QM: Phonons

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Phonons are collective atomic vibrations

C is spring constant;
u_s is sth atomic position
spring compression i.e. $x=u_s-u_{s-1}$

Force $$F_s = C(u_{s+1} - u_s) + C(u_{s-1} - u_s) \; .$$

Using Newton's laws

$$M\frac{d^2u_s}{dt^2} = C(u_{s+1} + u_{s-1} - 2u_s)$$

Assume a plane wave solution

$$\psi = e^{i(kx-\omega t)}$$

where $x = sa$ as each site is a lattice point cf. electron where any x is allowed

$$-M\omega^2 u_s = C(u_{s+1} + u_{s-1} - 2u_s) \; .$$

Assume $$u_{s\pm1} = u\,\exp(isKa)\exp(\pm iKa)$$

$$-\omega^2 Mu\,\exp(isKa) = Cu\{\exp[i(s+1)Ka] + \exp[i(s-1)Ka] - 2\exp(isKa)\}$$

We cancel $u\,\exp(isKa)$ from both sides, to leave

$$\omega^2 M = -C[\exp(iKa) + \exp(-iKa) - 2] \; .$$

$$\omega^2 = (2C/M)(1 - \cos Ka)$$

$$\omega = (4C/M)^{1/2}\left|\sin \tfrac{1}{2}Ka\right|$$

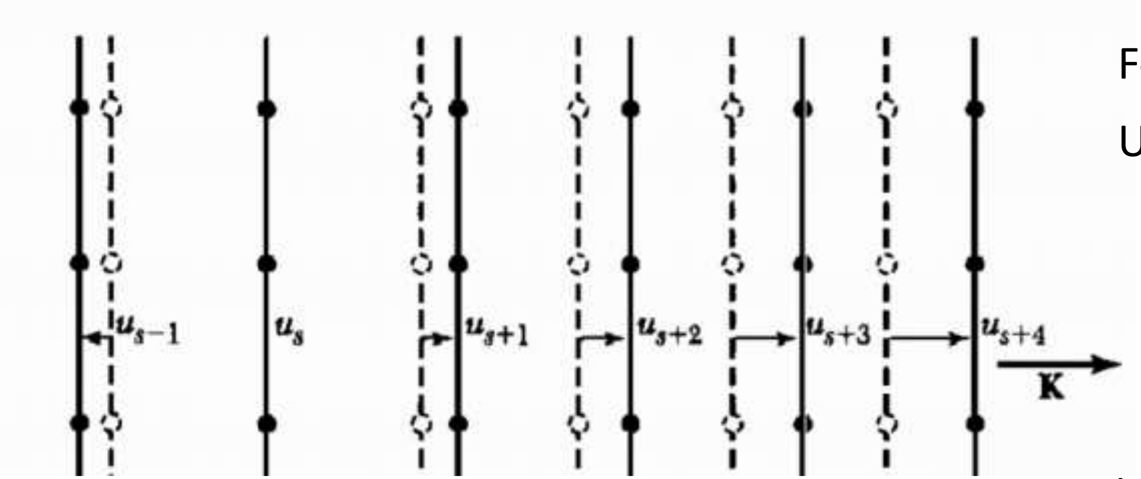
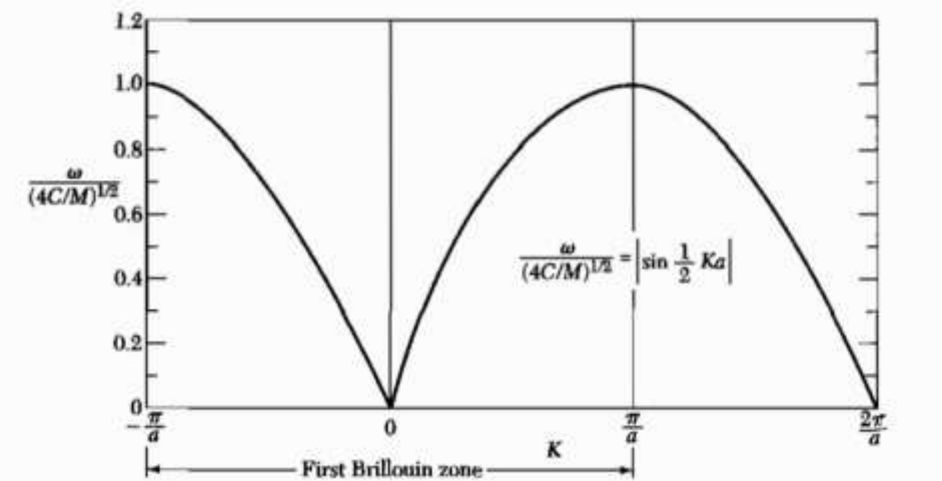


Figure 2 (Dashed lines) Planes of atoms when in equilibrium. (Solid lines) Planes of atoms when displaced as for a longitudinal wave. The coordinate u measures the displacement of the planes.



Phonon: A pseudo-particle

- The ω-k or E-k diagram is shown where $E=\hbar\omega$
- Each k crystal plane wave modes
- Like electrons; pseudo-particle can be generated as wave packets where
  - velocity = group velocity
  - Mass is $\hbar$/curvature
- Note: Electrons are charge waves in a crystal that are treated as particles; phonons are collective atomic oscillations in a crystal that can be treated as particles.

What is the group velocity and mass at $k \rightarrow 0$? As phonons are bosons, most particles are at $k \rightarrow 0$ or lowest energy

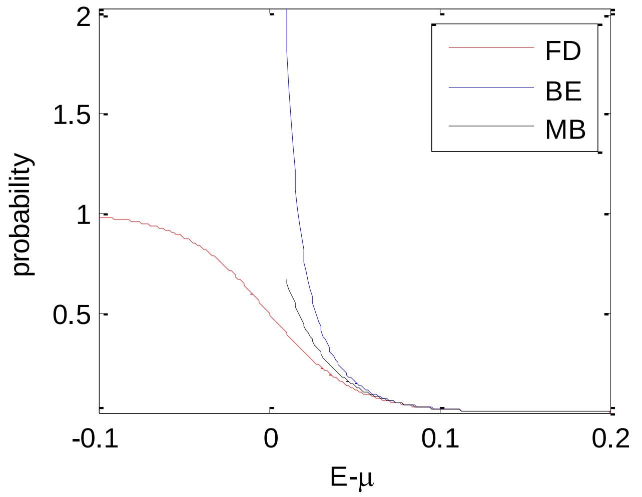
Bose-Einstein Statistics

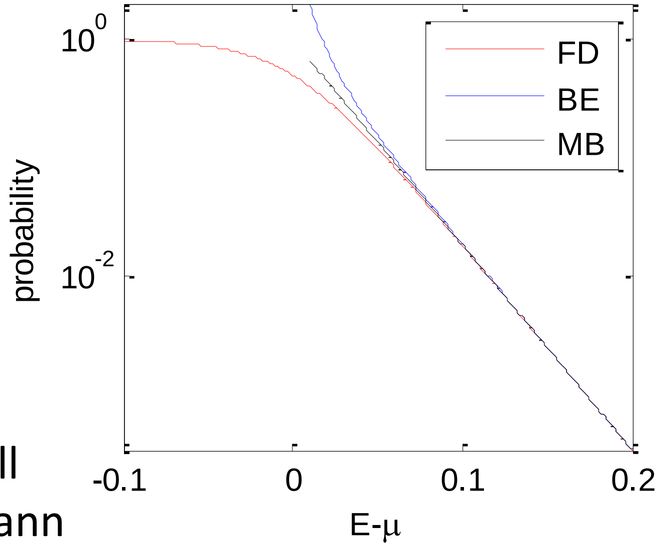
- Phonons are bosons i.e. they obey Bose Einstein Distribution
- Unlike FD, bosons can occupy the same state (no Pauli's exclusion); Hence μ (chemical potential) is zero and most particle populate lowest energy
- At higher energies, both FD and BE tend to MB distribution

$$f(E) = \frac{1}{\exp\left(\frac{E-E_F}{kT}\right) \pm 1} \sim \exp\left(-\frac{E-E_F}{kT}\right)$$

Maxwell Boltzmann Distribution

+ Fermi Dirac Distribution
- Bose Einstein Distribution





Try this demo http://demonstrations.wolfram.com/BoseEinsteinFermiDiracAndMaxwellBoltzmannStatistics/

Two types of phonons

- Acoustic phonons: Like sounds waves where adjacent atoms are in phase ➔ generally low energy ➔ causes normal scattering

- Optical phonon: When light moves through an ionic crystal, adjacent ions feel opposite force for same E field due to opposite charge ➔ they move out of phase; High energy ➔ causes velocity saturation

- Which States are primarily filled by phonons?
- Approx. above kT from zero energy

http://en.wikipedia.org/wiki/Phonon