equilibrium
   Harmonic approximation - energy expanded to second order in the $\mathbf{u}_i$
   Breaks down for high temperature (near melting), near certain phase transitions (where the lattice is very soft), and in 'quantum' solids (H and He).

4. General Expansion: $E = E_0 + 1/2 \sum_{ij} \mathbf{u}_i D_{ij} \mathbf{u}_j$, where $D_{ij} = d^2E/d\mathbf{u}_i d\mathbf{u}_j$
   For a crystal D_{ij} is function only of the relative positions of the cell of atom i and atom j

5. Pair Approximation: $E = 1/2 \sum_{ij} \phi(|\mathbf{R}_i - \mathbf{R}_j|)$
   Convenient form - accurate for rare gases, ionic crystals, some metals

6. One dimensional chain: Positions of atoms $R_n^0 = na$.
   Nuclei of mass M, connected by springs of force constant K.
   Displacements must obey the relation $u_n(t) = \exp(ikna - i\omega t)$ (easier than sin or cos functions)
   Dispersion relation $(\omega(k))^2 = 2(K/M)[1 - \cos(ka)]$ or $\omega(k) = 2(K/M)^{1/2} \sin(ka/2)$
   Describes the"Normal modes", independent modes of vibration of the crystal
   Vibrations at one wavevector k independent of vibrations at other k'
   Allowed values of $k = (2\pi/a)(m/N)$; $-\pi/a < k < \pi/a$ (First Brillouin Zone).
   Velocity of sound $v_s = \frac{lim}{k\to 0} d\omega/dk = a(K/M)^{1/2}$
   Group velocity $v_{group} = d\omega/dk$ goes to zero at BZ boundary.

7. One dimensional chain with basis.
   2 atoms per cell: 2x2 determinant; 2 dispersion curves $\omega_m(k)$; acoustic, optic
   For S atoms per cell: S dispersion curves; 1 acoustic; S-1 optic

8. Counting of modes
   N nuclei in a ring: N degrees of freedom give N normal modes.
   $k = (2\pi/a)(M/N)$; $(1/L)\sum_k \to (1/2\pi)\int_{BZ} dk$

9. Typical magnitudes:
   $K \approx E_{coh}/(bondlength)^2$; $\omega \approx 10^{13} rad/sec$; $v_{sound} \approx 10^5 cm/sec$