HW 11 20202010 신현석

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i) Assume $L_x, L_y \gg L_z$.

ii) Hamiltonian

$$\mathcal{H} = -\frac{\hbar^2}{2m_{xx}}\frac{\partial^2}{\partial x^2} - \frac{\hbar^2}{2m_{yy}}\frac{\partial^2}{\partial y^2} - \frac{\hbar^2}{2m_{zz}}\frac{\partial^2}{\partial z^2}.$$

iii) Energy eigen value of 3-D infinite potential well.

(i) periodic boundary condition.

$$\psi_{xyz} = \psi_x(x)\psi_y(y)\psi_z(z)$$

$$\Rightarrow \left(\begin{aligned} &\psi_x(0) = \psi_x(L_x) = 0 \\ &\psi_y(0) = \psi_y(L_y) = 0 \\ &\psi_z(0) = \psi_z(L_z) = 0 \end{aligned} \right)$$

$$\hookrightarrow \psi_{lmn} = A_{lmn}\sin\left(\frac{l\pi}{L_x}x\right)\sin\left(\frac{m\pi}{L_y}y\right)\sin\left(\frac{n\pi}{L_z}z\right)$$

where $E_{lmn} = \frac{\hbar^2}{2m_{xx}}\frac{l^2\pi^2}{L_x^2} + \frac{\hbar^2}{2m_{yy}}\frac{m^2\pi^2}{L_y^2} + \frac{\hbar^2}{2m_{zz}}\frac{n^2\pi^2}{L_z^2}.$

iV) Subbands.

because we assume that

$L_x, L_y \gg L_z$

different n gives big difference in E_{lmn}

V) if L_z is so small.

there are only 1 possible state along z-direction.

$\rightarrow$ quantum confinement.

Vi) Calculate the number of possible state of n-th subband.

$$\text{(i)} \quad \underbrace{2}_{\text{spin degeneracy.}}\sum_l \sum_m f_{FD}(E_{l,m,n}) = 2\cdot\frac{L_xL_y}{(2\pi)^2}\int_{-\infty}^{\infty} dk_x\int dk_y\, f_{FD}\left(\frac{\hbar^2k_x^2}{2m_{xx}} + \frac{\hbar^2k_y^2}{2m_{yy}} + E_{z,n}\right)$$

$$= \frac{\sqrt{m_{xx}m_{yy}}}{\cancel{m_d}}\, 2\cdot\frac{L_xL_y}{(2\pi)^2}\int_{-\infty}^{\infty} dk_x'\int_{-\infty}^{\infty} dk_y'\, f_{FD}\left(\frac{\hbar^2k'^2}{2m_d} + E_{z,n}\right)$$

$$\left(k_x' = k_x\sqrt{\frac{m_d}{m_{xx}}},\quad k_y' = k_y\sqrt{\frac{m_d}{m_{yy}}} \right.$$
$$\left. k' = k_x'^2 + k_y'^2;\quad m_d = \sqrt{m_{xx}m_{yy}} \right)$$

$$= 2\cdot\frac{L_xL_y}{(2\pi)^2}(2\pi)\int_0^{\infty} dk'\,k' f_{FD}\left(\frac{\hbar^2k'^2}{2m_d} + E_{z,n}\right)$$

$$= 2\cdot \frac{L_x L_y}{(2\pi)^2}(2\pi)\frac{m_d}{\hbar^2}\int_0^\infty dE_{xy}\, f_{FD}(E_{xy}+E_{z,n})$$

where $E_{xy} \equiv \frac{\hbar^2 k'^2}{2m_d}$

$$f_{FD}(E_{xy}+E_{z,n}) = \frac{1}{1+\exp\left(\frac{E_{xy}+E_{z,n}-E_F}{k_BT}\right)}$$

Say $\frac{E_{xy}}{k_BT} = e_{xy}$

And $\eta = \frac{E_{z,n}-E_F}{k_BT}$

then $\int_0^\infty dE_{xy}\, f_{FD}(E_{xy}+E_{z,n})$

$$= k_BT \int_0^\infty de_{xy}\, \frac{1}{1+\exp[e_{xy}-(-\eta)]}$$

$$= k_BT \ln\left(1+\exp\left(\frac{-E_{z,n}+E_F}{kT}\right)\right)$$

total number of electrons.

$$2\cdot \sum_{n=1}^{\infty} \frac{L_xL_y}{(2\pi)^2}(2\pi)\frac{m_d}{\hbar^2}k_BT\ln\left(1+\exp\left(\frac{-E_{z,n}+E_F}{kT}\right)\right)$$

Result