Lecture 13

Semi-Classical EOM

Semiconductors

Sometimes less is more.

Semi-Classical Equation of Motion

- $\hbar\, d\mathbf{k}/dt = -\,\text{grad}\, V$

  Here, V is the potential for electron.

  Much like Newton's law, except for "crystal momentum."

  Assumptions for this EOM are

  1. Wave packet: $\Delta k << \text{BZ size}$
  2. V varies slowly in space – wave packet can be thought of as a point particle in considering V

- Energy conservation from the EOM

  $d\varepsilon(\mathbf{k}) / dt = -\,\mathbf{v} \cdot \text{grad}\, V$

  $\mathbf{v} = \text{grad}_{\mathbf{k}}\, \varepsilon(\mathbf{k}) / \hbar \quad \rightarrow$ group velocity

- <u>Derived and NOT equivalent</u>: $m^* d\mathbf{v}/dt = -\,\text{grad}\, V$

  $m^* = \hbar^2 [d^2\varepsilon(k) / dk^2]^{-1}$

  This form is NOT as fundamental as the above. E.g., it cannot be used if $\varepsilon(\mathbf{k})$ is linear (as in metal).

- Generalized to the Lorenz force case, too (see A&M).

General (also for metal)

Note

Equation of Motion for Transport

- Simple relaxation time approximation as we discussed and used for metal

$$\hbar\,(d/dt + 1/\tau)\,\delta\mathbf{k} = -\,\mathrm{grad}\,V = \mathbf{F}$$

or

$$m^*\,(d/dt + 1/\tau)\,\mathbf{v}_d = \mathbf{F}$$

- $\delta\mathbf{k}$ is a net displacement of the whole
- The first form is more fundamental
- The second form simply defines $\mathbf{v}_d$ by $\hbar\,\delta\mathbf{k} = m^*\,\mathbf{v}_d$ where m* is an "effective mass"

General (also for metal)

General Results from SC-EOM

- Bravais Lattice of ions gives perfect conductivity – the source of a finite conductivity is imperfections, phonons, other electrons.
- Completely filled bands or completely empty bands are as good as nothing. ⇔ Only partially filled bands do things like conduct electricity and heat. (This is why a FS is so important! Distinction between metal and non-metals.)
- A few electrons missing from a completely filled band are best described by "holes."

Triumph of Band Theory

- Metal – has Fermi surface (FS) at T=0
- Insulators, Semiconductors – no FS at T=0

- Metal – resitivity increases as T increases
- Insulators, Semiconductors – opposite

- Resitivity can range from 10^{-10} Ωcm (good metal) to 10^{22} Ωcm (32 orders of magitude!)

- Triumph of Quantum Mechanics applied to periodic potential (band theory) – Si is the "poster child" of band theory

Hole

- As in metal, consider the vacuum as the T=0 state – hole is a fermionic excitation of the valence band, completely full at T=0
- EOM $\hbar\, d\mathbf{k}/dt = \mathbf{F}$ was derived for an electron. When a band is full and there is one electron missing, however, it is better to think of a "hole."
    1. The energy, (crystal or angular) momentum, and charge for a hole is the opposite of that for an electron.
    2. The righ hand side (force) has to change sign from e to h.
    3. The group velocity of a hole is the same as the group velocity of an electron.
- The motion of all electrons except one is more conveniently, or more "correctly," discussed as the motion of one hole and nothing else.

General (also for metal)

Note

Effective mass

1. At band maximum or minimum, the energy band can be written as $\propto k^2/m^*$, where m^* is the "effective mass," which can be defined as $\hbar^2[d^2\varepsilon(\mathbf{k})/dk^2]^{-1}$.
2. The definition above is useful mainly for semiconductors and semi-metals.
3. m^* tends to be small ~ a tenth of the mass of free electron (i.e. actual excitation is <u>lighter</u> than free electron). [HW]
4. For metals, energy dispersion near E_F is approximated as linear – effective mass m^* is then defined in terms of v_F ($v_F = v_{F0}/m^*$) and it tends to be larger than the mass of free electron (i.e. actual excitation is <u>heavier</u> than free electron), due to the electron-electron interaction or a "tight-binding-like" nature of band, both important for TM or RE materials.

Note