Lecture12

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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)

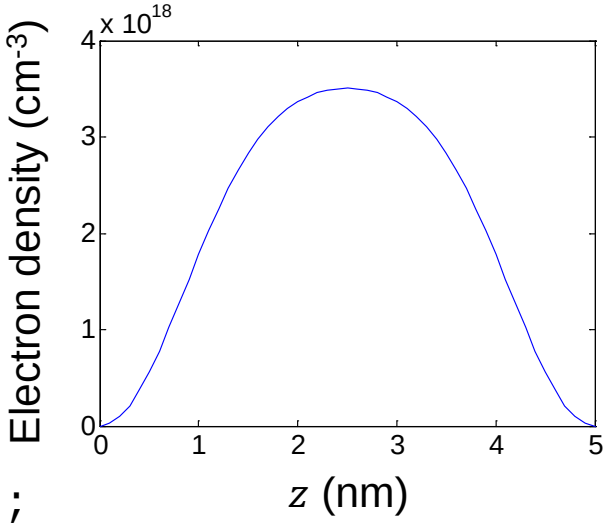
- Preparing some constants (the same as before)

```
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)
```



Potential energy

- In the case of the infinite potential well, the potential energy is 0 eV.
  - Of course, in the realistic case, the potential energy is provided from the Poisson equation.
  - When the electrostatic potential, $\phi(z)$, is given, the potential energy is written as

$$V(z) = -q\phi(z) + (E_c - E_i)$$

$E_c - E_i$: Constant for a given material

Schrödinger equation

- For the z-directional Schrödinger equation,
  - We have the following form:

$$-\frac{\hbar^2}{2m_{zz}}\frac{d^2}{dz^2}\psi_{z,n}(z)+V(z)\,\psi_{z,n}(z)=E_{z,n}\psi_{z,n}(z)$$

  - After a simple manipulation,

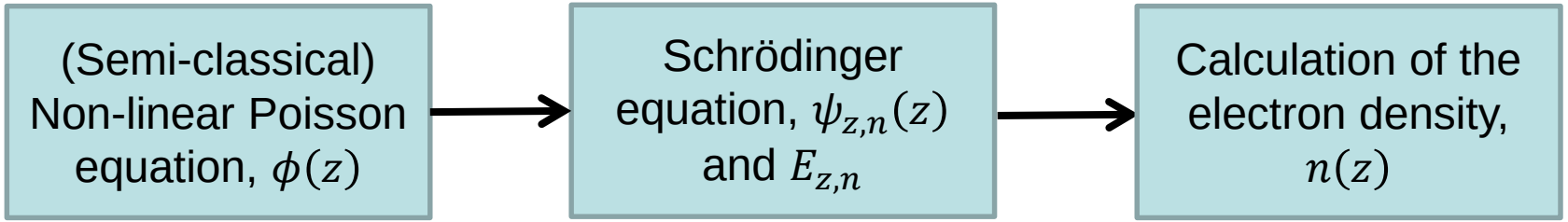
$$\frac{d^2}{dz^2}\psi_{z,n}(z)-\frac{2m_{zz}}{\hbar^2}V(z)\,\psi_{z,n}(z)=-\frac{2m_{zz}}{\hbar^2}E_{z,n}\psi_{z,n}(z)$$

  - Discretized version

$$\psi_{z,n,i+1}-2\psi_{z,n,i}+\psi_{z,n,i-1}-\frac{2m_{zz}}{\hbar^2}V(z_i)(\Delta z)^2\psi_{z,n,i}=-\frac{2m_{zz}}{\hbar^2}E_{z,n}(\Delta z)^2\psi_{z,n,i}$$

Simulation flow

- Anyway, we need the initial solution.
  - It can be obtained from the semi-classical simulation.
  - Then, under the given potential energy, we can calculate the electron density.



  - Of course, the electron density is not fully consistent with the Poisson equation. It should be improved later.

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

- Its normalization condition
  - Integration form

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

  - Discretized version (Be careful for the interface nodes!)

$$\sum_i \Delta z \left|\psi_{z,n,i}\right|^2 = 1$$

  - Eigenfunctions should be normalized accordingly.

Six valleys in silicon

- Up to now, we have considered only one band.
  - In silicon, we need to consider three valley pairs.
  - They can be characterized by (for a certain channel direction)

$m_{xx} = 0.91m_0, m_{yy} = 0.19m_0, m_{zz} = 0.19m_0$

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  - Each of them has two-fold degeneracy.

Homework#12

- Due: AM08:00, October 19 (Next Monday)
- Problem#1
  - It is based upon your Homework#8.
  - Consider the gate voltages from 0 V to 1 V.
  - For each gate voltage, first solve the nonlinear Poisson equation. (It has been done in Homework#8.)
  - By using the electrostatic potential, calculate the electron density. Of course, you must consider six valleys.
  - For each gate voltage, draw the electron densities calculated by two ways in the z axis.