

Lecture 1 – Nanoscale MOSFETs

- Course Structure
- Basic Concepts (1-38)

Course Layout

- 7.5 ECTS
- 7 Lectures
- 7 Exercises
- Written exam (t.b.d)

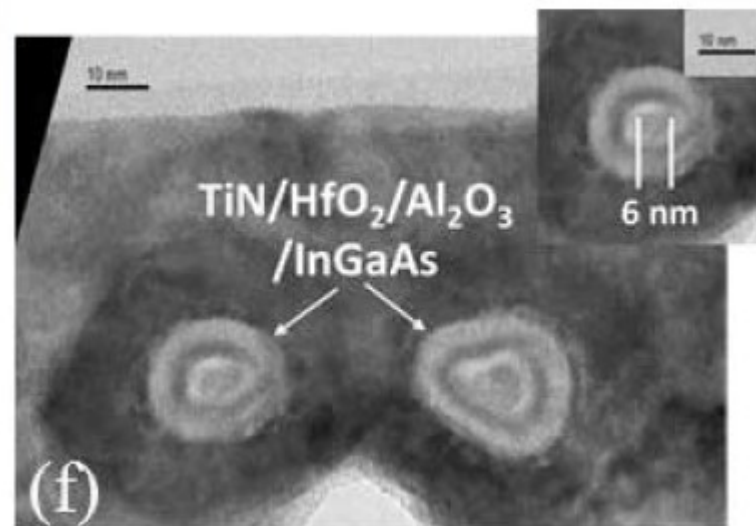
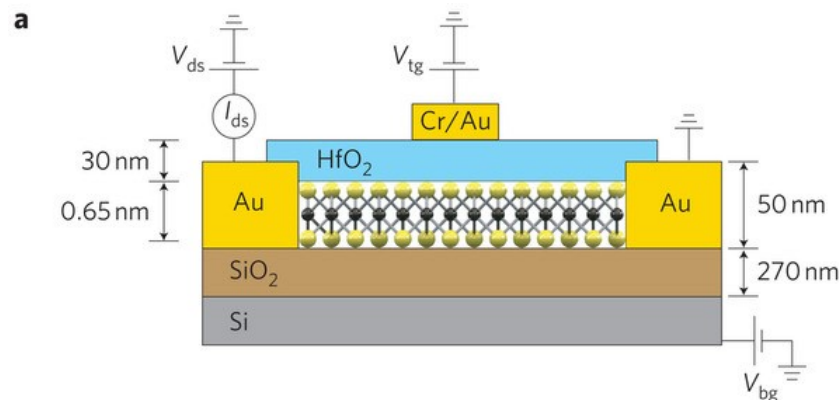
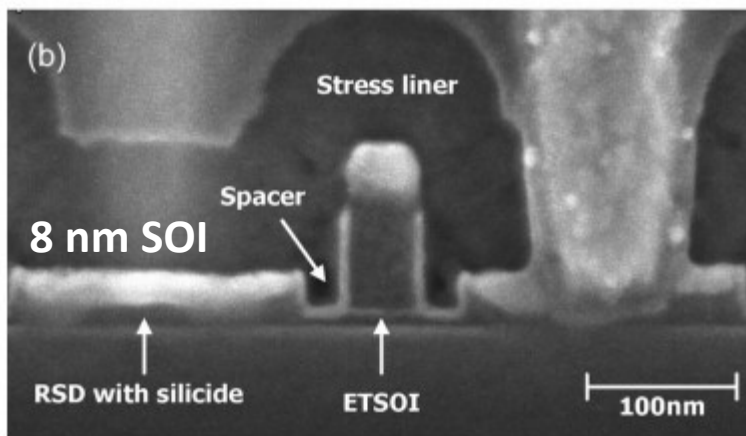
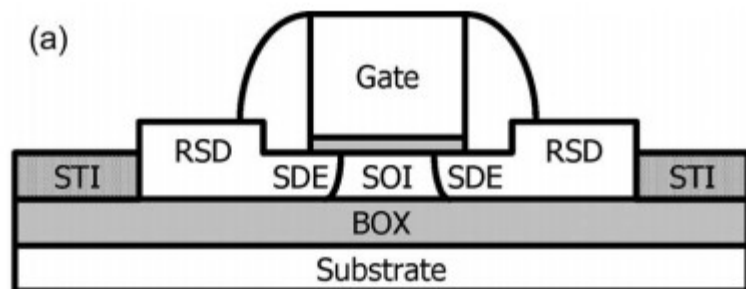
Textbook:

Nanoscale Transistors: Device Physics, Modeling and Simulation
by Lundstrom/Guo. *Available electronically.*

We will cover everything except the last chapter(1-181).

Motivation I

Modern transistors have *thin* 1D or 2D bodies

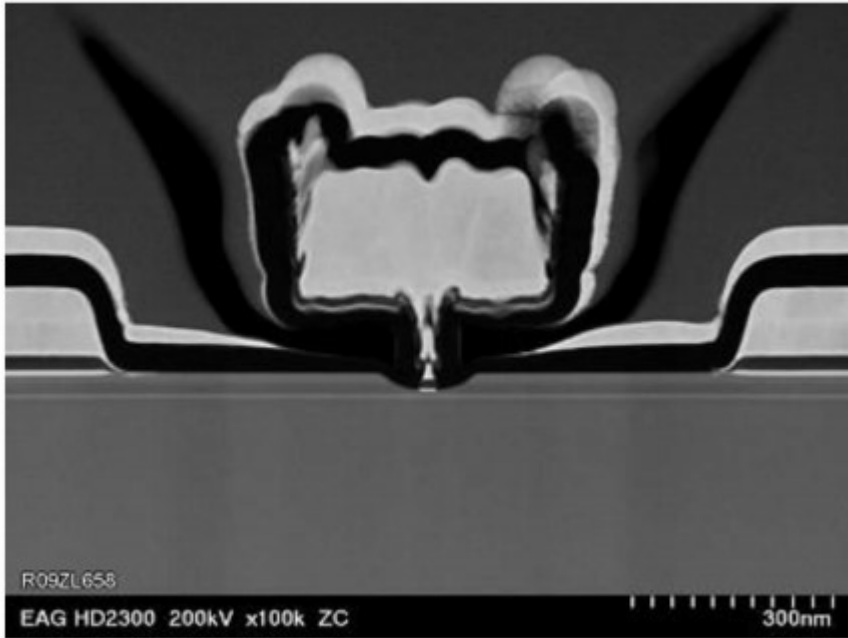


Undoped-Body Extremely Thin SOI MOSFETs With Back Gates

Amlan Majumdar, Zhibin Ren, Steven J. Koester, *Senior Member, IEEE*, and Wilfried Haensch, *Senior Member, IEEE*

Motivation II

Modern transistors have very short gate lengths



A STEM image of a 30 nm InP HEMT.

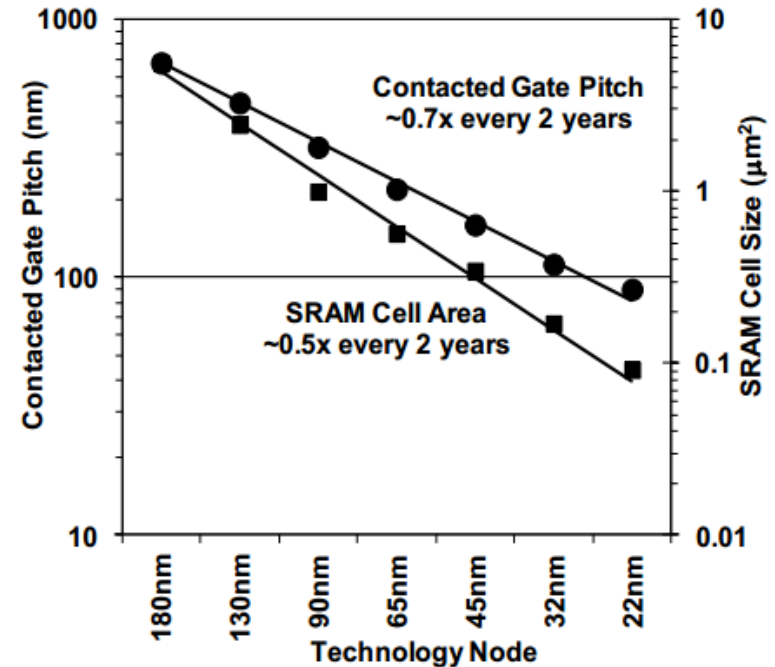


Fig. 4. Contacted gate pitch and SRAM cell size scaling trend for Intel's technology nodes.

$L_g < \lambda$ – diffusive transport gives a poor description of the device performance

HEMTs: 10-30 nm L_g . 14 nm Si FINFET: 20 nm L_g .

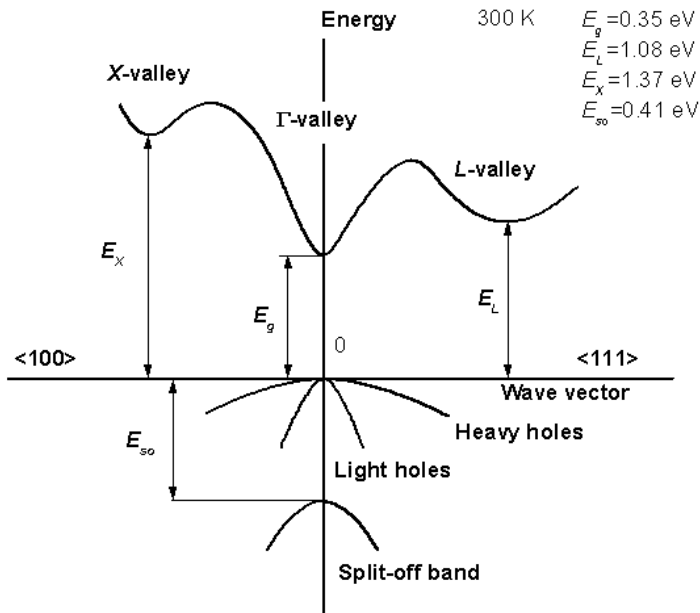
We need to understand the behaviour of close to ballistic FETs

Course Topics

Contemporary description of MOSFETs

- Basic semiconductor concepts (1)
- Basic MOSFET / CMOS physics (2)
 - 2D Ballistic FETs (3-4)
 - Scattering (5)
 - 1D Nanowire and CNT FETs (6)
 - ~~• Molecular FETs – Single Electron Transistors (7)~~
- 1D Tunneling Field Effect Transistors. Ferroelectric FETs. (7).

Band Structure, Group Velocity



- Direct band gap semiconductors
- Isotropic Γ -valley
- Parabolic bands for small E

$$E(\mathbf{k}) = E_C + \frac{\hbar^2}{2m^*} (k_x^2 + k_y^2 + k_z^2)$$

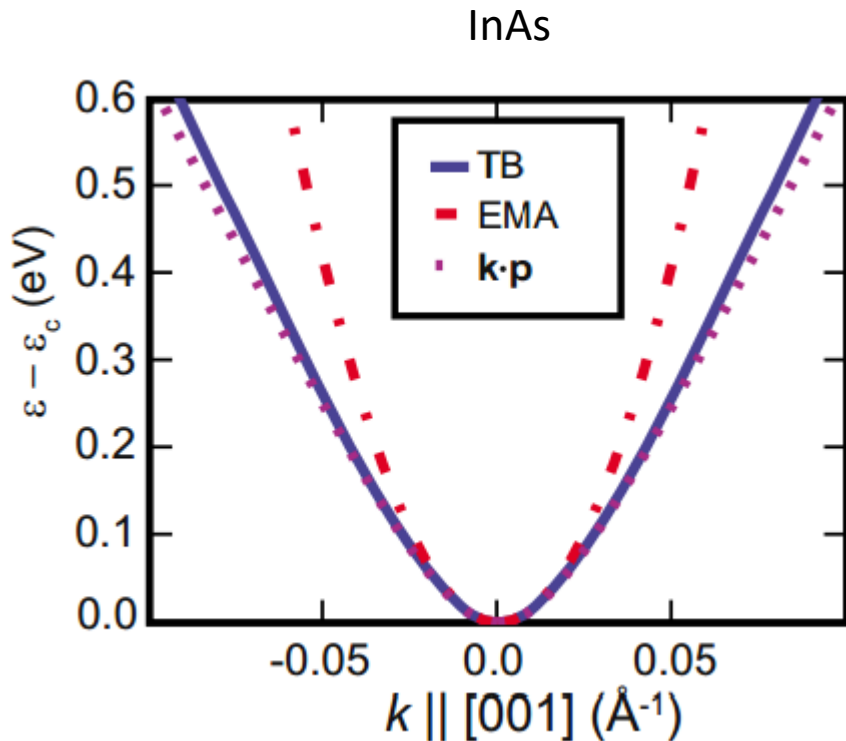
- Indirect band gap semiconductors (Si, Ge)
- Multiple *anisotropic* X/L-valleys
- Parabolic bands for small E

$$E(\mathbf{k}) = E_C + \frac{\hbar^2}{2} \left(\frac{k_x^2 + k_y^2}{m_t} + \frac{k_z^2}{m_l} \right)$$

The group velocity for a conduction band electron

$$v_x = \frac{1}{\hbar} \frac{dE}{dk_x}$$

Nonparabolicity



$E \gg E_c$ introduces nonparabolicity

$$E(k)(1 + \alpha E(k)) = \frac{\hbar^2}{2m^*} (k_x^2 + k_y^2 + k_z^2)$$

(2-band kp)

α : 2 eV⁻¹ (InAs)
0.5 eV⁻¹ (Si)

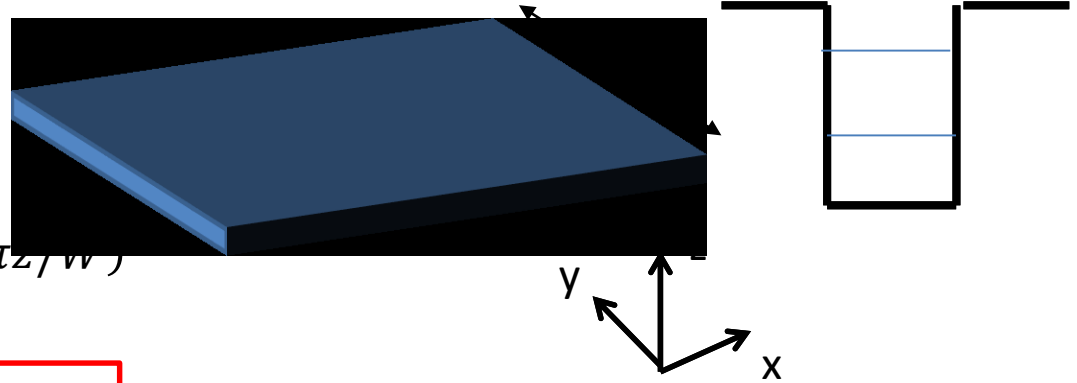
TB: Atomistic bandstructure modeling
EMA: Effective mass
kp: 2-band k dot p

2D / 1D structures

The channel of a modern FET is 2D today - 1D tomorrow (?)

$$\psi(r) = \phi(z) \frac{1}{\sqrt{A}} e^{ik_x x + ik_y y}$$

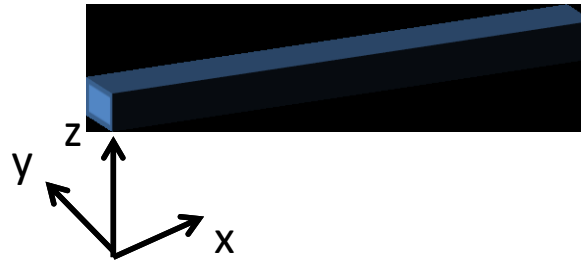
$$\phi(z) = \sqrt{\frac{2}{W}} \sin(k_n z) = \sqrt{\frac{2}{W}} \sin(n\pi z / W)$$



$$\varepsilon_n = \frac{\hbar^2 n^2 \pi^2}{2m^* W^2} \quad E(\mathbf{k}) = \varepsilon_n + \frac{\hbar^2 k_{\parallel}^2}{2m^*}$$

$$\psi(r) = \phi(y, z) \frac{1}{\sqrt{L}} e^{ik_x x}$$

$$\phi(y, z) \propto \sin\left(\frac{n\pi z}{W_z}\right) \sin\left(\frac{n\pi y}{W_y}\right)$$



$$\varepsilon_{n,m} = \frac{\hbar^2 \pi^2}{2m^*} \left(\frac{n^2}{W_z^2} + \frac{m^2}{W_y^2} \right)$$

$$E(k) = \varepsilon_{n,m} + \frac{\hbar^2 k_x^2}{2m^*}$$

Fermi-Dirac Integrals

$$F_j(\eta_F) = \frac{1}{\Gamma(j+1)} \int_0^\infty \frac{\xi^j}{1 + e^{\xi - \eta_F}} d\xi$$

$$\frac{dF_j}{d\eta_F} = F_{j-1}$$

$$F_0(\eta_F) = \log(1 + e^{\eta_F})$$

$$\eta_F = \frac{E_F - E_n}{kT}$$

In the non-degenerate limit:

$$F_j(\eta_F) \approx e^{\eta_F}$$

$$\eta_F \ll 0$$

In the degenerate limit:

$$F_j(\eta_F) \approx \eta_F^{j+1} / \Gamma(j+2)$$

$$\eta_F \gg 0$$

Gamma function

$$\Gamma(0.5) = \sqrt{\pi}$$

$$\Gamma(1) = 1$$

$$\Gamma(1.5) = \frac{\sqrt{\pi}}{2}$$

$$\Gamma(2) = 1$$

$$\Gamma(2.5) = \frac{3\sqrt{\pi}}{4}$$

n positive integer

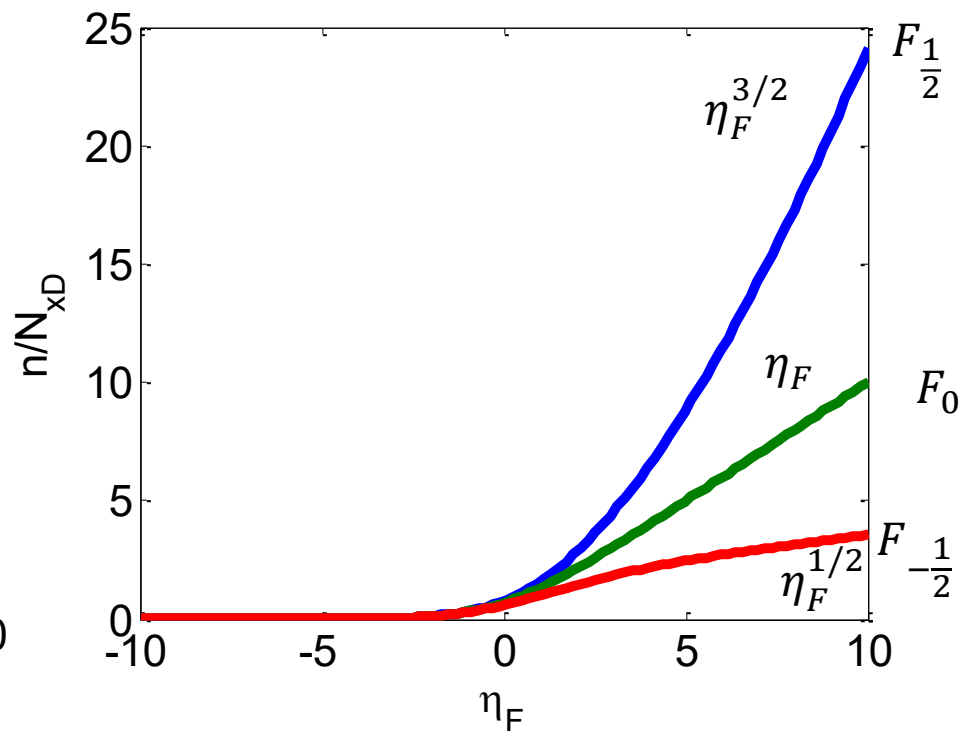
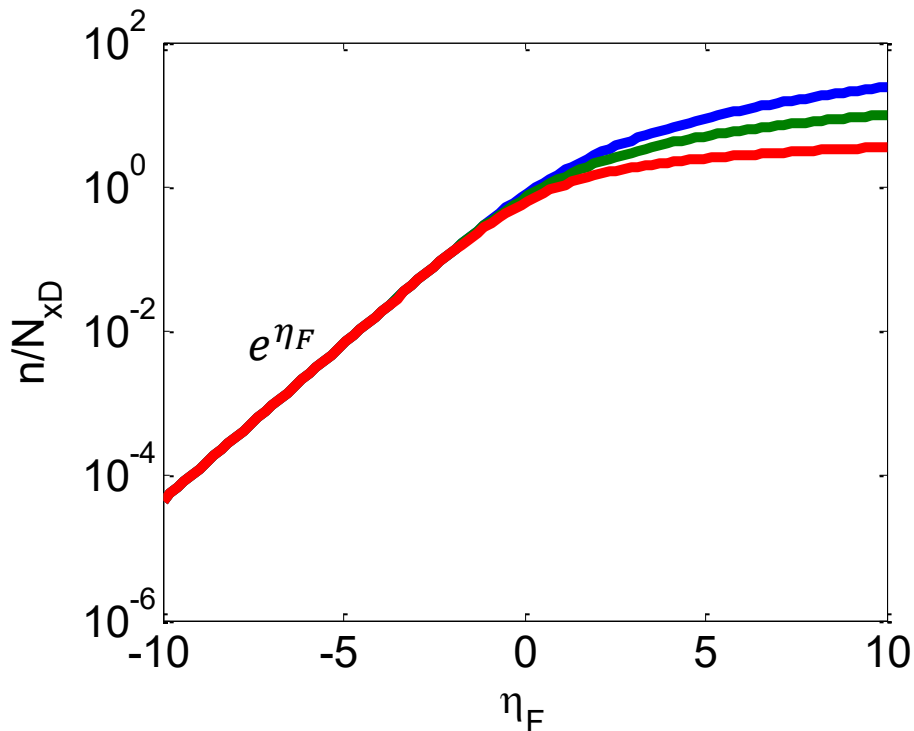
$$\Gamma(n) = (n-1)!$$

$$\Gamma(p+1) = p\Gamma(p)$$

Notes on FD/integrals:

<http://arxiv.org/ftp/arxiv/papers/0811/0811.0116.pdf>

Fermi-Dirac Integrals



In the non-degenerate limit:

$$F_j(\eta_F) \approx e^{\eta_F}$$

In the degenerate limit:

$$F_j(\eta_F) \approx \eta_F^{j+1} / \Gamma(j+2)$$

$$\eta_F = \frac{E_F - E_n}{kT}$$

$$\Gamma(0.5 + 2) = \frac{3\sqrt{\pi}}{4}$$

$$\Gamma(0 + 2) = 1$$

$$\Gamma(-0.5 + 2) = \frac{\sqrt{\pi}}{2}$$

Carrier Statistics: 3D,2D,1D

Density of states:

$$D_{3D} = \frac{(2m^*)^{\frac{3}{2}}}{2\pi^2 \hbar^3} \sqrt{E - E_C}$$

$$D_{2D} = \frac{m^*}{\pi \hbar}$$

$$D_{1D} = \frac{\sqrt{2m^*}}{\pi \hbar} \frac{1}{\sqrt{E - E_C}}$$

Effective density of states:

$$N_{3D} = 2 \left(\frac{2\pi m^* kT}{h^2} \right)^{\frac{3}{2}}$$

$$N_{2D} = \frac{m^* kT}{\pi \hbar^2}$$

$$N_{1D} = \frac{\sqrt{2m^* kT}}{\hbar}$$

$$v_x = \frac{1}{\hbar} \frac{dE}{dk_x}$$

We will derive these later on.

$$n_0(k_F) = \sum_k f_0(k, k_F) = \int_0^\infty f_0(E, E_F) D(E) dE$$

$$F_j(\eta_F) = \frac{1}{\Gamma(j+1)} \int_0^\infty \frac{\xi^j d\xi}{1 + e^{\xi - \eta_F}}$$

$$\eta_F = (E_F - E_C)/kT$$

$$n_0 = N_{3D} F_{1/2}(\eta_F) \quad 3D$$

$$n_s = N_{2D} F_0(\eta_F) \quad 2D$$

$$n_L = N_{1D} F_{-1/2}(\eta_F) \quad 1D$$

Semi-classical transport

$$\frac{\partial f(x, p, t)}{\partial t} + v_x \frac{\partial f}{\partial x} - qE_x \frac{\partial f}{\partial p_x} = \hat{C}(x, p, t)f$$

Boltzmann Transport Equation

f : distribution function. C : collision operation

Zeroth Moment: continuity equation

First Moment: drift diffusion

2nd Moment: energy balance

$$J_{nx} = qn\mu_n E_x + \frac{2}{3}\mu_n \frac{dW}{dx}$$
$$\mu_n = \frac{q\tau_m}{m^*}$$

$$W \approx \frac{3}{2}nkT$$

Kinetic energy near equilibrium

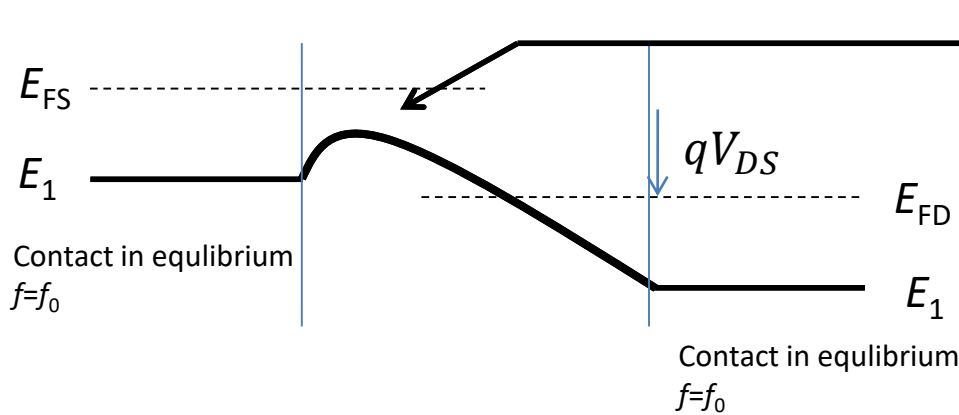
High field, short devices:

$\tau_m(E)$ Scattering increases with energy

$W > \frac{3}{2}nkT$ Mean energy larger

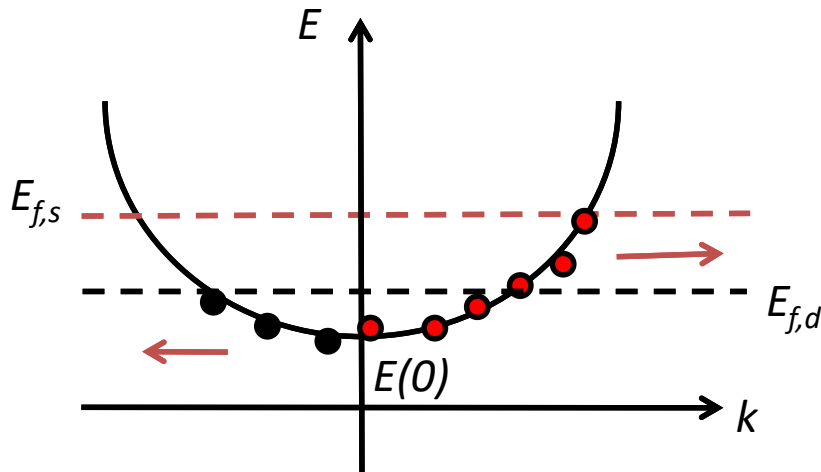
Drift-diffusion is a poor approximation for nm-scale transistors!

Ballistic Transport – Directed moments



$$v_x \frac{\partial f_0}{\partial x} - qE_x \frac{\partial f_0}{\partial p_x} = 0$$

$f=f_0$ in the active region – but with two Fermi levels!



$$n_s^+ = \frac{1}{A} \sum_{k_x, k_y > 0} f_0(E_{F,d}, E(k))$$

$$J^+ = \frac{1}{A} \sum_{k_x, k_y > 0} qv_x f_0(E(k) - E_{F,d})$$

$$\sum_{\mathbf{k}} g(\mathbf{k}) \rightarrow \frac{L^d}{(2\pi)^d} \int_{\mathbf{k}} g(\mathbf{k}) d\mathbf{k}$$

We will work out these expressions in detail for the 1D and 2D FETs in coming lectures

Quantum Transport – 1D

The Schrödinger Equation with open boundary conditions:

$$\left. \begin{aligned} \psi(x) &= 1e^{ik_1x} + re^{-ik_1x} & x < 0 \\ \psi(x) &= te^{-ik_2x} & x > L \end{aligned} \right\} \psi(x, k)$$

Local Density of states / electron density:

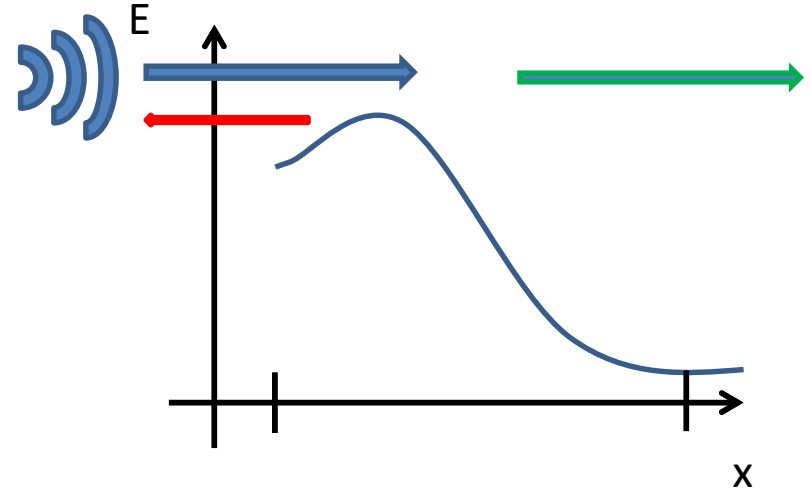
$$LDOS_1(x, E) \equiv \left[\frac{1}{\pi} \frac{dk_1}{dE} |\psi(x, k_1)| \right]$$

$$n_1(x, E) = f_0(E - E_F) LDOS_1(x, E)$$

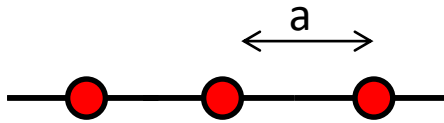
Current:

$$I_D(E) = \frac{2q}{h} T_{1-2}(E) [f_0(E - E_F) - f_0(E - E_F - qV_D)]$$

$$T_{1-2}(E) = 1 - |\psi(0, E) - 1|^2$$



Quantum Transport – Numerical Solutions



$$\frac{d^2}{dx^2} f(x_n) \rightarrow \frac{(-f(x_{n-1}) + 2f(x_n) - f(x_{n+1})))}{a^2}$$

$$[E\mathbf{I} - \mathbf{H} - \mathbf{\Sigma}_1 - \mathbf{\Sigma}_2]\psi = i\boldsymbol{\gamma}_1 \quad \text{N}\times\text{N matrix}$$

Self-Energies – models the open boundary contacts:

$$\Sigma_1(i, j) = -t_0 e^{ik_1 a} \delta_{1,i} \delta_{1,j}$$

N×N matrices with 1
element ≠ 0

$$t_0 = \frac{\hbar^2}{2m^* a^2}$$

$$\Sigma_2(i, j) = -t_0 e^{ik_1 a} \delta_{N,i} \delta_{N,j}$$

Source Injection:

$$\boldsymbol{\gamma}_1 = i[\Sigma_1(1,1) - \Sigma_1^*(1,1)] = \hbar \frac{v(k)}{a} \quad \text{N}\times\text{1 vector with (1,1) element } \neq 0$$

$$\psi = i\mathbf{G}\boldsymbol{\gamma}$$

$$\mathbf{G} = [E\mathbf{I} - \mathbf{H} - \mathbf{\Sigma}_1 - \mathbf{\Sigma}_2]^{-1}$$

Retarded Green's function

$$\left. \begin{array}{l} \psi = i\mathbf{G}\boldsymbol{\gamma} \\ \mathbf{G} = [E\mathbf{I} - \mathbf{H} - \mathbf{\Sigma}_1 - \mathbf{\Sigma}_2]^{-1} \end{array} \right\} \psi_{x_n}(E)$$

Quantum Transport – NEFG

$$\mathbf{G}_r = [\mathbf{E}\mathbf{I} - \mathbf{H} - \mathbf{\Sigma}_1 - \mathbf{\Sigma}_2]^{-1}$$

$$A_1(E) = \mathbf{G}\mathbf{\Gamma}_1\mathbf{G}^\dagger \quad \text{Spectral Density} \approx \text{LDOS}$$

$$\mathbf{\Gamma}_1 = i(\mathbf{\Sigma}_1 - \mathbf{\Sigma}_1^\dagger)$$

$$G_1^n(E) = f_0(E_{F1} - E) \frac{A_1}{2\pi} \quad \text{Correlation Function}$$

$$T_{1-2}(E) = \text{trace}(\mathbf{\Gamma}_1\mathbf{G}\mathbf{\Gamma}_2\mathbf{G}^\dagger) \quad \text{Transmission}$$

$$I_D(E) = \frac{2q}{h} T_{1-2}(E) [f_0(E - E_F) - f_0(E - E_F - qV_D)]$$

If \mathbf{H} is a real space representation:

$\text{Tr}(A_1)$ equals to the local density of states

$\text{Tr}(G_1^n)$ equals to the position dependent electron concentration

Can treat **scattering** and **many-body** effects.

$$\mathbf{G} = [\mathbf{E}\mathbf{I} - \mathbf{H} - \mathbf{\Sigma}_1 - \mathbf{\Sigma}_2 - \mathbf{\Sigma}_s]^{-1}$$



Self-Energy due to scattering

Excercises

Download and work on the excercise sets – 1 every week.