Condensed Matter Physics – FK7042, Feb. 18, 2016.

Lecture 9 – Lattice vibrations

Reading

Ashcroft & Mermin, Ch. 21, Ch. 22 (p. 422, 428 - 437. p. 438 - 443 for overview)

Content

- Failures of the static lattice
- Harmonic approximation
- Adiabatic approximation
- Law of Dulong and Petit
- Normal modes
- One-dimensional case
- Velocities
- Dispersion relation
- Polarization vectors
- Acoustic and optical branches

Central concepts

- **Failures of the static lattice (Ch. 21)**

  Failures to explain **equilibrium properties**:
  - *Specific heat*, $C(T) \sim T^3$ for both metals and insulators at low T.
  - *Thermal expansion*
  - *Melting*

  Failures to explain **transport properties**:
  - Temperature dependence of relaxation time τ, *resistivity* etc.
  - Failure of *Wiedemann-Franz law* at intermediate temperature
  - Appearance of *superconductivity*
  - Thermal conductivity of insulators
  - Transmission of *sound* in insulators

  Failure to explain **interaction with radiation**:
  - Maximum in *reflectivity* at infrared frequencies for ionic crystals
  - *Inelastic scattering* (frequency shift of relected light)
  - Decreased amplitude of *x-ray* Bragg peaks, background
  - *Neutron scattering* show loss of energy in definite, discrete amounts

- **Harmonic approximation**

  Each ion is displaced only small distances compared with the interionic spacing. This gives a harmonic force, proportional to the displacement.

- **Adiabatic approximation**

  Electrons have time to assume their ground states for a particular ionic configuration even when the ions move.

- **Law of Dulong and Petit**

  Classical result for specific heat due to the lattice vibrations

  $$c_v = \frac{\partial u}{\partial T} = 3nk_B$$

  Deviations are observed at low temperature, where c_v decreases, but also at higher temperatures because of anharmonic terms.

- **Normal modes**

  A general motion of N ions is represented as a superposition (linear combination) of $3N$ *normal modes* of vibration, each with its own characteristic frequency.

  The allowed energies of an oscillator with frequency ν are given by

  $$\left(n + \frac{1}{2}\right)h\nu, \qquad n = 0, 1, 2, \ldots \qquad (h\nu = \hbar\omega)$$

  The $3N$ normal modes correspond to $3N$ oscillators, each with the above possible energies.

- **One-dimensional case**

  Lattice spacing a, length $L = Na$, ion mass M, lattice vectors $R = na$, $n = 0, 1, 2, \ldots$

  Displacements

  $$u_n(t) = Ae^{i(Kna-\omega t)}$$

  where $K = 2\pi/\lambda$ is the wave vector and ω is the angular frequency.

  The solution has N distinct values of K ranging from $-\pi/a$ to π/a (contained to the 1st Brillouin zone), each with a unique frequency

  $$\omega(K) = \sqrt{\frac{4C}{M}}\left|\sin\frac{Ka}{2}\right|$$

  For a *lattice with a basis*, there are pN normal modes, where p is the number of ions in each of the N primitive cells. There are still N values of K, so each K will give p solutions for ω.

- **Velocities**

  Group velocity

  $$v = \frac{\partial\omega}{\partial K}$$

  The group velocity goes to zero at the Brillouin-zone boundary.

  Phase velocity

  $$c = \frac{\omega}{K}$$

  Sound waves propagate with a velocity $v_s = (\partial\omega/\partial K)|_{K\to 0}$

- **Dispersion relation**

  The relation between ω and K is known as the dispersion relation.

- **Polarization vectors**

  The vibrations have different polarization directions. There is always a longitudinal polarization. In 3D crystals, there are also 2 transverse polarizations, and in 2D crystals one transverse polarization.

  In a crystal with N ions there are N vibration modes per polarization direction. For each K, there are thus $3p$ solutions for ω in 3D crystals.

- **Acoustic and optical branches**

  The $3p$ curves of ω vs. K (in 3D) are known as *branches*. Three branches are known as the *acoustic branches*, and follow $\omega = cK$ at small K. The $3(p-1)$ other branches (depending on how many ions p there are per primitive cell) are known as *optical branches*. Such branches have a finite ω at long wavelengths (K near 0), and can interact with electromagnetic radiation.

  In an acoustic mode, all ions within a primitive cell move essentially in phase, as a unit. In an optical mode, the ions in each cell are resembling molecular vibrations, which are broadened into a band of frequencies due to intercellular interactions.