EE 232 Lightwave Devices
Lecture 4: Quantum Wells

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Review of Quantum Mechanics

Schrodinger Equation

$$H\Psi(\vec{r},t) = i\hbar\frac{\partial}{\partial t}\Psi(\vec{r},t)$$

$$H = \frac{P^2}{2m_0} + V(\vec{r},t)$$ Hamiltonian = Kinetic + Potential Energy

$\Psi(\vec{r},t)$ Wavefunction

$\left|\Psi(\vec{r},t)\right|^2 = \Psi(\vec{r},t)\cdot\Psi(\vec{r},t)^*$ Probability of finding particle at $\vec{r}$

$\vec{P} = -i\hbar\nabla$ Momentum operator

$\left\langle\vec{P}\right\rangle = -i\hbar\int\Psi(\vec{r},t)^*\nabla\Psi(\vec{r},t)d\vec{r}$ Average Momentum

$\left\langle\vec{r}\right\rangle = \int\Psi(\vec{r},t)^*\vec{r}\Psi(\vec{r},t)d\vec{r}$ Average Position

Solution in Free Space

Consider 1-d case, and separation of variables

$$\Psi(\vec{r},t)=\Psi(x,t)=\phi(x)e^{-i\omega t}$$

$$\frac{-\hbar^2}{2m_0}\frac{d^2\phi(x)}{x^2}e^{-i\omega t}=i\hbar\cdot(-i\omega)\cdot\phi(x)e^{-i\omega t}$$

$$\frac{d^2\phi(x)}{x^2}+\frac{2m_0\hbar\omega}{\hbar^2}\cdot\phi(x)=0$$

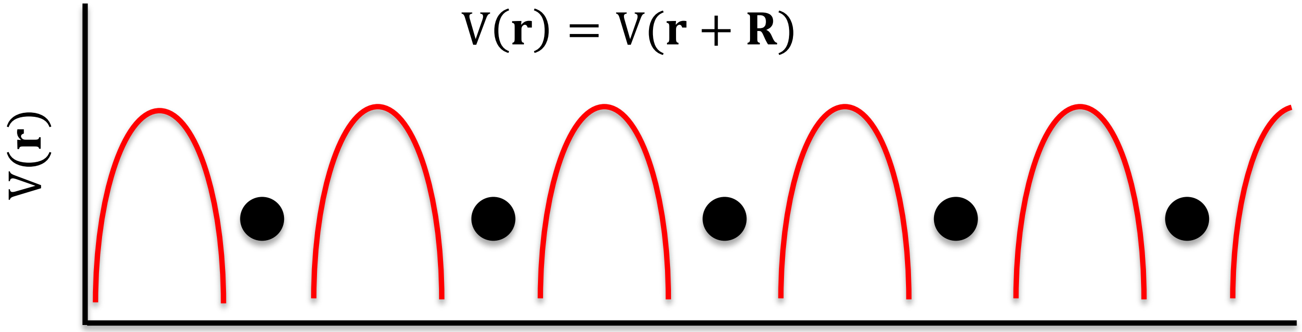
Let $k=\sqrt{\frac{2m_0\hbar\omega}{\hbar^2}}$

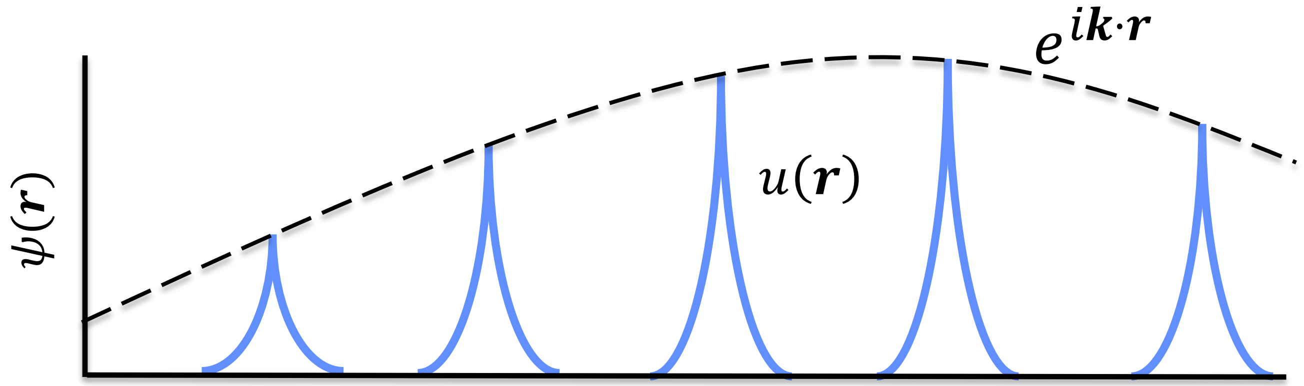
$$\frac{d^2\phi(x)}{x^2}+k^2\cdot\phi(x)=0$$

Solution: $\phi(x)=e^{i\vec{k}\cdot\vec{r}}$ or $e^{-i\vec{k}\cdot\vec{r}}$

$\Psi(\vec{r},t)=e^{\pm i\vec{k}\cdot\vec{r}-i\omega t}$: Plane waves

In Uniform Crystals: Bloch Theorem





$$\psi(r) = u(r)e^{ik\cdot r}$$ (Bloch Theorem)

In Heterostructures: Envelope wave function

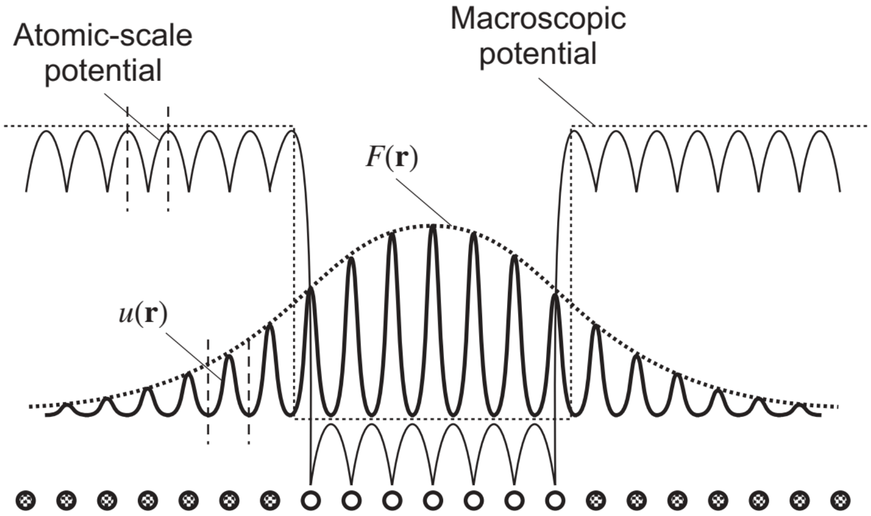


Figure from Coldren et al.
Diode Lasers and Photonic Integrated Circuits

General linear superposition of Bloch states (i.e. a wave-packet)

$$\Psi(\mathbf{r},t)=\sum_k C_k u_k(\boldsymbol{r})exp(i\mathbf{k}\cdot\mathbf{r})exp(-iE_k t/\hbar)$$

$$\Psi(\mathbf{r},t)\cong u_0(\boldsymbol{r})\left(\sum_k C_k exp(i\mathbf{k}\cdot\mathbf{r})exp(-iE_k t/\hbar)\right)$$

$$\Psi(\mathbf{r},t)=u_0(\boldsymbol{r})\cdot\psi_{env}(\mathbf{r},t)$$

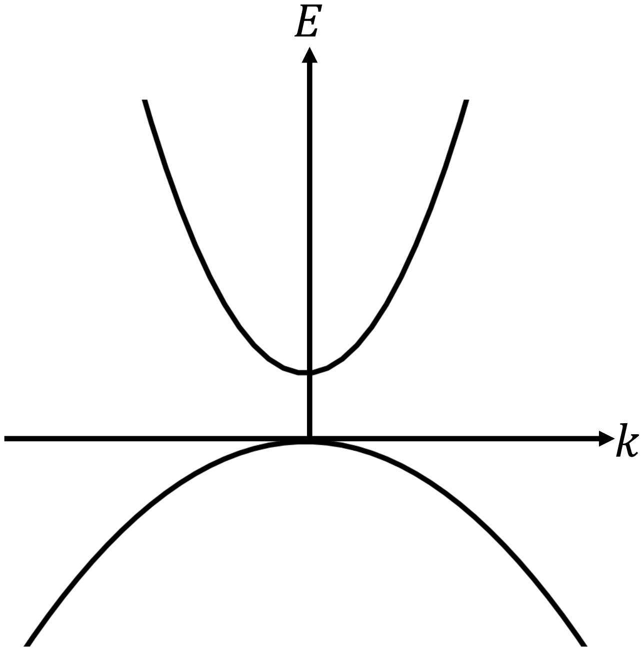
Assumptions:

(1) Include only one band and

(2) electrons are near bandedge

$u_k(\boldsymbol{r})\approx u_0(\boldsymbol{r})$

Effective Mass Approximation



$$E_k = \frac{\hbar^2 k^2}{2m_e^*} + V(r)$$

kinetic energy

potential energy

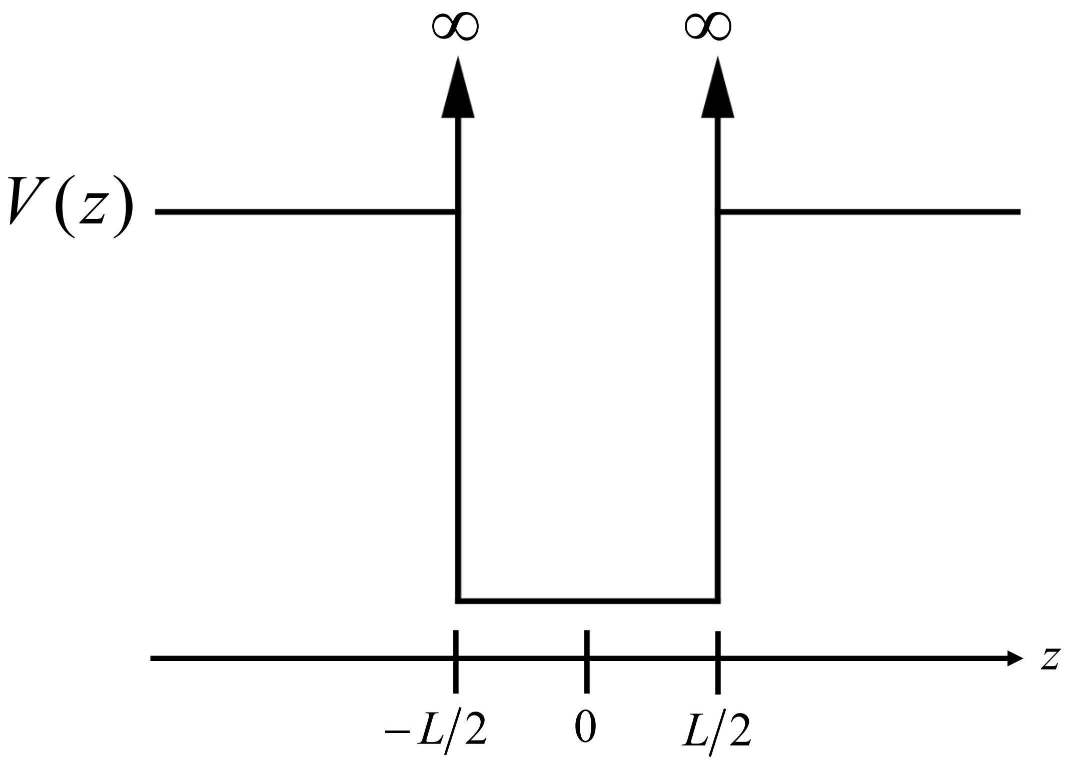
Schrodinger Equation for Envelope wave function

$$
\begin{aligned}
i\hbar \frac{\partial \psi_{env}(\mathbf{r},t)}{\partial t} &= \sum_k C_k E_k exp(i\mathbf{k}\cdot\mathbf{r}) exp(-iE_k t/\hbar) \\
&= \sum_k C_k \left(\frac{\hbar^2 k^2}{2m_e^*} + V(\mathbf{r}) \right) exp(i\mathbf{k}\cdot\mathbf{r}) exp(-iE_k t/\hbar) \\
&= \sum_k C_k \left(\frac{\hbar^2 k^2}{2m_e^*} \right) exp(i\mathbf{k}\cdot\mathbf{r}) exp(-iE_k t/\hbar) + V(\mathbf{r})\psi_{env}(\mathbf{r},t) \\
&= \frac{\hbar^2}{2m_e^*} \sum_k [-C_k \nabla^2 exp(i\mathbf{k}\cdot\mathbf{r}) exp(-iE_k t/\hbar)] + V(\mathbf{r})\psi_{env}(\mathbf{r},t)
\end{aligned}
$$

$$
\boxed{i\hbar \frac{\partial \psi_{env}(\mathbf{r},t)}{\partial t} = \left[\frac{-\hbar^2}{2m_e^*} \nabla^2 + V(\mathbf{r}) \right] \psi_{env}(\mathbf{r},t)}
$$

Schrodinger equation in terms of envelope wave function and macro potential
Periodicity of crystal potential is captured in m_e^*

Infinite potential well



$$V(z) = \begin{cases} 0 & \text{for } z < |L/2| \\ \infty & \text{for } z > |L/2| \end{cases}$$

Separation of variables

$$\left[-\frac{\hbar^2}{2m^*}\nabla^2+V(x,y,z)\right]\psi(x,y,z)=E\psi(x,y,z)$$

$$\psi(x,y,z)=\phi_x(x)\phi_y(y)\phi_z(z)$$

$$-\frac{\hbar^2}{2m^*}\frac{\partial^2\phi_x}{\partial x^2}+V(x)\phi_x=E_x\phi_x \qquad -\frac{\hbar^2}{2m^*}\frac{\partial^2\phi_y}{\partial y^2}+V(y)\phi_y=E_y\phi_y \qquad -\frac{\hbar^2}{2m^*}\frac{\partial^2\phi_z}{\partial z^2}+V(z)\phi_z=E_z\phi_z$$

If $V(x,y,z)=V(z)$

$$\psi(x,y,z)=\phi_x(x)\phi_y(y)\phi_z(z)$$

$$-\frac{\hbar^2}{2m^*}\frac{\partial^2\phi_x}{\partial x^2}=E_x\phi_x$$

$$-\frac{\hbar^2}{2m^*}\frac{\partial^2\phi_y}{\partial y^2}=E_y\phi_y$$

$$-\frac{\hbar^2}{2m^*}\frac{\partial^2\phi_z}{\partial z^2}+V(z)\phi_z=E_z\phi_z$$

$$\phi_x=Ae^{ik_xx}$$

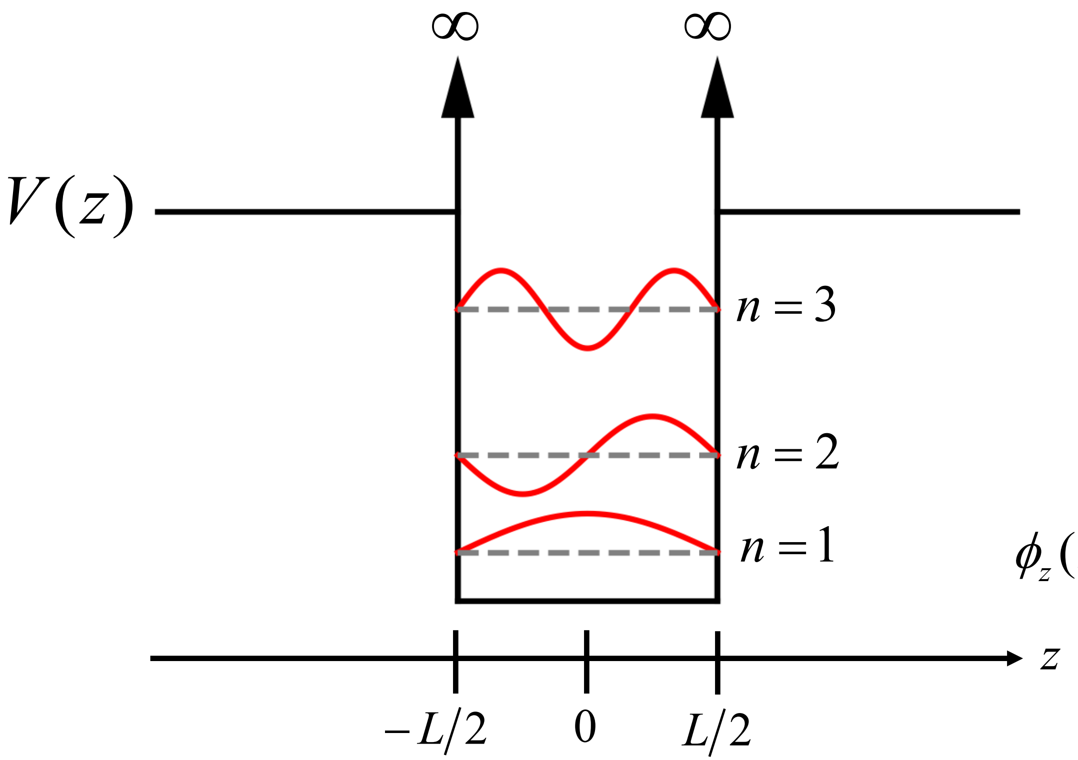
$$\phi_y=Be^{ik_yy}$$

$$\phi_t=\phi_x\phi_y=Ce^{i(k_xx+k_yy)}$$

$$1=\int|\phi_t|^2\,dxdy\rightarrow C=\frac{1}{\sqrt{A}}$$

$$\phi_t=\frac{1}{\sqrt{A}}e^{i(k_xx+k_yy)}$$

Infinite potential well



$$\psi(x,y,z)=\phi_t(x,y)\phi_z(z)$$

$$\phi_t=\frac{1}{\sqrt{A}}e^{i(k_x x+k_y y)}$$

$$\phi_z(z)=\begin{cases}\sqrt{\frac{2}{L}}\cos\left(\frac{n\pi}{L}z\right) & n=1,3,5,\ldots\\ \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi}{L}z\right) & n=2,4,6,\ldots\end{cases}$$

$$E=\frac{\hbar^2}{2m_w^*}\left[k_x^2+k_y^2+\left(\frac{n\pi}{L}\right)^2\right]$$

$$V(z)=\begin{cases}0 & \text{for } z<|L/2|\\ \infty & \text{for } z>|L/2|\end{cases}$$

Typical Examples

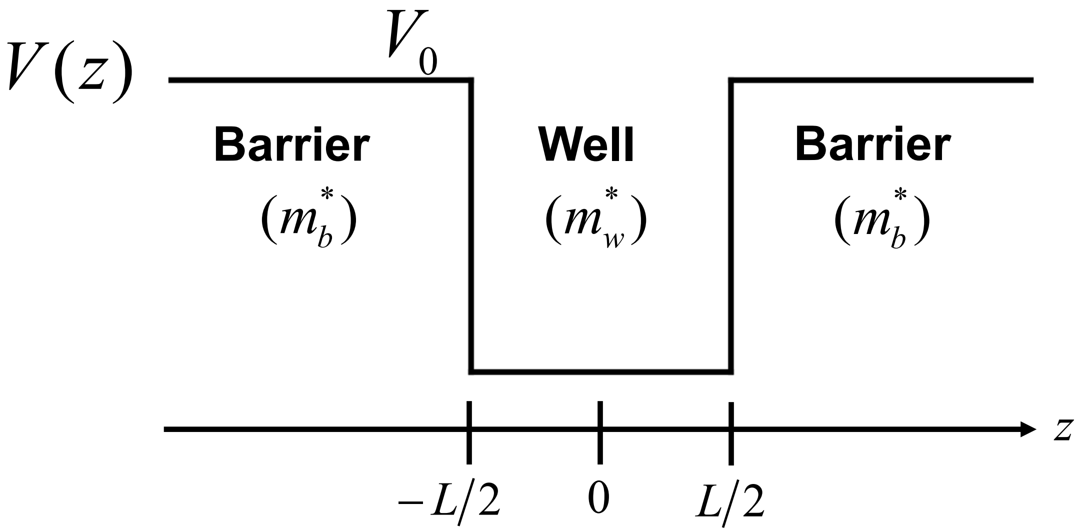
In GaAs, $m_e^* = 0.067 m_0$

For a 10-nm-wide potential well ($L = 10nm$)

$E_1 = 56$ meV

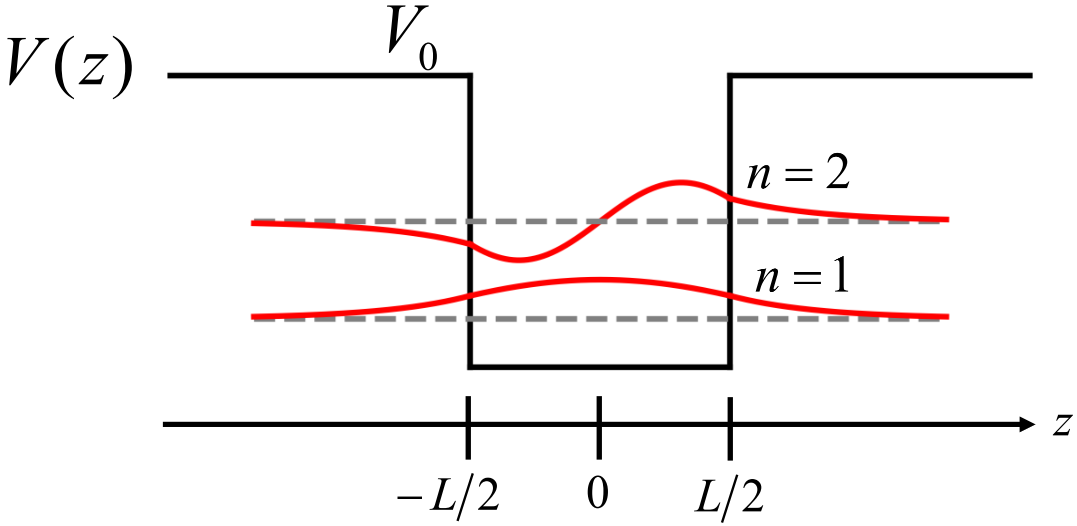
$E_2 = 4E_1 = 224$ meV

Finite potential well



$$V(z) = \begin{cases} 0 & \text{for } z < |L/2| \\ V_0 & \text{for } z > |L/2| \end{cases}$$

Finite potential well



$$V(z)=\begin{cases}0 & \text{for } z<|L/2| \\ V_0 & \text{for } z>|L/2|\end{cases}$$

$$\psi(x,y,z)=\phi_t(x,y)\phi_z(z)$$

$$\phi_t=\frac{1}{\sqrt{A}}e^{i(k_x x+k_y y)}$$

Barrier solution

$$\phi_z(z)=\begin{cases}Ce^{-\alpha(z-L/2)} & z>\frac{L}{2} \\ Ce^{\alpha(z+L/2)} & z<\frac{L}{2}\end{cases}$$

Well even solution

$$\phi_z(z)=B\cos(k_z z) \quad \tfrac{-L}{2}<z<\tfrac{L}{2}$$

Well odd solution

$$\phi_z(z)=A\sin(k_z z) \quad \tfrac{-L}{2}<z<\tfrac{L}{2}$$

Finite potential well

Barrier solution

$$\phi_z(z) = \begin{cases} Ce^{-\alpha(z-L/2)} & z > \frac{L}{2} \\ Ce^{\alpha(z+L/2)} & z < \frac{L}{2} \end{cases}$$

Well even solution

$$\phi_z(z) = B\cos(k_z z) \qquad \tfrac{-L}{2} < z < \tfrac{L}{2}$$

Well odd solution

$$\phi_z(z) = A\sin(k_z z) \qquad \tfrac{-L}{2} < z < \tfrac{L}{2}$$

① Plug into Schrodinger's Equation

$$\longrightarrow \quad \alpha = \frac{\sqrt{(V_0 - E)2m_b^*}}{\hbar}, \qquad k_z = \frac{\sqrt{2m_w^* E}}{\hbar}$$

② Apply boundary conditions

$$\phi_z\left(L^+/2\right) = \phi_z\left(L^-/2\right)$$

$$\frac{1}{m_b^*}\frac{d}{dz}\phi_z\left(L^+/2\right) = \frac{1}{m_w^*}\frac{d}{dz}\phi_z\left(L^-/2\right)$$

$$\longrightarrow$$

$$\alpha = k_z \frac{m_b^*}{m_w^*}\tan\left(k_z \frac{L}{2}\right) \quad \textbf{(even)}$$

$$\alpha = -k_z \frac{m_b^*}{m_w^*}\cot\left(k_z \frac{L}{2}\right) \quad \textbf{(odd)}$$

Finite potential well

Barrier solution

$$\phi_z(z) = \begin{cases} Ce^{-\alpha(z-L/2)} & z > \frac{L}{2} \\ Ce^{\alpha(z+L/2)} & z < \frac{L}{2} \end{cases}$$

Well even solution

$$\phi_z(z) = B\cos(k_z z) \quad \frac{-L}{2} < z < \frac{L}{2}$$

Well odd solution

$$\phi_z(z) = A\sin(k_z z) \quad \frac{-L}{2} < z < \frac{L}{2}$$

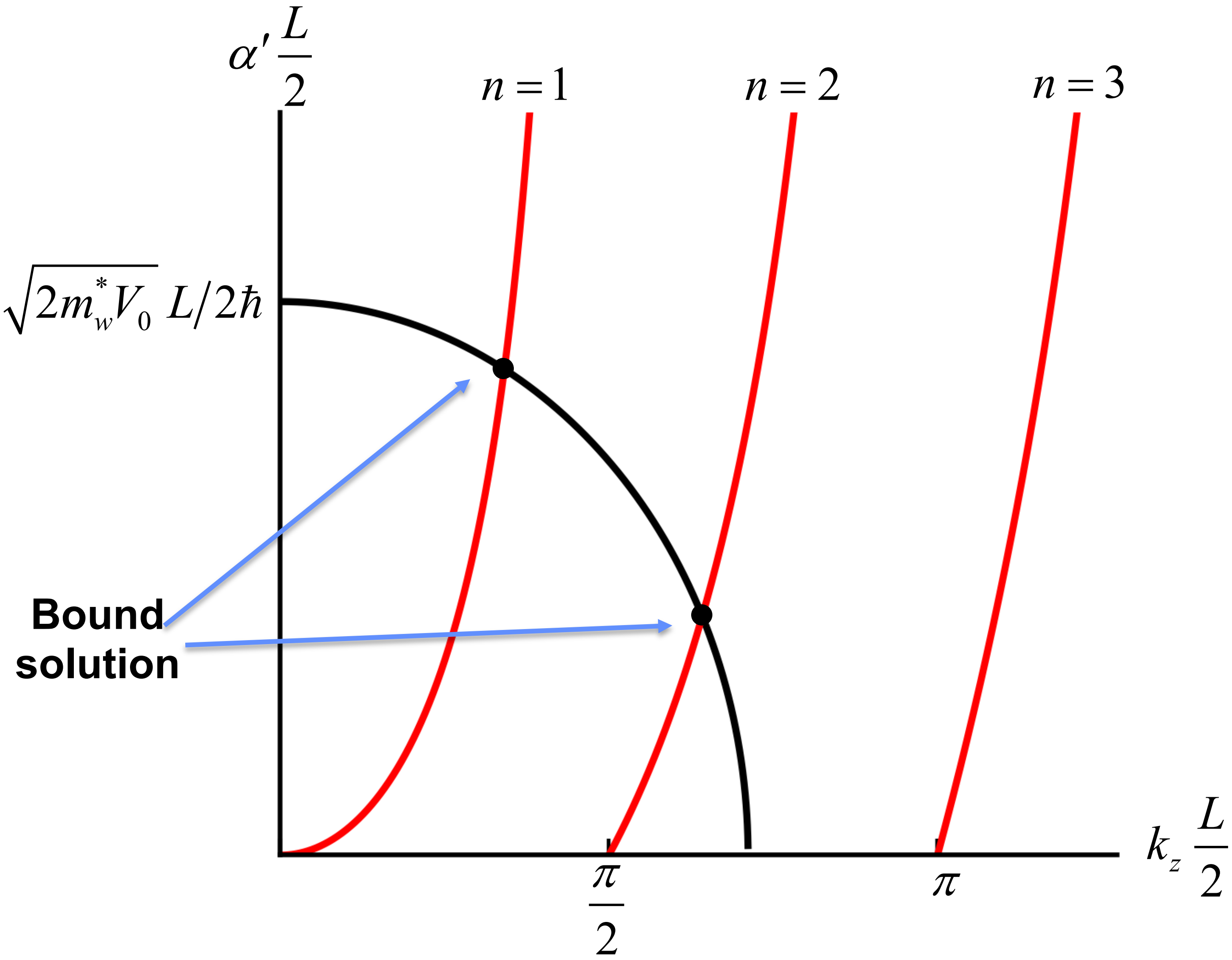
③ After rearranging →

$$\boxed{\begin{aligned} &\left(\alpha'\frac{L}{2}\right)^2 + \left(k_z\frac{L}{2}\right)^2 = \frac{2m_w^* V_0}{\hbar^2}\left(\frac{L}{2}\right)^2 \\ &\alpha'\frac{L}{2} = k_z\frac{L}{2}\sqrt{\frac{m_b^*}{m_w^*}}\tan\left(k_z\frac{L}{2}\right) \quad \textbf{(even)} \\ &\alpha'\frac{L}{2} = -k_z\frac{L}{2}\sqrt{\frac{m_b^*}{m_w^*}}\cot\left(k_z\frac{L}{2}\right) \quad \textbf{(odd)} \end{aligned}}$$

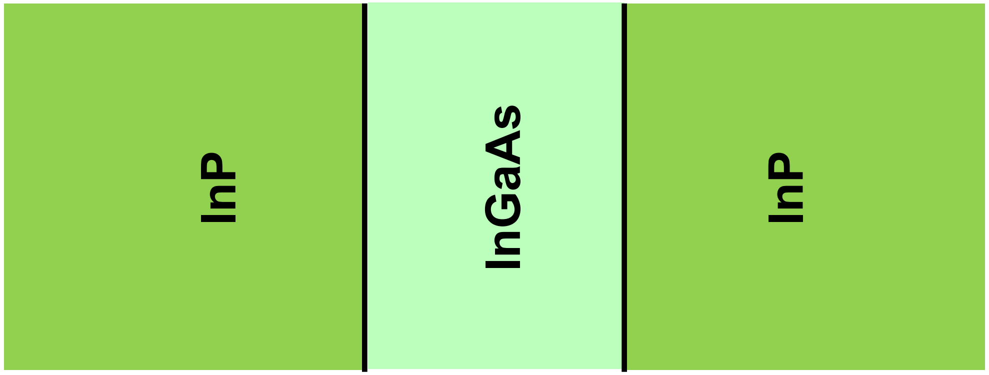
where $\alpha' = \alpha\sqrt{\frac{m_w^*}{m_b^*}}$

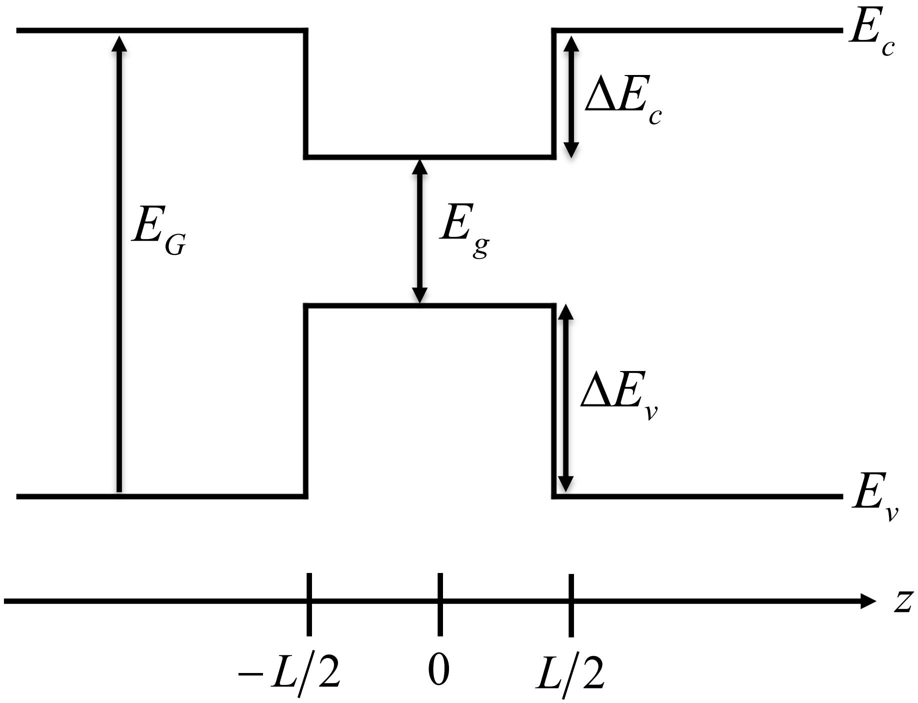
Finite potential well

④ Solve graphically

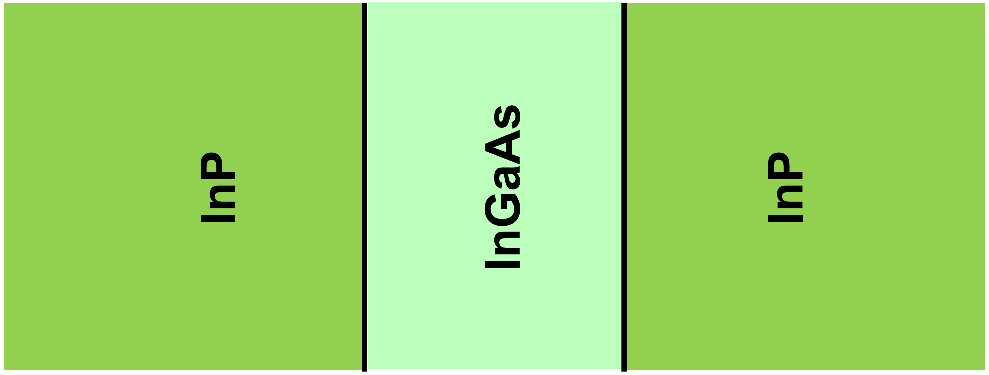


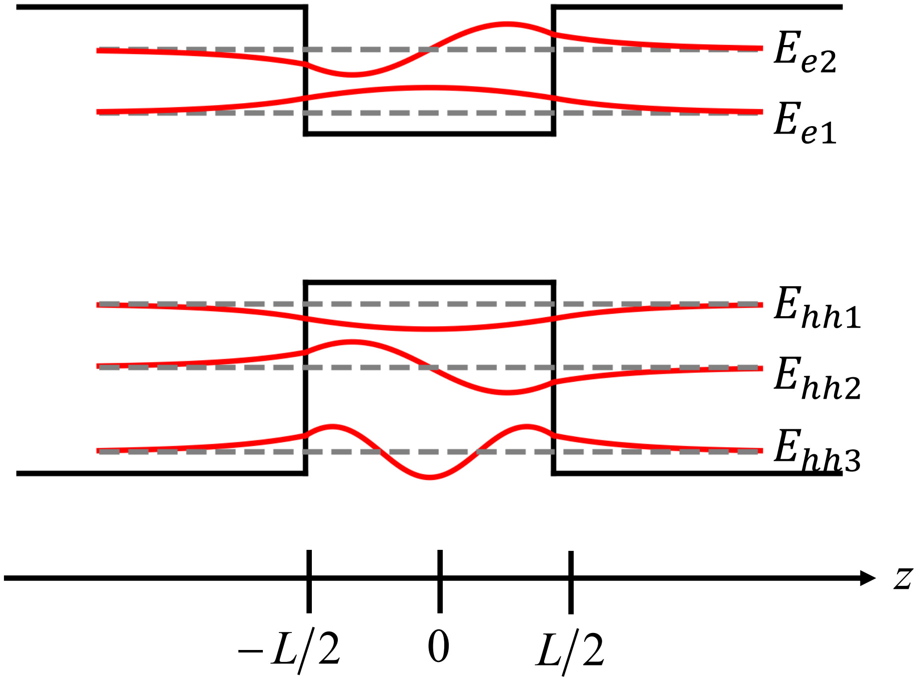
Semiconductor quantum well





Semiconductor quantum well

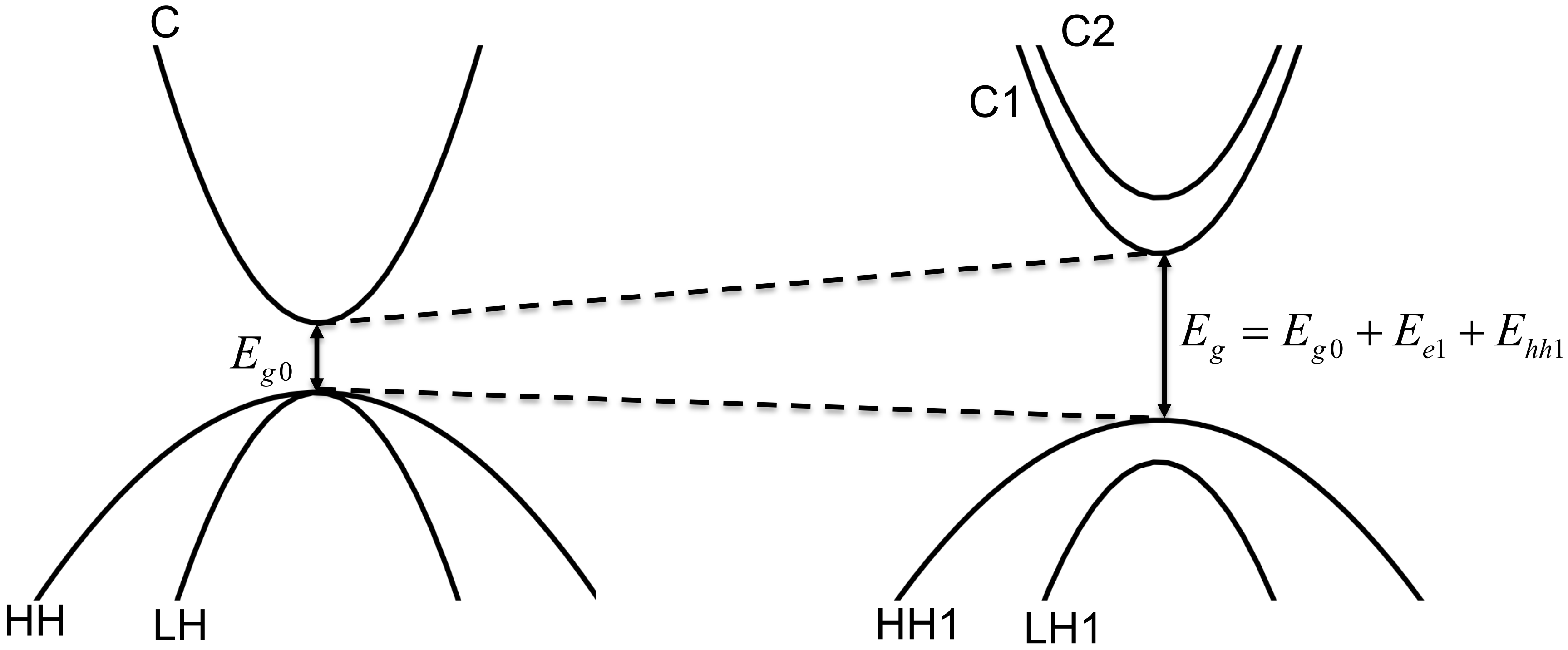




Only heavy-hole showed for clarity

Semiconductor quantum well

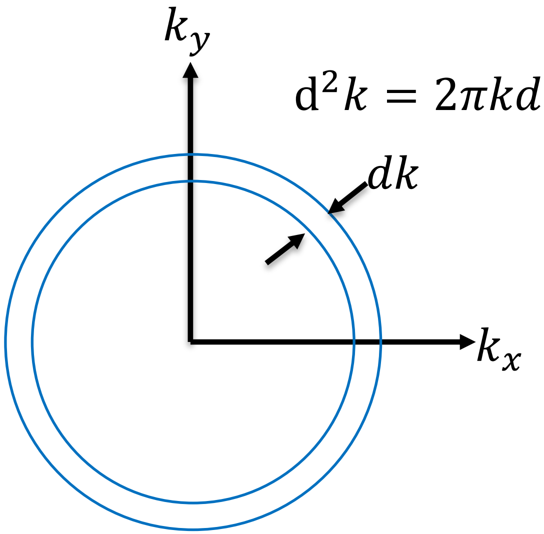
$$E = \frac{\hbar^2}{2m_w^*}\left[k_x^2 + k_y^2 + \left(\frac{n\pi}{L}\right)^2\right]$$



“Bulk” material
No quantum confinement

Quantum well

Density of states (2D)



Conduction Band

$$E = \frac{\hbar^2 k^2}{2m_e^*} + E_c + E_{en}$$

$$dE = \frac{\hbar}{m_e^*} k dk$$

$$N = 2\int_{-\infty}^{\infty} \frac{1}{(2\pi)^2} d^2\mathbf{k} = 2\int_{0}^{\infty} \frac{2\pi k}{(2\pi)^2} dk = \int_{0}^{\infty} \frac{k}{\pi} dk = \int_{E_c+E_{en}}^{\infty} \frac{m_e^*}{\pi\hbar^2} dE$$

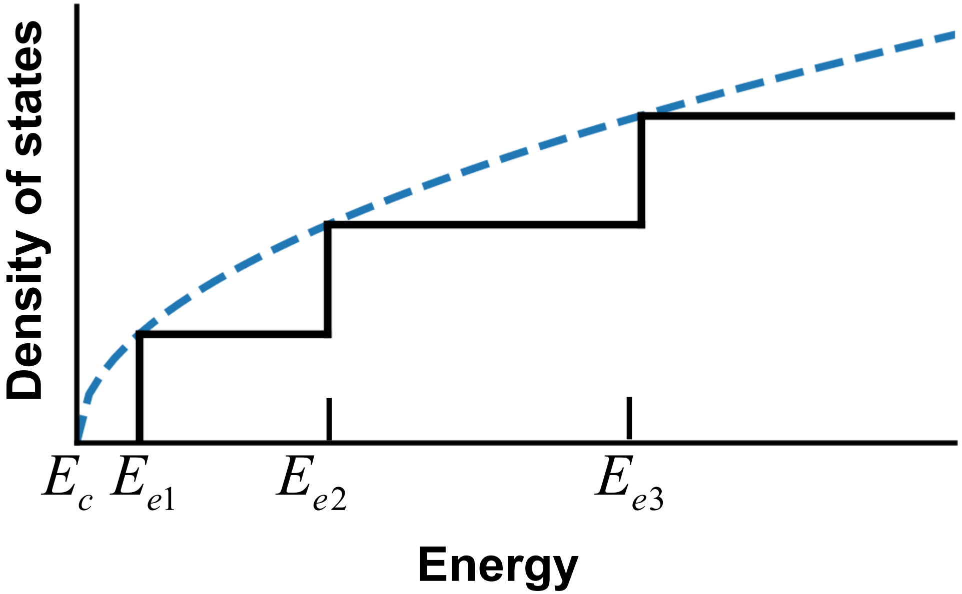
$$= \int_{0}^{\infty} \frac{m_e^*}{\pi\hbar^2} H(E - E_c - E_{en}) dE$$

$$\boxed{g(E) = \frac{m_e^*}{\pi\hbar^2} H(E - E_c - E_{en})}$$

$$H(x) = \begin{cases} 1 & x \geq 0 \\ 0 & x < 0 \end{cases}$$

(Heaviside step function)

Quantum well density of states



$$g(E) = \begin{cases} 0 & 0 < E - E_c < E_{e1} \\ \dfrac{m_e^*}{\pi\hbar^2} & E_{e1} < E - E_c < E_{e2} \\ 2\dfrac{m_e^*}{\pi\hbar^2} & E_{e2} < E - E_c < E_{e3} \\ 3\dfrac{m_e^*}{\pi\hbar^2} & E_{e3} < E - E_c < E_{e4} \end{cases}$$

(and so on…)

$$g_c(E) = \frac{m_e^*}{\pi\hbar^2}\sum_n H(E - E_c - E_{en})$$

2-d Electron/Hole Concentration

Electron and hole concentrations:

$$n = \int_{E_C}^{\infty} f_n(E)\rho_{e,2d}(E)\,dE$$

$$p = \int_{-\infty}^{E_V} f_p(E)\rho_{h,2d}(E)\,dE$$

At T = 0K, and for $E_1 < E < E_2$

$$n = \left(F_n - E_1\right)\cdot \rho_{e,2d}(E_1 < E < E_2)$$

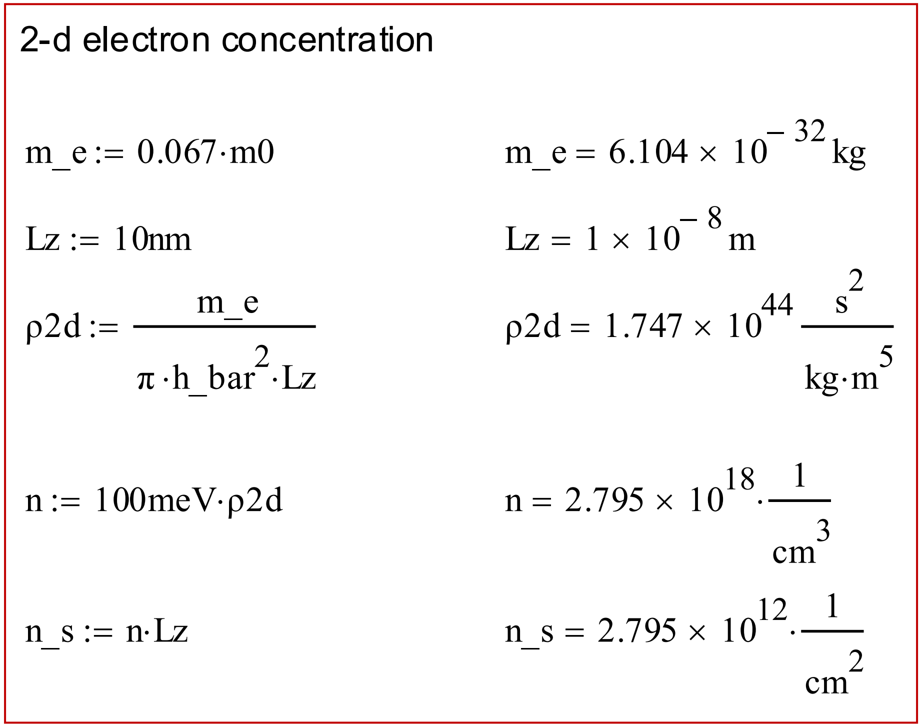
$$n = \left(F_n - E_1\right)\frac{m_e^*}{\pi\hbar^2 L_z}$$

Example:

10-nm-wide GaAs quantum well

quasi-Fermi energy is 100 meV

above E_1



2-d electron concentration

$\text{m\_e} := 0.067\cdot \text{m0}$ $\qquad$ $\text{m\_e} = 6.104\times 10^{-32}\,\text{kg}$

$\text{Lz} := 10\text{nm}$ $\qquad$ $\text{Lz} = 1\times 10^{-8}\,\text{m}$

$\rho\text{2d} := \dfrac{\text{m\_e}}{\pi\cdot \text{h\_bar}^2\cdot \text{Lz}}$ $\qquad$ $\rho\text{2d} = 1.747\times 10^{44}\,\dfrac{\text{s}^2}{\text{kg}\cdot\text{m}^5}$

$\text{n} := 100\text{meV}\cdot\rho\text{2d}$ $\qquad$ $\text{n} = 2.795\times 10^{18}\cdot\dfrac{1}{\text{cm}^3}$

$\text{n\_s} := \text{n}\cdot\text{Lz}$ $\qquad$ $\text{n\_s} = 2.795\times 10^{12}\cdot\dfrac{1}{\text{cm}^2}$

General Expression of Electron Concentration in Quantum Wells (or 2D Materials)

Electron concentration:

$$N = \int dE\, \rho_e^{2d}(E) f_C^n(E)$$

$$\rho_e^{2d}(E) = \frac{m_e^*}{\pi\hbar^2 L_z}\sum_{n=1}^{\infty} H(E-E_{en})$$

$$f_C^n(E) = \frac{1}{1+e^{\frac{E_{en}+E_t-F_C}{k_BT}}}$$

Use $\int \frac{dx}{1+e^x} = -\ln(1+e^{-x})$

$$N = \sum_n \frac{m_e^* k_BT}{\pi\hbar^2 L_z}\ln\left(1+e^{\frac{F_C-E_{en}}{k_BT}}\right)$$

For large quasi-Fermi Energy:

$F_C \gg E_{en}$

$$\ln\left(1+e^{\frac{F_C-E_{en}}{k_BT}}\right) \approx \frac{F_C-E_{en}}{k_BT}$$

$$N = \sum_n \frac{m_e^*}{\pi\hbar^2 L_z}(F_C-E_{en})$$

For small quasi-Fermi Energy:

$F_C \ll E_{en}$

$$\ln\left(1+e^{\frac{F_C-E_{en}}{k_BT}}\right) \approx e^{\frac{F_C-E_{en}}{k_BT}} = e^{-\frac{E_{en}-F_C}{k_BT}}$$

$$\boxed{N = \frac{m_e^* k_BT}{\pi\hbar^2 L_z} e^{-\frac{E_{e1}-F_C}{k_BT}} = N_C e^{-\frac{E_{e1}-F_C}{k_BT}}}$$