Week 1 Summary

Professor Mark Lundstrom
Electrical and Computer Engineering
Purdue University, West Lafayette, IN USA
DLR-103 and EE-334C / 765-494-3515
lundstro at purdue.edu
topics

1) Bandstructure review
2) Quantum confinement
3) Heterostructures
4) Counting states
5) Sums in k-space / integrals in energy space
wave equation

\[- \frac{\hbar^2}{2m_0} \nabla^2 \psi(\vec{r}) + U(\vec{r}) \psi(\vec{r}) = E \psi(\vec{r}) \]

\[\Psi(\vec{r}, t) = \psi(\vec{r}) e^{i\omega t}\]

free space, constant potential:

\[- \frac{\hbar^2}{2m_0} \nabla^2 \psi(\vec{r}) = E \psi(\vec{r}) \]

\[\psi(\vec{r}) = A e^{i\vec{k} \cdot \vec{r}} \]

\[k = \sqrt{2m_0 E / \hbar}\]

momentum:

\[\vec{p} = \hbar \vec{k}\]

position:

\[\psi^*(\vec{r}) \psi(\vec{r}) = |A|^2\]

Lundstrom ECE-656 F13
electrons in crystals

\[- \frac{\hbar^2}{2m_0} \nabla^2 \psi(\vec{r}) + U_C(\vec{r}) \psi(\vec{r}) = E \psi(\vec{r}) \quad U_C(\vec{r} + \vec{a}) = U_C(\vec{r}) \]

\[
\psi(\vec{r}) = u_\vec{k}(\vec{r}) e^{i\vec{k} \cdot \vec{r}} \quad u_\vec{k}(\vec{r} + \vec{a}) = u_\vec{k}(\vec{r}) \quad k: \text{ Brillouin zone}
\]

“Bloch wave”

\[\vec{p} \neq h\vec{k}\quad \text{but…. “crystal momentum”}\]
bandstructure (dispersion)

$E(k) \neq \frac{\hbar^2 k^2}{2m}$

DFT calculations of Bi$_2$Te$_3$ by Dr. J. Maassen, Purdue
near-equilibrium, ballistic transport

Electrons in a solid behave as both particles (quasi-particles) and as waves.

Electron waves are described by a “dispersion:”

Because the crystal is periodic, the dispersion is periodic in $k$ (Brillouin zone).

Particles described by a “wavepacket.”

The “group velocity” of a wavepacket is determined by the dispersion:
model bandstructure

silicon

\[ E(k) = E_C + \frac{\hbar^2 k^2}{2m_w} \]

\[ m^*_x = 0.92m_0 \]
\[ m^*_y = 0.19m_0 \]
\[ m^*_z = 0.16m_0 \]

GaAs

\[ E(k) = E_C - \frac{\hbar^2 k^2}{2m'_w} \]

\[ m^* = 0.063m_0 \]

\[ \Delta E = 1.12 \text{ eV} \]
\[ \Delta E = 1.42 \text{ eV} \]
$E(k)$ for graphene

Recall:

$$v_x(k) = \frac{1}{\hbar} \frac{dE(k)}{dk}$$

For graphene:

$$v_x(k) = v_F$$

Also recall:

$$m^* = \left( \frac{1}{\hbar^2} \frac{d^2E(k)}{dk^2} \right)^{-1}$$

For graphene:

$$m^* = ?$$
1) Bandstructure review

2) Quantum confinement

3) Heterostructures

4) Counting states

5) Sums in k-space / integrals in energy space
particle in a box

\[ \frac{d^2 \psi(z)}{dz^2} + k^2 \psi = 0 \quad k^2 = \frac{2m^* (E - E_c(z))}{\hbar^2} \]

\[ \psi(z) = \sin k_n z \quad k_n = \frac{n\pi}{t} \quad n = 1, 2, 3... \]

\[ \varepsilon_n = \frac{\hbar^2 k_n^2}{2m^*} = \frac{\hbar^2 n^2 \pi^2}{2m^* t^2} \]

Light mass or narrow well \( \rightarrow \) high subband energy, but specifics depend on the shape of the well.

Note: electrons are free to move in the x-z plane. **2D electrons.**
2D electrons

Semi-infinite in the x-y plane, but very thin in the z-direction.

\[ \psi(\vec{r}) \sim e^{i\vec{p} \cdot \vec{r}} \rightarrow \sin(k_z z) \times e^{i\vec{k}_{x,y} \cdot \vec{r}} \]

Lundstrom ECE-656 F13
“subbands”

\[ \varepsilon_j = \frac{\hbar^2 j^2 \pi^2}{2m^* i^2} \]

\[ k_\parallel = \sqrt{k_x^2 + k_y^2} \]

\[ E = \varepsilon_j + \frac{\hbar^2 k_\parallel^2}{2m^*} \]
ex. quantum confinement in Si cond. band.

Si conduction band

\[ m_{i}^* = 0.9m_v \]
\[ m_i = 0.19m_0 \]

\[ \varepsilon_{j} = \frac{\hbar^2 j^2 \pi^2}{2m_i^* t_{Si}^2} \]

\[ m^* = ? \]

unprimed ladder: \[ m^* = m_{\ell}^* \quad g_v = 2 \]

primed ladder: \[ m_{\ell}^* = m_{\ell}^* \quad g_v = 13 \]
quantum confinement in SOI

\[ \Delta \psi_S^{QM} = \frac{\varepsilon_1}{q} \]

(D. Esseni et al. IEDM 2000 and TED 2001)
1) Bandstructure review
2) Quantum confinement
3) Heterostructures
4) Counting states
5) Sums in k-space / integrals in energy space
heterojunctions

$E_0$ (field-free vacuum level)

$E_C$  

$E_G = 1.80 \text{ eV}$

$qV_{bi} = E_{FN} - E_{FP}$

$E_G = 1.42 \text{ eV}$
Type I HJ e-band

“band spike”

\[ V_{jk} = V_j \]

\[ E_C \]

\[ E_C \]

\[ E_G \approx 1.80 \text{ eV} \]

\[ E_v \]

\[ \Delta E_v \]

\[ E_v \]

\[ E_{VR} \]

\[ E_{VR} \]

\[ E_G \approx 1.42 \text{ eV} \]
general, graded heterostructure

\[ E_C(x) = E_0 - \chi(x) - qV(x) \]

\[ E_v(x) = E_v(x) - E_C(x) \]
1) Bandstructure review
2) Quantum confinement
3) Heterostructures
4) **Counting states**
5) Sums in k-space / integrals in energy space
energy levels in Si

Si atom (At. no. 14)

4S\(^0\)

3P\(^2\)

3S\(^2\)

2P\(^6\)

2S\(^2\)

1S\(^2\)

4 valence electrons
8 valence states

“core levels”

Lundstrom ECE-655 F13
states in a Si crystal

- Only the valence states are of interest to us.

- The 8 valence states give rise to $8N_{\text{atoms}}$ states per cm$^3$ in the solid.

- But the interaction of the electron wavefunctions alters the discrete energy levels of the isolated Si atoms.
energy levels $\rightarrow$ energy bands

Si atom (At. no. 14)  Si crystal

- $3P^2$
- $3S^2$

energy

conduction "band"

"forbidden gap"

valence "band"

$4N_{\text{atoms}}$ states

$4N_{\text{atoms}}$ states

22
states in a finite volume of semiconductor

Finite volume, $\Omega$

(part of an infinite volume)

Finite number of states

Periodic boundary conditions:
\[ \psi(x) = u_k(x)e^{ik_xx} \]

\[ \psi(0) = \psi(L_x) \rightarrow e^{ik_xL_x} = 1 \]

\[ k_xL_x = 2\pi j \quad j = 1, 2, 3, \ldots \]

\[ k_x = \frac{2\pi}{L_x} j \]

\[ k_x = \pi/a \]

\# of states = \( \frac{dk_x}{(2\pi/L_x)} \times 2 = N_c dk \)

\[ N_c = \frac{L_x}{\pi} \] = density of states in k-space
density-of-states in k-space

1D:
\[ N_k = 2 \times \left( \frac{L}{2\pi} \right) = \frac{L}{\pi} \quad dk \]

2D:
\[ N_k = 2 \times \left( \frac{A}{4\pi^2} \right) = \frac{A}{2\pi^2} \quad dk_x dk_y \]

3D:
\[ N_k = 2 \times \left( \frac{\Omega}{8\pi^2} \right) = \frac{\Omega}{4\pi^3} \quad dk_x dk_y dk_z \]
DOS: k-space vs. energy space

but non-uniformly distributed in energy space.

Depends on $E(k)$ (e.g. different for parabolic bands and linear bands)

States are uniformly distributed in k-space.

$D(E) dE = N(k) dk$
1) Bandstructure review
2) Quantum confinement
3) Heterostructures
4) Counting states
5) Sums in k-space / integrals in energy space
splits in k-space

\[ N = \sum_k f_0(E_k) \quad f_0 = \frac{1}{1 + e^{(E - E_F)/k_B T}} \]

\[ n = \frac{1}{\Omega} \sum_k f_0(E_k) \text{ cm}^{-3} \]

\[ n = \frac{1}{\Omega} \frac{\Omega}{4\pi^3} \int_{\mathbb{R}^3} f_0(E_k) d^3k \text{ cm}^{-3} \]
\[ n = \frac{1}{4\pi^3} \int_{\mathbb{R}^3} f_0(E_k) \, d^3k \]

\[ n = \frac{1}{4\pi^3} \int_0^{\infty} \frac{4\pi k^2 \, dk}{1 + e^{(E - E_F)/k_B T}} \]

\[ f_0 = \frac{1}{1 + e^{(E_0 - E)/k_B T}} \]

\[ E = E_C + \mathcal{E}(k) = E_C + \frac{\hbar^2 k^2}{2m^*} \]

Note: We extend the integral to infinity because we can usually assume that the higher energy states at large \( k \) have \( E >> E_F \), so they are not occupied.
\[ n = \frac{1}{\Omega} \sum_k f_0(E_k) \rightarrow N_c F_{1/2}(\eta_F) \text{ cm}^{-3} \]

\[ E = E_C + E(k) = E_C + \frac{\hbar^2 k^2}{2m^*} \]

\[ \eta_F = (E_F - E_C)/k_B T \]

\[ N_c = \frac{1}{4} \left( \frac{2m^* k_B T}{\pi \hbar^2} \right)^{3/2} \]

\[ F_{1/2}(\eta_F) = \frac{2}{\sqrt{\pi}} \int_0^\infty \frac{\eta^{1/2} \, d\eta}{1 + e^{\eta - \eta_F}} \]
k-space vs. energy space

\[ n = \frac{1}{\Omega} \sum_k f_0(E_k) \rightarrow N_c F_{1/2}(\eta_F) \text{cm}^{-3} \]

\[ n = \int_{E_c}^{\infty} D_c(E) f_0(E) dE \]

\[ D(E) = \frac{(2m^*)^{3/2}}{2\pi^3\hbar^3} (E - E_c)^{1/2} \]

\[ E = E_c + E(k) = E_c + \frac{\hbar^2 k^2}{2m^*} \]
1) Bandstructure review
2) Quantum confinement
3) Heterostructures
4) Counting states
5) Sums in k-space / integrals in energy space