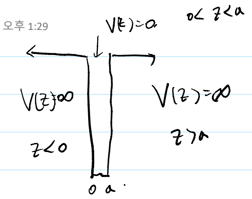
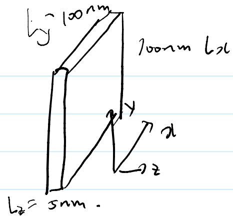
Hw 12

2020년 10월 14일 수요일 오후 1:29





※ infinite potential well 에서 전자농도 구하기.

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

$$\left|\psi_{k_x k_y n}(x,y,z)\right|^2 = |A_{k_x k_y n}|^2 \, |\psi_{z,n}(z)|^2$$: probability density of particle at (x,y,z)

$$\iiint |\psi_{k_x k_y n}|^2 \, dx dy dz = L_x L_y |A_{k_x k_y n}|^2 \int |\psi_{z,n}(z)|^2 dz$$
$$= 1.$$: integration of probability density of space = 1.

If $\int |\psi_{n,z}(z)|^2 dz = 1.$ (normalized)
then $|A|^2 = \dfrac{1}{L_x L_y}$

When $\psi_{z,n}(z) = A_{z,n} \sin\left(\dfrac{n\pi}{L_z} z\right)$

$\Rightarrow \int |\psi_z|^2 dz = 1$

$\therefore A_{z,n} = \sqrt{\dfrac{2}{L_z}}$

$\therefore |\psi(x,y,z)|^2$
$= \dfrac{2}{L_x L_y L_z} \sin^2\left(\dfrac{n\pi}{L_z} z\right)$; 1-D infinite potential well 의 경우.

만약, $\psi_{n,z}(z)$ 가 normalized 된 wavefunction 일 경우,
electron density $n(z)$는 다음과 같다.

$$n(z) = \frac{1}{L_x L_y} \sum_n |\psi_n(z)|^2 \times \underline{f_{FD}(E_{z,n})} \times 2$$ ← spin degeneracy.

↳ $E_{z,n}$ 의 energy 를 갖을 때 Fermi-dirac distribution.

probability density.

◎ $\psi_n(z)$, $E_{z,n}$ 계산을 위한 flow charts.

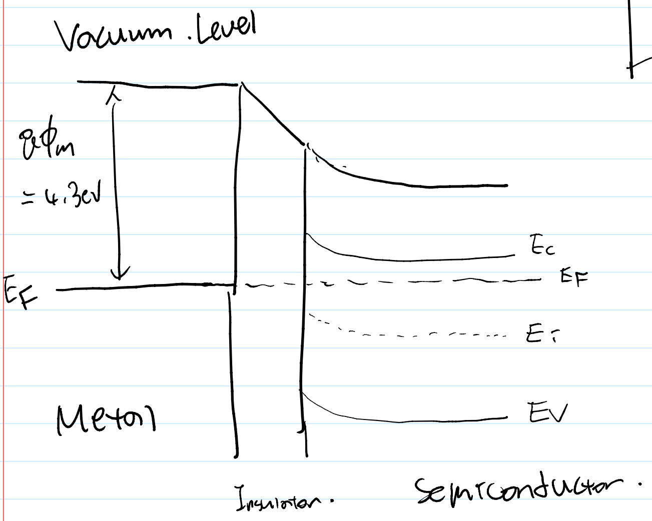
$\boxed{\text{HW 8에서 구한 electostatic potential } \phi}$ $\xrightarrow{\text{Semi-classical.}}$ $n(z)_{semiclassical.} = n_i \exp\left(q\phi / k_B T\right)$

↓ quantum mechanical.

$\boxed{\text{Solve Schrodinger eq.}}$ → $\boxed{\text{get } \cdot \psi_n(z) \text{ eigen function. } \cdot E_n, \text{ eigen-value}}$

↓

$n(z)_{quantum}$
$= \dfrac{1}{\ldots} \sum f_{FD}(E_{z,n}) |\psi_n(z)|^2 \times 2.$



$$\boxed{n(z)_{quantum} = \frac{1}{L_x L_y} \sum f_{FD}(E_{z,n}) |\psi_n(z)|^2 \times 2.}$$

$$n = N_c \exp\left(\frac{E_F - E_c}{k_B T}\right)$$

$$= N_c \exp\left(\frac{-E_c}{kT}\right) \quad (E_F = 0)$$

$$= N_c \exp\left(\frac{E_i - E_c}{kT}\right) \exp(-E_i/kT)$$

$$= n_i \exp(q\phi_i/k_B T) \quad (E_i = -q\phi_i)$$

슈뢰딩거 방정식.

$$\frac{\hbar^2}{2m_{zz}} \partial_z^2 \psi_n(z) + V(z)\psi_n(z) = E_{n,z}\psi_n(z)$$

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

$\boxed{HW8}$

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

Set $\alpha \equiv \frac{\hbar^2}{2m_{zz}(\Delta z)^2}$

$$\begin{pmatrix} -2\alpha+V & \alpha & 0 & \cdots & \cdots & 0 \\ +\alpha & -2\alpha+V & \alpha & 0 & \cdots & 0 \\ 0 & \alpha & -2\alpha+V & \alpha & \cdots & 0 \\ \vdots & & \ddots & & & \vdots \\ \vdots & & & \ddots & & \\ \vdots & & 0 & \alpha & -2\alpha+V & \alpha \\ 0 & \cdots & 0 & \cdots & \alpha & -2\alpha+V \end{pmatrix} \psi_{n,z} = E_{n,z}\psi_n(z).$$

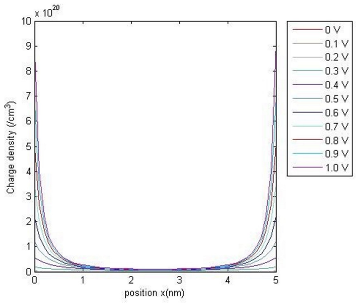
위의 eigenvalue problem 을 풀어주면.

Eigenvalue, eigen vector 들을 구할 수 있음.

이때, eigenvector 들은, $\psi_n(z) \times \sqrt{\frac{1}{\Delta z}}$ 를 통해 normalization 해줘야 한다.

결과.

① Semiclassical electron density.



② quantum mechanical

i) when $m_{zz} = 0.91\, m_e$ ii) when $m_{zz} = 0.19\, m_e$.