6.730 Physics for Solid State Applications

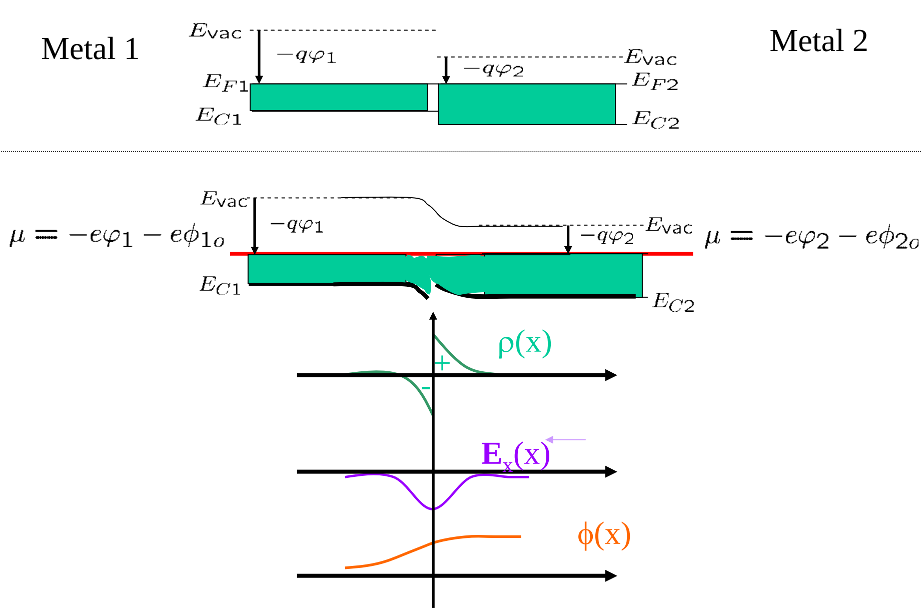
Lecture 27: Quasi-fermi levels and Non-equilibrium

<u>Outline</u>

- •Review of Equilbrium of inhomogeneous materials
  - •Metal-Metal, PN and hetero-junctions- fermi levels
- •Rate Equations for Non-equilibrium Electrons
- • Quasi-Fermi Levels

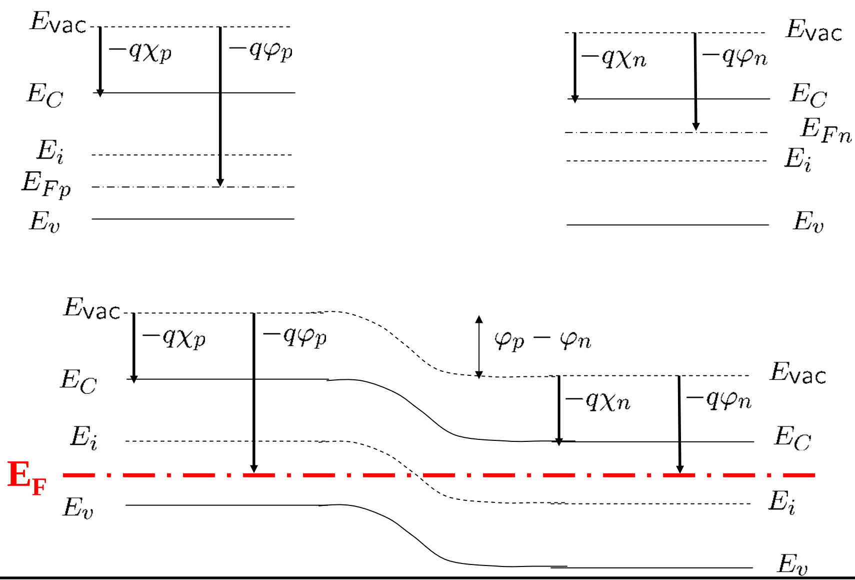
April 12, 2004

Metal-Metal contact

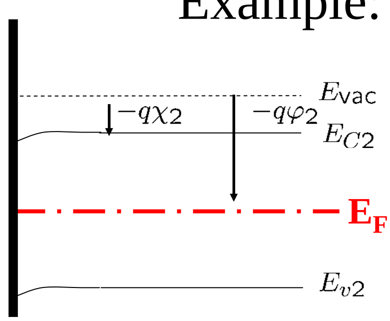


Example: PN-junction

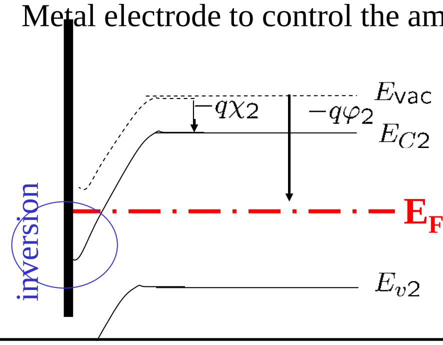
p-doped Si n-doped Si



Example: MOS

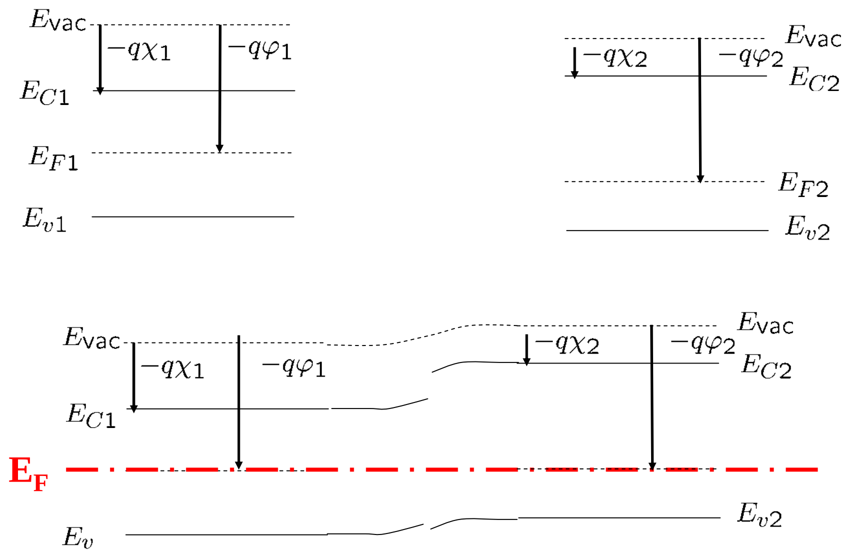


Metal electrode to control the amount of bandbending at the surface



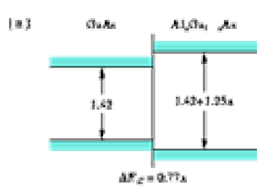
Inversion region looks like the electrons are near the surface, confined by the potential, resulting in a 2D electron gas parallel to the surface.

Example: hetero-junction

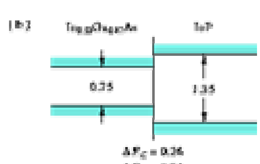


Species of Heterjunctions

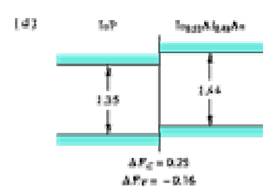
Type I



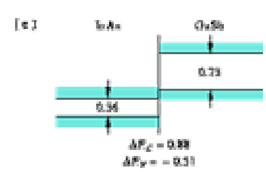
Type I



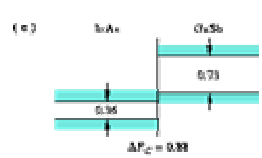
Type II



Type III



Type III



http://www.utdallas.edu/~frensley/technical/hetphys

6.730 Physics for Solid State Applications

Lecture 27: Quasi-fermi levels and Non-equilibrium

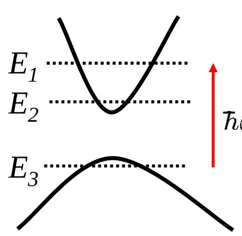
Outline

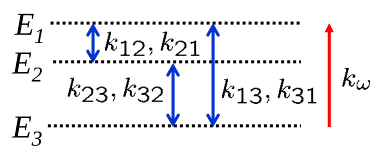
- PN and hetero-junctions- fermi levels
- **Rate Equations for Non-equilibrium Electrons**
- **Quasi-Fermi Levels**

April 12, 2004

Near Equilibrium Electron Distributions

Informative Example: Optical Excitations





k_{12}, k_{21}	Intraband scattering:	electron-electron electron-acoustic phonon
k_{23}, k_{32} k_{13}, k_{31}	Interband scattering:	electron-hole electron-phonon with defects

What are f_1, f_2, & f_3 under illumination (non-equilibrium) ?

Classical Rate Equation Formalism

number of electrons = number of states x probability of occupancy

$$n_1 = N_1 f_1 \qquad n_2 = N_2 f_2 \qquad n_3 = N_3 f_3$$

$$\frac{dn_1}{dt} = -k_{12} N_1 f_1 N_2(1-f_2) + k_{21} N_2 f_2 N_1(1-f_1)$$

$$-k_{13} N_1 f_1 N_3(1-f_3) + k_{31} N_3 f_3 N_1(1-f_1) + k_\omega N_3 f_3 N_1(1-f_1)$$

$$\frac{dn_2}{dt} = +k_{12} N_1 f_1 N_2(1-f_2) - k_{21} N_2 f_2 N_1(1-f_1)$$

$$-k_{23} N_2 f_2 N_3(1-f_3) + k_{32} N_3 f_3 N_2(1-f_2)$$

$$\frac{dn_3}{dt} = -\left(\frac{dn_1}{dt} + \frac{dn_2}{dt}\right)$$

assume total number of electrons in N_1, N_2, & N3 is contant

Rate Constants in Equilibrium

Detailed Balance

In equilibrium: $f^o(E) = \dfrac{1}{1 + \exp\left(\frac{E-E_F}{k_B T}\right)}$

Detailed balance:

In equilibrium, <u>each</u> scattering process balances with its inverse

$$k_{12} N_1 f_1^o N_2(1 - f_2^o) = k_{21} N_2 f_2^o N_1(1 - f_1^o)$$

$$k_{21} = k_{12} \frac{f_1^o}{(1 - f_1^o)} \frac{(1 - f_2^o)}{f_2^o}$$

$$= k_{12}\, e^{-(E_1-E_F)/k_B T}\, e^{(E_2-E_F)/k_B T}$$

$$= k_{12}\, \underbrace{e^{-(E_1-E_2)/k_B T}}_{A_{12}}$$

$$k_{21} = k_{12} A_{12} \qquad k_{32} = k_{23} A_{23} \qquad k_{31} = k_{13} A_{13}$$

Rate Equations

Assume the rate constants don't change out of equilibrium...

$$N_1 \frac{df_1}{dt} = -k_{12} N_1 N_2 [f_1(1-f_2) - A_{12} f_2 (1-f_1)]$$
$$-k_{13} N_1 N_3 [f_1(1-f_3) - A_{13} f_3 (1-f_1)] + k_\omega N_3 N_1 f_3 (1-f_1)$$

$$N_2 \frac{df_2}{dt} = +k_{12} N_1 N_2 [f_1 (1-f_2) - A_{12} f_2 (1-f_1)]$$
$$-k_{23} N_2 N_3 [f_2(1-f_3) - A_{23} f_3 (1-f_2)]$$

Steady-State Solutions

Non-equilibrium

$$\frac{dn_3}{dt} = \frac{dn_1}{dt} = \frac{dn_2}{dt} = 0$$

$$\frac{dn_2}{dt} = 0 \Rightarrow \frac{f_1 (1-f_2) - A_{12} f_2 (1-f_1)}{f_2(1-f_3) + A_{23} f_3 (1-f_2)} = \frac{k_{23} N_3}{k_{12} N_1}$$

For example when intraband scattering is much faster than interband scattering...

$$N_1 \sim N_3 \qquad k_{12} \gg k_{31}, k_{23}$$

$$f_1 (1-f_2) - A_{12} f_2 (1-f_1) \approx 0$$

$$\frac{f_1}{(1-f_1)} \approx A_{12} \frac{(1-f_2)}{f_2}$$

Steady-State Solutions
Non-equilibrium

Equilibrium Fermi-Dirac distribution:

$$f^o(E) = \frac{1}{1+\exp\left(\frac{E-E_F}{k_BT}\right)}$$

Non-equilibrium Quasi-Fermi-Dirac distribution is defined by:

$$f_j(E_j) = \frac{1}{1+\exp\left(\frac{E_j-E_{F_j}}{k_BT}\right)}$$

$$\frac{f_1}{(1-f_1)} \approx A_{12}\frac{(1-f_2)}{f_2}$$

$$e^{-(E_1-E_{F_1})/k_BT} \approx e^{-(E_1-E_2)/k_BT}\, e^{(E_2-E_{F_2})/k_BT}$$

$$E_{F_1} \approx E_{F_2}$$

Intraband states have same chemical potential

➡ in 'equilibrium' with each other because of fast intraband scattering

Steady-State Solutions
Non-equilibrium

$$N_1\frac{df_1}{dt} \to 0 = -k_{12}\,N_1\,N_2\,[f_1(1-f_2) - A_{12}\,f_2\,(1-f_1)]$$

$$-k_{13}\,N_1\,N_3\,[f_1(1-f_3) - A_{13}\,f_3\,(1-f_1)] + k_\omega\,N_3\,N_1\,f_3(1-f_1)$$

$$E_{F_3} = E_{F_1} - k_BT\ln\left[\frac{k_\omega e^{(E_1-E_3)/k_BT} + k_{13}}{k_{13}}\right]$$

Interband states have different chemical potentials

unless $k_\omega \to 0$ $\quad E_{F_3} = E_{F_1}$

Counting in Non-equilibrium Semiconductors

Equilibrium

$$n_o = N_c \exp\left(\frac{-(E_c - E_{F_o})}{k_B T}\right)$$

$$p_o = N_v \exp\left(\frac{-(E_{F_o} - E_v)}{k_B T}\right)$$

$$n_o p_o = N_c N_v \exp\left(\frac{-E_g}{k_B T}\right) = n_i^2$$

Quasi-equilibrium

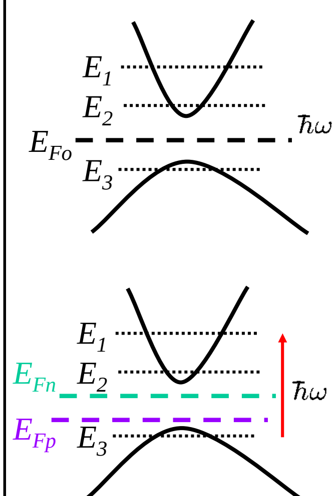
$$n \approx N_c \exp\left(\frac{-(E_c - E_{F_n})}{k_B T}\right)$$

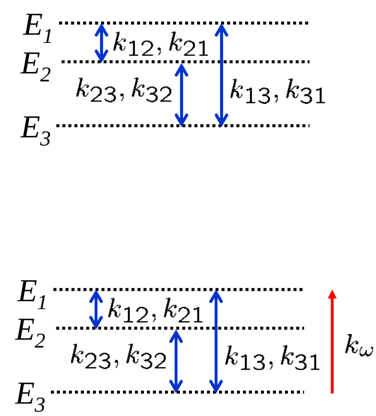
$$p \approx N_v \exp\left(\frac{-(E_{F_v} - E_p)}{k_B T}\right)$$

$$np = n_i^2 \exp\left(\frac{-(E_{F_n} - E_{F_p})}{k_B T}\right)$$

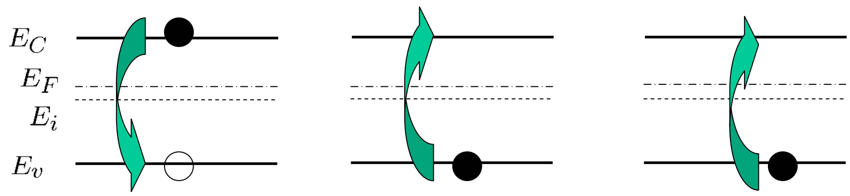
Near Equilibrium Electron Distributions

Optical Excitation





Example: Generation and Recombination



Recombination	Thermal Generation	External Generation
R = A n p	$\mathbf{G_{th}}$	$\mathbf{G_L}$

Charge conservation: $\frac{d}{dt}(n+p) = 0$

Rate equation: $\frac{d}{dt}n = G_{\text{th}} + G_{\text{L}} - R$

In equilibrium, every process and its reverse balances, and no drive (G_L=0)

$$G_{\text{th}} = R_o = A n_o p_o \qquad G_{\text{th}} = A n_o p_o$$

Rate equation becomes: $\frac{d}{dt}n = G_{\text{L}} - A[np - n_o p_o]$

Example

$$\frac{d}{dt}n = G_{\text{L}} - A[np - n_o p_o]$$

Define the excess carriers as n', then n = n_o + n' and p = p_o + p'

$$\frac{d}{dt}n' = G_{\text{L}} - A[n'(n_o + p_o) - n'^2]$$

Consider a special case of low level injection in n-type, that is, n_o >> p_o, and n' << n_o, then

$$\frac{d}{dt}n' = G_{\text{L}} - \underbrace{A n_o}_{\tau}\ n'$$

$$n' = n'(0)e^{-t/\tau} + G_{\text{L}}\tau(1 - e^{-t/\tau}) \rightarrow G_{\text{L}}\tau$$

Steady state solution

In steady state $n' = G_L \tau$ so that

$$n = n_o + n' \approx n_o \quad \text{and} \quad p = p_o + n'$$

Recall that in the Boltzmann limit,

$$n = N_c \exp\left(\frac{-(E_c - E_{F_n})}{k_B T}\right) = n_o \exp\left(\frac{-(E_F - E_{F_n})}{k_B T}\right)$$

$$p = N_v \exp\left(\frac{-(E_{F_p} - E_v)}{k_B T}\right) = p_o \exp\left(\frac{-(E_{F_p} - E_F)}{k_B T}\right)$$

Since we know n and p from the rate equations we can find

$$E_{Fn} = E_{Fo} + k_B T \ln(1 + n'/n_o) \approx E_{Fo} + k_B T (n'/n_o) \approx E_{Fo}$$

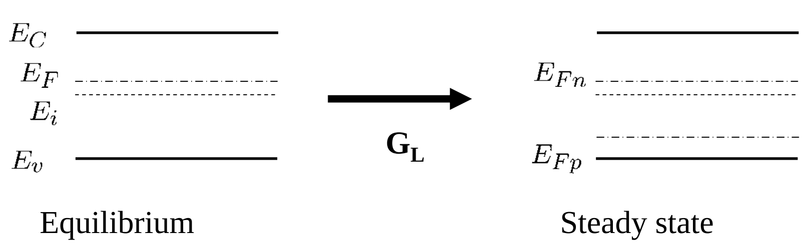
$$E_{Fp} = E_{Fo} - k_B T \ln(1 + n'/p_o)$$ Moves towards the holes

Summary: Steady state solution

In steady state $n' = G_L \tau$

$$E_{Fn} = E_{Fo} + k_B T \ln(1 + n'/n_o) \approx E_{Fo} + k_B T (n'/n_o) \approx E_{Fo}$$

$$E_{Fp} = E_{Fo} - k_B T \ln(1 + n'/p_o)$$ Moves towards the holes



Quasi-equilibrium Transport

Peek into future lectures: Assume that during steady state transport the system can be described by quasi-fermi levels:

$$n(r) \approx N_c \exp\left(\frac{-(E_c(r) - E_{F_c})}{k_B T}\right) \quad \Rightarrow \quad E_{F_c} = E_c(r) + k_B T \ln \frac{n(r)}{N_c}$$

Furthermore assume that the current density given by

$$E_c(x) = E_{co} - q\phi(x)$$

$$\frac{dE_c(x)}{dx} = -q\frac{d\phi(x)}{dx} = qE_x$$

$$J_{n_x} \approx \mu_n n \frac{dE_{F_c}}{dx}$$

$$= \mu_n n \frac{dE_c}{dx} + \mu_n n k_B T \frac{N_c}{n} \frac{1}{N_c} \frac{dn}{dx}$$

$$= \mu_n n \frac{dE_c}{dx} + \mu_n k_B T \frac{dn}{dx}$$

$$= \mu_n n q E_x + \mu_n k_B T \frac{dn}{dx}$$

Assuming $\frac{\mu}{q} = \frac{D}{k_B T}$ $\Rightarrow$ $J_{n_x} \equiv q\mu_n n E_x + qD_n \frac{dn}{dx}$

We still have lots to do before we can prove each major assumption