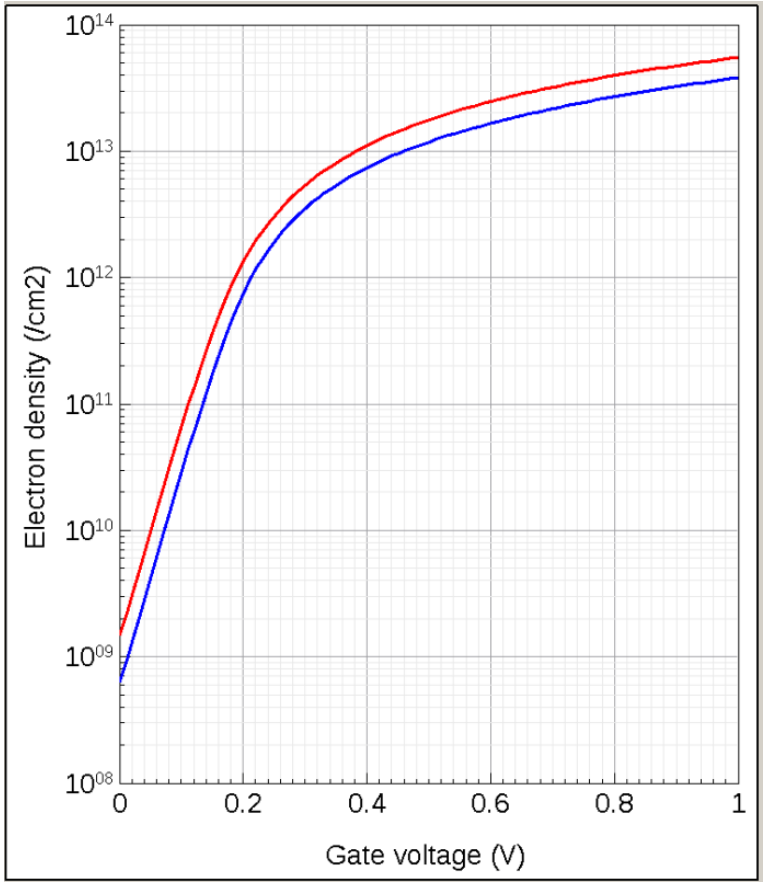
Lecture11

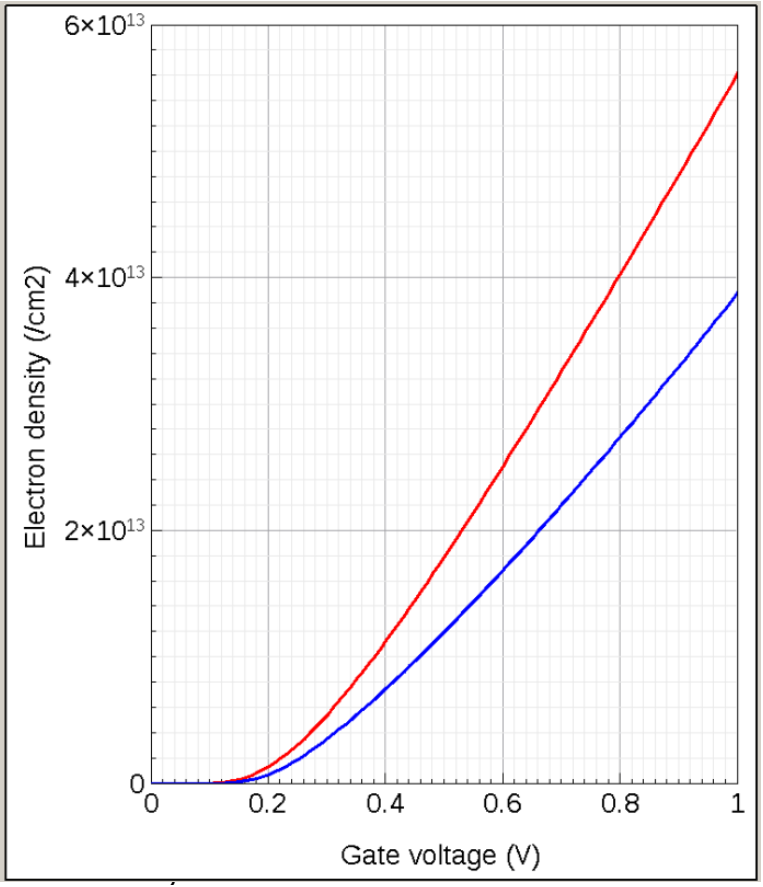
Sung-Min Hong (smhong@gist.ac.kr)

Semiconductor Device Simulation Lab.
School of Electrical Engineering and Computer Science
Gwangju Institute of Science and Technology

GIST Lecture on October 17, 2018

Answer of Homework#6





Notice

- No lecture on October 29
  - Currently, no make-up session will be provided.

- No lecture on December 3 and 5
  - One make-up session on October 31
  - We need one more!

How to find $n(x, y, z)$

- The total number is known. But, how can we find $n(x, y, z)$?
  - Each state, $\psi_{k_x,k_y,n}(x, y, z)$, contributes $\left|\psi_{k_x,k_y,n}(x, y, z)\right|^2$.
  - Recall that the wavefunction can be written as

$$\psi_{k_x,k_y,n}(x, y, z) = A_{k_x,k_y,n} e^{+ik_x x} e^{+ik_y y} \psi_{z,n}(z)$$

  - Then, $\left|\psi_{k_x,k_y,n}(x, y, z)\right|^2 = \left|A_{k_x,k_y,n}\right|^2 \left|\psi_{z,n}(z)\right|^2$
  - Integration of $\left|\psi_{k_x,k_y,n}(x, y, z)\right|^2$ over the box should give unity.

$$L_x L_y \left|A_{k_x,k_y,n}\right|^2 \int_0^{L_z} dz \left|\psi_{z,n}(z)\right|^2 = 1$$

Normalization of $\psi_{z,n}(z)$

- If $\psi_{z,n}(z)$ is normalized in the 1D structure,
  - We have the following condition:

$$\left|A_{k_x,k_y,n}\right|^2 = \frac{1}{L_x L_y}$$

  - Therefore, each state contributes

$$\left|\psi_{k_x,k_y,n}(x,y,z)\right|^2 = \frac{1}{L_x L_y}\left|\psi_{z,n}(z)\right|^2$$

  - Note that every state in a subband has the same electron density. (In general, it does not hold.)

1D infinite potential well

- When $\psi_{z,n}(z) = A_{z,n} \sin\left(\frac{n\pi}{L_z} z\right)$,
  - The value of $A_{z,n}$ is $\sqrt{\frac{2}{L_z}}$.
  - Therefore, when fully occupied, a state in the n-th subband contributes an electron density of (per spin)

$$\frac{2}{L_x L_y L_z} \sin^2\left(\frac{n\pi}{L_z} z\right)$$

  - Finally, the electron density can be obtained by considering all subbands.

MATLAB example (1)

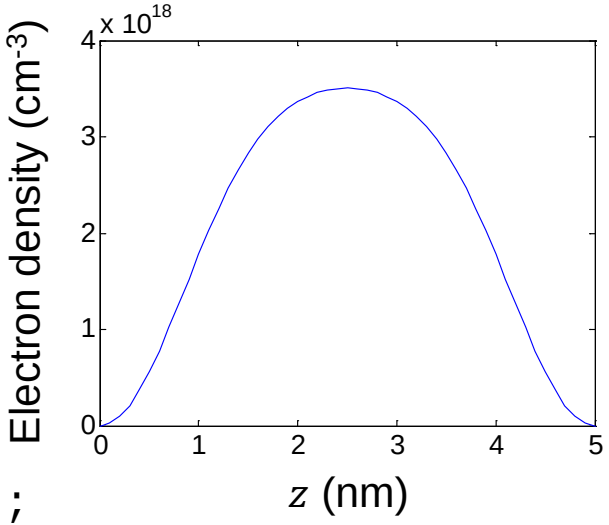
- Preparing some constants (the same as before)

```
h = 6.626176e-34; % Planck constant, J s
hbar = h / (2*pi); % Reduced Planck constant, J s
q = 1.602192e-19; % Elementary charge, C
m0 = 9.109534e-31; % Electron rest mass, kg
k_B = 1.380662e-23; % Boltzmann constant, J/K
T = 300.0; % Temperature, K
Lx = 100e-9; Ly = 100e-9; Lz = 5e-9; % Lenghs, m
mxx = 0.19; myy = 0.19; mzz = 0.91; % Masses, m0
nmax = 10;
coef = 2*Lx*Ly/(2*pi)*sqrt(mxx*myy)*m0/(hbar^2)*(k_B*T);
```

MATLAB example (2)

- Calculation of `elec`

```
totalNumber = 0;
Nz = 51;
z = transpose([0:Nz-1])*Lz/(Nz-1);
elec = zeros(Nz,1); % Electron density, /m^3
for n=1:nmax
  Ez = (hbar^2)/(2*mzz*m0)*(pi*n/Lz)^2;
  subbandNumber = coef*log(1+exp(-Ez/(k_B*T)));
  totalNumber = totalNumber + subbandNumber;
  elec = elec + 2/(Lx*Ly*Lz)*(sin(n*pi*z/Lz).^2)*subbandNumber;
end
plot(z/1e-9,elec/1e6)
```



Homework#7

- Due: AM08:00, October 22
- Problem#1
  - Up to now, we have assumed that the Fermi energy is 0 eV.
  - In this problem, a 5-nm-thick potential well is considered again.
  - You can set it to any value. (-0.1 eV to +0.1 eV)
  - Calculate the integrated electron density (/cm^2) as a function of the Fermi energy.
  - Show snapshots of the electron density for different Fermi energies.