6.730 Physics for Solid State Applications

Lecture 26: Inhomogeneous Solids

Outline

• Last Time: Quasi-Fermi Levels
• Inhomogenous Solids in Equilibrium
• Quasi-equilibrium Transport
• Heterostructures
Near Equilibrium Electron Distributions

Optical Excitation

\[ E_1 \quad E_2 \quad E_3 \]

\[ E_3 \quad k_{12}, k_{21} \quad k_{23}, k_{32} \quad k_{13}, k_{31} \]

- Intraband scattering: electron-electron
- Intraband scattering: electron-acoustic phonon
- Interband scattering: electron-hole
- Interband scattering: electron-phonon with defects

What are \( f_1, f_2, \) & \( f_3 \) under illumination (non-equilibrium)?
Steady-State Solutions
Non-equilibrium

\[ \frac{dn_3}{dt} = \frac{dn_1}{dt} = \frac{dn_2}{dt} = 0 \]

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

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

\[ N_1 \sim N_3 \]
\[ k_{12} \gg k_{31}, k_{23} \]

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

\[ \frac{f_1}{(1 - f_1)} \approx A_{12} \frac{f_2}{(1 - f_2)} \]
Steady-State Solutions

Non-equilibrium

Equilibrium Fermi-Dirac distribution:

\[ f^o(E) = \frac{1}{1 + \exp\left(\frac{E - E_{F}}{k_B T}\right)} \]

Non-equilibrium Quasi-Fermi-Dirac distribution:

\[ f_i(E_i) = \frac{1}{1 + \exp\left(\frac{E_i - E_{F_i}}{k_B T}\right)} \]

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

\[ e^{-(E_1 - E_{F_1})/k_B T} \approx e^{-(E_1 - E_2)/k_B T} \ e^{-(E_2 - E_{F_2})/k_B T} \]

\[ E_{F_1} \approx E_{F_2} \]

Intraband states have same chemical potential in ‘equilibrium’ with each other because of fast intraband scattering
Steady-State Solutions
Non-equilibrium

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

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

\[ E_{F3} = E_{F1} - k_B T \ln \left[ \frac{k_\omega e^{(E_1-E_3)/k_B T} + A}{A} \right] \]

\[ A = k_{13} + \frac{N_2}{N_1} k_{21} e^{(E_1-E_2)/k_B T} \]

Interband states have different chemical potentials
unless \( k_\omega \to 0 \quad E_{F3} = E_{F1} \)
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**

\[ N \approx N_c \exp \left( \frac{-(E_c - E_{F_c})}{k_B T} \right) \]

\[ P \approx N_v \exp \left( \frac{-(E_{F_v} - E_v)}{k_B T} \right) \]

\[ N P = N_i^2 \exp \left( \frac{-(E_{F_c} - E_{F_v})}{k_B T} \right) \]
Consider a solid with a spatially varying impurity concentration...

\[ N_d = 10^{16} \quad N_d = 10^{17} \]

In equilibrium, the carrier concentration is balanced by an internal electrostatic potential...
Inhomogeneous Semiconductors in Equilibrium

If electrostatic potential varies slowly compared to wavepacket...

\[
\left( -\frac{\hbar^2 \nabla^2}{2m^*} + E_{co} - q\phi(r) \right) G(r) = EG(r)
\]

Dividing solid into slices where \( \phi_i \) is uniform...

\[
-\frac{\hbar^2 \nabla^2}{2m^*} G_i(r) = (E_i - E_{co} + q\phi_i) G_i(r)
\]

...the envelope function has solutions of the form...

\[
G_i(r) = (A_i e^{ik_xx} + B_i e^{-ik_xx}) e^{ik_yy} e^{ik_zz}
\]

...therefore the eigenenergies are...

\[
E_i = E_{co} - q\phi_i + \frac{\hbar^2 k^2}{2m^*}
\]

\[
E(r) = E_{co} - q\phi(r) + \frac{\hbar^2 k^2}{2m^*}
\]
Inhomogeneous Semiconductors in Equilibrium

Given the modified energy levels, the 3-D DOS becomes...

\[ g(E, r) = \frac{1}{2\pi^2 \hbar^3 (2m^*)^{3/2}} [E - E_{co} + q\phi(r)]^{1/2} \]

...in equilibrium the carrier concentration is...

\[ N_o(r) = \int_{E_{co} - q\phi(r)}^{\infty} g(E, r) \frac{1}{1 + e^{(E - E_{F_o})/k_BT}} dE \]

\[ N_o(r) = \frac{2}{\sqrt{\pi}} N_c F_{1/2} \left( \frac{E_{F_o} - E_{co} + q\phi(r)}{k_BT} \right) \]

Boltzmann approx. \[ \approx N_c \exp \left( \frac{-(E_{co} - q\phi(r) - E_{F_o})}{k_BT} \right) \]
Inhomogeneous Semiconductors in Equilibrium

\[ N_0(r) = \frac{2}{\sqrt{\pi}} N_c F_{1/2} \left( \frac{E_{F_0} - E_{co} + q\phi(r)}{k_B T} \right) \]

\[ \approx N_c \exp \left( \frac{-(E_{co} - q\phi(r) - E_{F_0})}{k_B T} \right) \]

\[ E_c(r) \equiv E_{co} - q\phi(r) \]

\[ N_0(r) = \frac{2}{\sqrt{\pi}} N_c F_{1/2} \left( \frac{E_{F_0} - E_c(r)}{k_B T} \right) \]

\[ \approx N_c \exp \left( \frac{-(E_c(r) - E_{F_0})}{k_B T} \right) \]

The slowly varying electrostatic potential can be incorporated in \( E_c(r) \).
Quasi-equilibrium Transport

\[ N(r) \approx N_c \exp \left( \frac{-(E_c(r) - E_{Fc})}{k_BT} \right) \]

\[ \Rightarrow E_{Fc} = E_c(r) + k_BT \ln \frac{N(r)}{N_c} \]

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

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

\[ J_{nx} \approx \mu_n N \frac{dE_{Fc}}{dx} \]

\[ = \mu_n N \frac{dE_c}{dx} + \mu_n k_BT \frac{N_c}{N} \frac{1}{N_c} \frac{dN}{dx} \]

\[ = \mu_n N qE_x + \mu_n k_BT \frac{dN}{dx} \]

\[ J_{nx} \equiv q\mu_n N E_x + qD_n \frac{dN}{dx} \]
Species of Heterjunctions

Type I

1.42

\( \Delta F_C = 0.77 \alpha \)
\( \Delta F_V = 0.43 \alpha \)

Type II

1.42 + 1.25 \alpha

\( \Delta F_C = 0.23 \)
\( \Delta F_V = -0.16 \)

Type III

\( \Delta F_C = 0.36 \)
\( \Delta F_V = 0.34 \)

http://www.utdallas.edu/~frensley/technical/hetphys
Tight-binding Calculation of Band Alignments

LCAO internally references bandstructures to each other...

\[ E_v(k = 0) = \frac{E_p^1 + E_p^2}{2} - \sqrt{\left(\frac{E_p^1 - E_p^2}{2}\right)^2 + \left(\frac{1.28\hbar^2}{md^2}\right)^2} \]

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GaAs \hspace{3cm} \text{InAs}

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\[ \Delta E_v \]

Unfortunately, this doesn’t take into account the details of the charges and bonding at the interface...

...need a self-consistent LCAO theory...still a research topic!
Tight-binding Calculation of Band Alignments

\[ E_v(k = 0) = \frac{E_p^1 + E_p^2}{2} - \sqrt{\left(\frac{E_p^1 - E_p^2}{2}\right)^2 + \left(\frac{1.28\hbar^2}{md^2}\right)^2} \]

Example GaAs/InAs

\( \text{Ga: } E_p = -4.9 \text{ eV} \quad \text{As: } E_p = -7.91 \text{ eV} \quad \text{In: } E_p = -4.69 \text{ eV} \)

\( \text{GaAs: } d = 2.45 \text{ Å} \quad \text{InAs: } d = 2.61 \text{ Å} \)

\( E_v = -8.61 \text{ eV} \quad E_v = -8.45 \text{ eV} \)

GaAs/InAs: \( \Delta E_v = 0.16 \text{ eV} \) (LCAO)

\( \Delta E_v = 0.17 \text{ eV} \) (experiment)
Experimentally Determined Band Alignment

Valence Band Alignment

Courtesy of Sandip Tiwari, Cornell University; Used with Permission
Experimentally Determined Band Alignment

Conduction Band Alignment

Energy (eV) vs. Lattice Constant (Å)

T=300K

GaP, AlAs, GaAs, Si, Ge, InP, GaSb, InAs, AlSb, InSb

 Courtesy of Sandip Tiwari, Cornell University; Used with Permission
Experimentally Determined Band Alignment

![Graph showing band alignment](image)

Energy (eV) vs. Lattice Constant (Å) for various materials at T=300K.

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SimWindows Software

Self-consistent solution of *modified* drift-diffusion & Poisson’s Equation...

http://www-ocs.colorado.edu/SimWindows/simwin.html