Lecture 7
Semiconductors

Sometimes less is more.

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

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).
4. For metals, energy dispersion near E_F is approximated as linear – effective mass m^* is then defined in terms of v_F 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

Equation of Motion

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

  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 << $ 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

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

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

- Derived and not equivalent: $m^* d\mathbf{v}/dt = -\,\mathrm{grad}\,V$

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

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

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)

Effect of Lattice on Conductivity

- This EOM was used (without proof) in considering the conductivity of metals.
- We have also stated then, without proving, that the perfect lattice does not cause any resistivity.
- Indeed, the conductivity in a periodic potential would be <u>infinite</u> if there is no other form of scattering, no matter what the band structure is (or no matter what the lattice constant is), as long as there are <u>some</u> carriers.

General (also for metal)

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

Charge Carriers in a Semiconductor

- Electrons in conduction band
- Holes in valence band
- Intrinsic Semiconductors: Carriers are created by excitation across the energy gap E_G
- Extrinsic Semiconductors: Carriers are provided by impurities (donors, acceptors)

Donors and Acceptors

- Consider Si or Ge, both with 4 valence electrons
- Substitutional impurities with 5 valence electrons (P, As) are donors
- Substitutional impurities with 3 valence electrons (B, Al) are acceptors
- Donors (acceptors) create impurity states just below (above) the conduction (valence) band, at energy ~ O(10) meV

Note

Charge Carrier Population (General)

- Define energy 0 = top of valence band
- Electron density: $\mathbf{n = N_c \exp(\beta(\mu - E_G))}$

  $N_c = 2\,(m_e k_B T/2\pi\hbar^2)^{3/2}$
- Hole density: $\mathbf{p = N_v \exp(-\beta\mu)}$

  $N_v = 2\,(m_h k_B T/2\pi\hbar^2)^{3/2}$
- $np = N_c N_v \exp(-\beta E_G) = n_i p_i = n_i(T)^2 = p_i(T)^2$

  Law of mass action

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Note

Charge Carrier Population (Intrinsic Semiconductors)

- $n_i = p_i$
- $n_i = p_i = (N_c N_v)^{1/2} \exp(-\beta E_G/2)$
- Intrinsic carrier density:

  $n_i = p_i \sim 10^{16}$ (Si) and 10^{19} (Ge) m^{-3}

  (fewer than in metals by ~ 10 orders of magnitude or more)
- Chemical Potential for Intrinsic Semi-cond:

  $$\mu = \tfrac{1}{2} E_G + \tfrac{3}{4} k_B T \ln (m_h/m_e)$$

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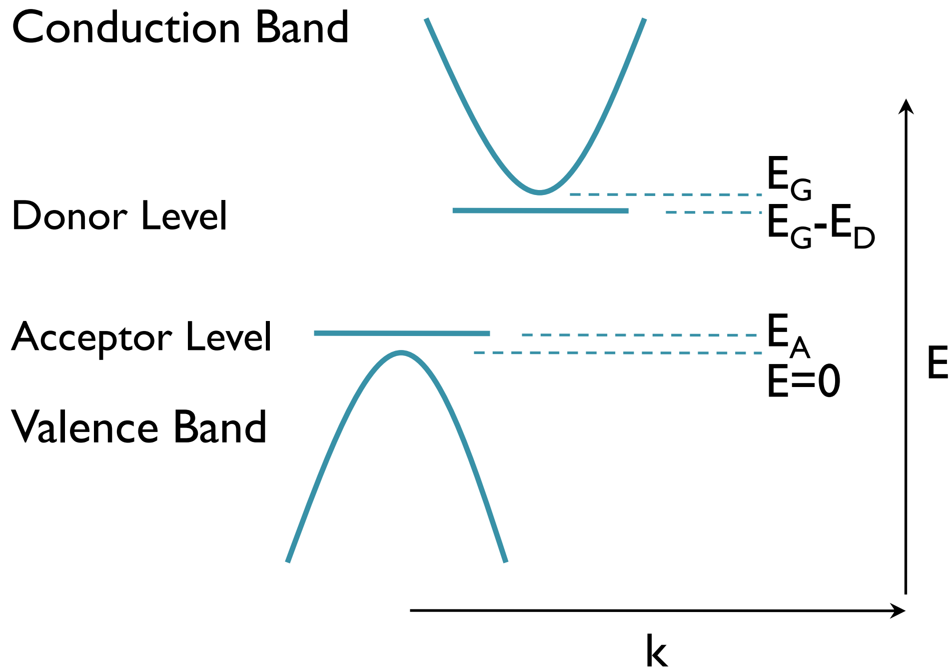
Note

Warning: In semi-conductor literature, the chemical potential is very often referred to as the "fermi level." This is an unfortunate and un-recommended mis-nomer, as there is no Fermi surface!

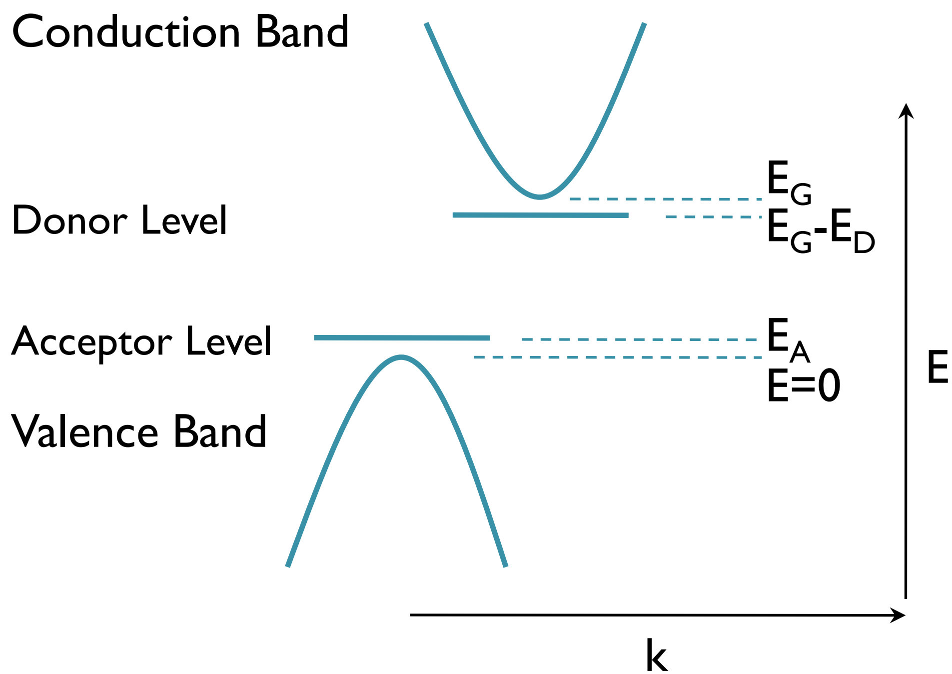
Charge Carrier Population (Extrinsic Semiconductors)



At T = 0

- Conduction Band A. is full B. is empty C. can have some electrons
- Valence Band is full
- Donors may have some electrons to spare, acceptors holes

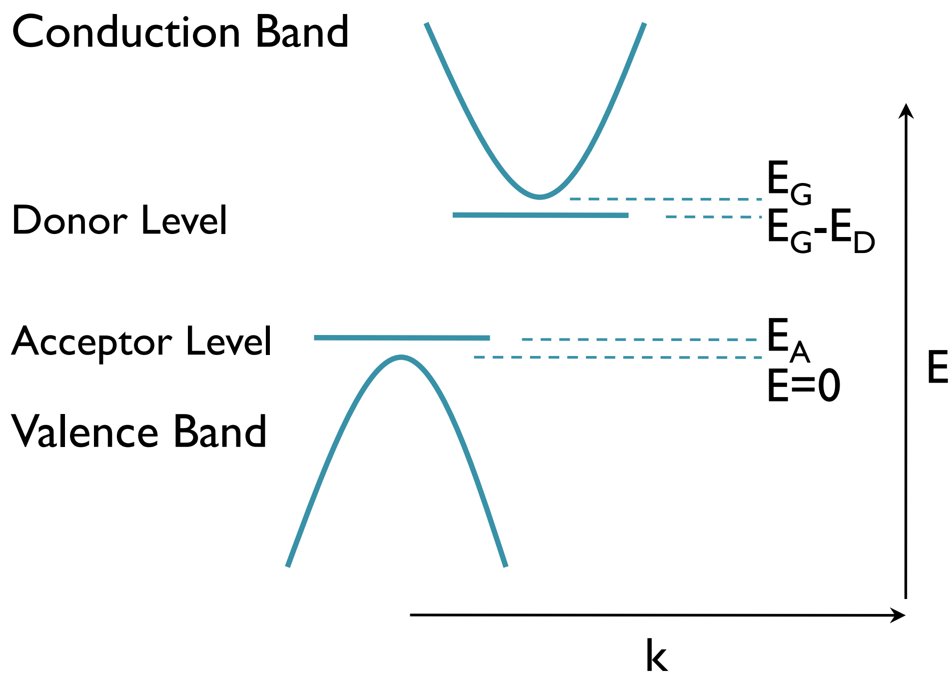
Charge Carrier Population (General)



At T = 0

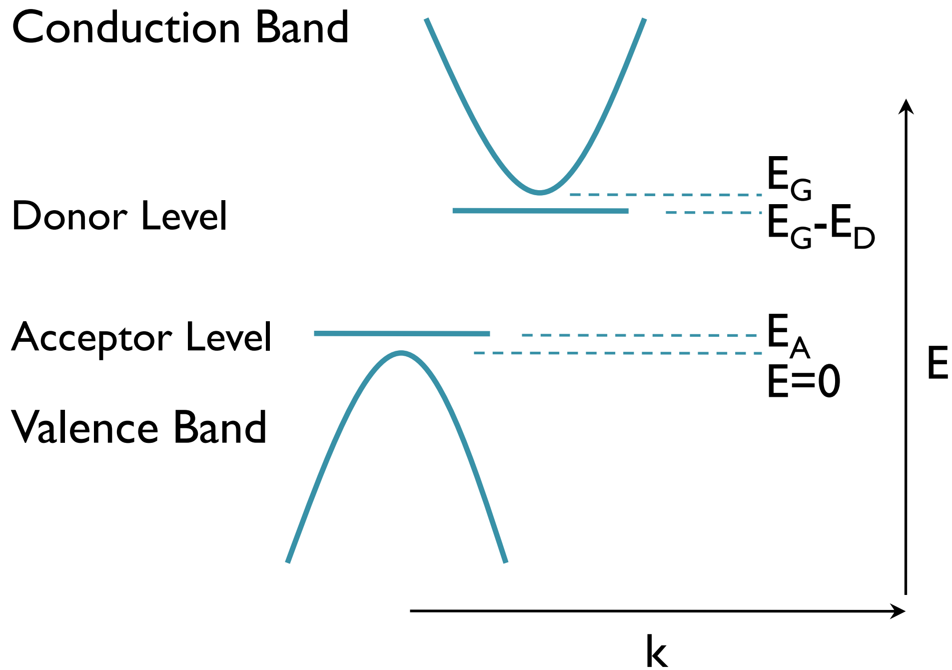
- Conduction Band is empty
- Valence Band is full
- Donors may have some electrons to spare, acceptors holes

Charge Carrier Population - Where is Chemical Potential at <u>T=0</u>?



- Common n-type (More donors than acceptors; <u>majority carriers</u> are electrons from donors, and <u>minority carriers</u> are holes from acceptors): A. $E_G/2$ B. E_G-E_D C. E_A
- Common p-type: E_A
- Pure n-type: A. $E_G/2$ B. E_G-E_D C. E_G-0.5E_D
- Pure p-type: $E_A/2$
- Intrinsic: $E_G/2$

Charge Carrier Population
- Where is Chemical Potential at T=0?



- Common n-type (More donors than acceptors; majority carriers are electrons from donors, and minority carriers are holes from acceptors): E_G-E_D
- Common p-type: E_A
- Pure n-type: E_G-0.5E_D
- Pure p-type: $E_A/2$
- Intrinsic: $E_G/2$

Extrinsic Semiconductors (n-type)

- For $T \approx 0$

  $\mu \approx E_G - E_D$ (common n-type: small # of acceptor impurities)
  $E_G - 0.5\ E_D$ (pure n-type: absolutely no acceptors)

  $n \approx N_c \exp(-\beta E_D)$ (common n-type)
  $N_c \exp(-\beta E_D/2)$ (pure n-type)
- $n >> n_i$: electron is **majority** carrier
- $p << p_i << n$ (recall $np = n_i p_i$): hole is **minority** carrier
- As T increases (~ E_D), all donors lose electrons

  $n \approx N_D - N_A$ (N_A: acceptor # density, N_D: donor # density)

  $\mu \approx E_G - k_B T \ln (N_c / (N_D - N_A)) \equiv$ ☆
- Intrinsic behaviors : at even higher T
- μ : E_G – [0.5] $E_D \rightarrow$ ☆ $\rightarrow 0.5\ E_G$ as T ↑
- n(T) : $\exp(-\beta\ [0.5]\ E_D) \rightarrow N_D - N_A \rightarrow \exp(-\beta\ 0.5\ E_G)$

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Extrinsic Semiconductors (p-type)

- For $T \approx 0$

  $\mu \approx E_A$ (common p-type: small # of donor impurities)

  $\quad 0.5\ E_A$ (pure p-type: absolutely no donors)

  $p \approx N_v \exp(-\beta E_A)$ (common p-type)

  $\quad N_v \exp(-\beta E_A/2)$ (pure p-type)

- $p >> p_i$: hole is **majority** carrier
- $n << n_i << p$ ($np = n_i p_i$): electron is **minority** carrier
- As T increases (~ E_A), all acceptors lose holes

  $p \approx N_A - N_D$

  $\mu \approx k_B T \ln (N_v / (N_A - N_D)) \equiv$ ☆

- Intrinsic behaviors : at even higher T
- μ : [0.5] $E_A \rightarrow$ ☆ $\rightarrow 0.5\ E_G$ as $T \uparrow$
- $n(T)$: $\exp(-\beta\ [0.5]\ E_A) \rightarrow N_A - N_D \rightarrow \exp(-\beta\ 0.5\ E_G)$

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Transport Properties (“hole” is real)

- Equation of Motion: $m^* (d/dt + 1/\tau)\, \mathbf{v}_d = \mathbf{F}$ (as we used in metal)
- Hall Effect (for single type of carrier) in B field

  $R_H \equiv E_y/(B_z j_x) = -1/(ne)$ or $1/(pe)$ [sign !]
- Thermo-electric Effect can probe the sign of the carrier charge as well
- Cyclotron Resonance in B field: $\omega_c = eB/m^*$ (SI unit)
- Conductivity

  $\sigma = ne\mu_e + pe\mu_h$

  $\mu_e = e\tau_e/m^*_e = v_{d,e}/E$, and similarly for μ_e

  μ_e, μ_h: mobility

  1. useful concept for semiconductors
  2. characterizes “quality” rather than “quantity” (n or p)
  3. not important for T dependence of σ (determined by exponentials in n or p – see slide “Charge Carrier Population”)

Note

Charge Carrier Motion (n-type)

- Definition

$$n = n_0 + n'(x,t), \quad p = p_0 + p'(x,t)$$

n_0: equilibrium, $n'(x,t)$: non-equilibrium
p_0: equilibrium, $p'(x,t)$: non-equilibrium

- Continuity Equation

$$\frac{\partial n}{\partial t} + \frac{\partial J_e}{\partial x} = g - r \qquad \frac{\partial p}{\partial t} + \frac{\partial J_h}{\partial x} = g - r$$

J: number current not charge current

g: generation rate (source term)

r: recombination rate (sink term)

- Majority Carrier Equation (for no ext. field)

$$\frac{\partial n'}{\partial t} = -\frac{n' - p'}{\tau_D} + \frac{\lambda_D^2}{\tau_D}\frac{\partial^2 n'}{\partial x^2}$$

Majority carriers screen non-equilibrium charge fast :
τ_D ~ psec (10^{-12} sec), λ_D ~ 100 Å

- Minority Carrier Equation

$$\frac{\partial p'}{\partial t} = -\frac{p'}{\tau_n} + D_h \frac{\partial^2 p'}{\partial x^2} - \mu_h E \frac{\partial p'}{\partial x}$$

Minority carriers have slower response :
τ_n ~ 10^{-7} sec, $\lambda = \sqrt{(D_h \tau_n)}$ ~ 10 μm

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Charge Carrier Motion (p-type)

- Definition

$$n = n_0 + n'(x,t), \quad p = p_0 + p'(x,t)$$

n_0: equilibrium, $n'(x,t)$: non-equilibrium
p_0: equilibrium, $p'(x,t)$: non-equilibrium

- Continuity Equation

$$\frac{\partial n}{\partial t} + \frac{\partial J_e}{\partial x} = g - r \qquad \frac{\partial p}{\partial t} + \frac{\partial J_h}{\partial x} = g - r$$

J: number current not charge current

g: generation rate (source term)

r: recombination rate (sink term)

- Majority Carrier Equation (for no ext. field)

$$\frac{\partial p'}{\partial t} = -\frac{p' - n'}{\tau_D} + \frac{\lambda_D^2}{\tau_D}\frac{\partial^2 p'}{\partial x^2}$$

Majority carriers screen non-equilibrium charge fast :
τ_D ~ psec (10^{-12} sec), λ_D ~ 100 Å

- Minority Carrier Equation

$$\frac{\partial n'}{\partial t} = -\frac{n'}{\tau_p} + D_e\frac{\partial^2 n'}{\partial x^2} + \mu_e E \frac{\partial n'}{\partial x}$$

Minority carriers have slower response :
$\tau_p \sim 10^{-7}$ sec, $\lambda = \sqrt{(D_e \tau_p)} \sim 10\ \mu m$

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