Applications of Schroedinger's Equation

$$E = E_K + E_p = E_K + V$$

E_K = Kinetic Energy

E_p = Potential Energy = V

- The Free Electron in One Dimension

Here, V = constant = 0

Time-Independent Equation:

$$-\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2} + V\psi(x) = E\psi(x)$$

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{2m}{\hbar^2}(E-V)\psi(x) = 0$$

Time-Independent Solution to this differential equation is:

$\psi(x) =$

Time-Dependent Equation:

$$\frac{\partial \phi(t)}{\partial t} = -j\frac{E}{\hbar}\phi(t)$$

Time-Dependent Solution is:

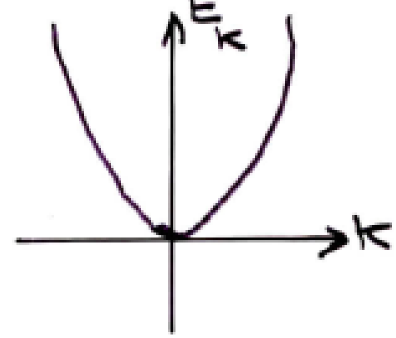
$$\phi(t) = \boxed{\phantom{e^{-j\frac{E}{\hbar}t}}}$$

Total Wavefunction solution is:

$$\Psi(x,t) = A e^{\frac{j}{\hbar}\left(\sqrt{2mE}\cdot x - Et\right)} + B e^{-\frac{j}{\hbar}\left(\sqrt{2mE}\cdot x + Et\right)}$$

Traveling Wave Solution

Define Wave Vector $k \equiv \frac{2\pi}{\lambda}$



parabolic

Recall $\lambda = \frac{h}{p}$

so $p = \frac{h}{2\pi} k = \hbar k$

$$E_k = \frac{1}{2} m v^2 = \frac{\hbar^2 k^2}{2m}$$

$$k = \sqrt{\frac{2mE_k}{\hbar^2}} = \sqrt{\frac{2m(E-V)}{\hbar^2}} = \frac{1}{\hbar}\sqrt{2m(E-V)}$$

and $\lambda = \frac{2\pi}{k} = \frac{2\pi}{\frac{1}{\hbar}\sqrt{2m(E-V)}} = \frac{h}{\sqrt{2m(E-V)}}$

Total Wave function $\Psi(x,t) =$

Total Wave function $\Psi(x,t) = Ae^{j(kx - \frac{E}{\hbar}t)} + Be^{-j(kx + \frac{E}{\hbar}t)}$

This has the form of two traveling in the $+x$ and the $-x$ directions.

Can define a $\omega = \frac{E}{\hbar}$ to produce the familiar $e^{j(kx-\omega t)}$ wave expression. Also $\omega =$

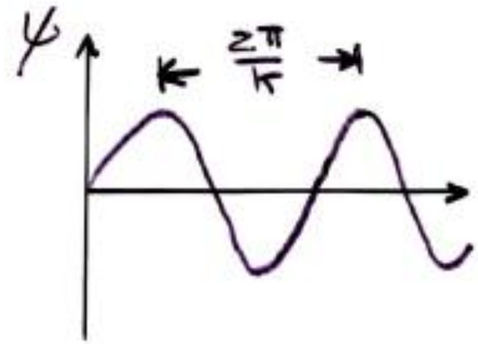
But, strictly speaking, the value of E depends on the choice of V, that is, the potential energy depends on a reference value.

Okay to use $\omega = \frac{\Delta E}{\hbar}$

(doesn't depend on reference)

Consider the first term,

$$Ae^{j(kx - \frac{E}{\hbar}t)}$$



For a point of constant phase of this +x traveling wave,

$$kx - \frac{E}{\hbar}t = \text{constant}$$

requires increasing x with increasing t.

Velocity of a point of constant phase of the wave

= <u>Phase</u> <u>Velocity</u>

$$v_p = \frac{x}{t} =$$

(Again, this depends on the potential energy reference)

Velocity of a point of constant phase of the wave

= Phase Velocity

$$v_p = \frac{x}{t} = \boxed{}$$

(Again, this depends on the potential energy reference)

Group Velocity = velocity of center of mass

$$v_g = \frac{dx}{dt} = \boxed{}$$

For $\psi(x,t) = A e^{j(kx - \frac{E}{\hbar}t)}$,

$$\langle p_x \rangle = \frac{\int \psi^* \frac{\hbar}{j} \frac{\partial}{\partial x} \psi \, dx}{\int \psi^* \psi \, dx} = \hbar k$$

as shown earlier (De Broglie)

Can in fact use this to derive De Broglie relation!

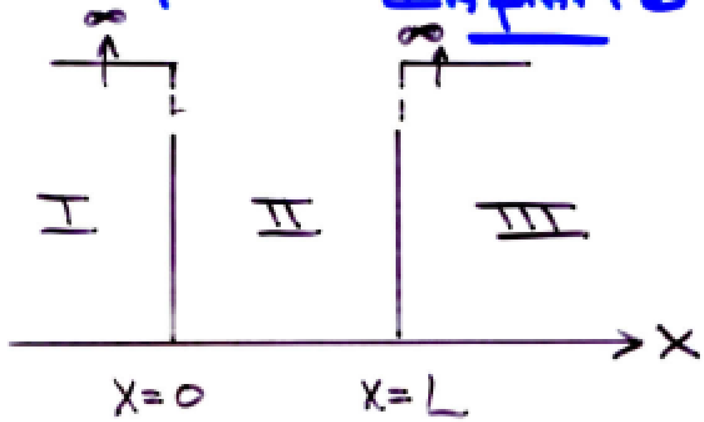
How To Solve Wave Equation Problems

1. Draw V diagram
2. Define Distinct V Regions
3. Write solution for Each Region
4. Determine Boundary Conditions on ψ
5. Solve for ψ: General Solution
6. Use Normalization to Specify ψ constants
7. Done - or - Use ψ to get requested parameter
   e.g., $\langle p(x) \rangle$, $\langle x \rangle$, E, ...

Example: Infinite Potential Well

1

2



Regions I and III: $V(x) = \infty$

Region II: $V(x) = 0$

$$\frac{\partial^2 \psi(x)}{\partial x^2} + \frac{2m}{\hbar^2}\left(E - V(x)\right)\psi(x) = 0$$

(Schroendinger equation in 1 dimension)

3a Since infinite barrier wall, no penetration into region I or III $\rightarrow \psi = 0$ in I and III

3b In region II, $\psi(x) = A \sin kx + B \cos kx$

$k = \sqrt{2mE}/\hbar$

4a $\psi(x)$ continuous boundary condition

so $\psi(x=0) = 0$

Therefore, $B=0$ and $\psi(x) = A \sin kx$

4b Boundary condition $\psi(x=L) = 0 = A \sin kx$

Therefore, $KL = n\pi$ where n = integer, positive (quantum number)

$K = \boxed{}$

5 $\psi(x) = A \sin\left(\frac{n\pi x}{L}\right)$

6 $\int_{-\infty}^{\infty} \psi^* \psi \, dx = 1 = \int_0^L A^2 \sin^2\left(\frac{n\pi x}{L}\right) dx$

$= \frac{L}{2} A^2 \longrightarrow A = \sqrt{\frac{2}{L}}$

Therefore, $\psi(x) = \boxed{}$

So Bound Particle in infinite well represented by standing wave.

Now go back to ③ : $K = \sqrt{2mE}/\hbar$

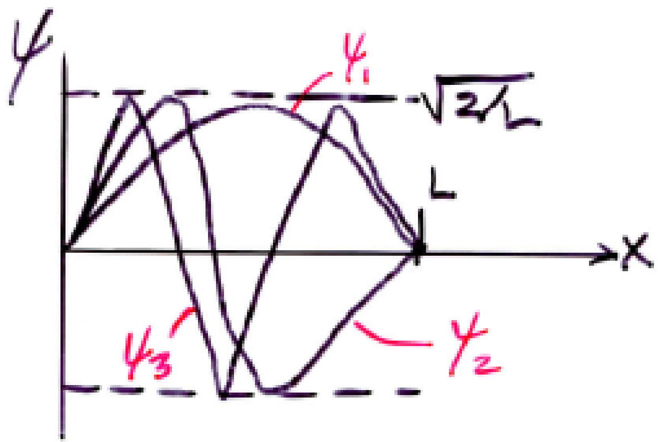
From ④, $K = \frac{n\pi}{L}$

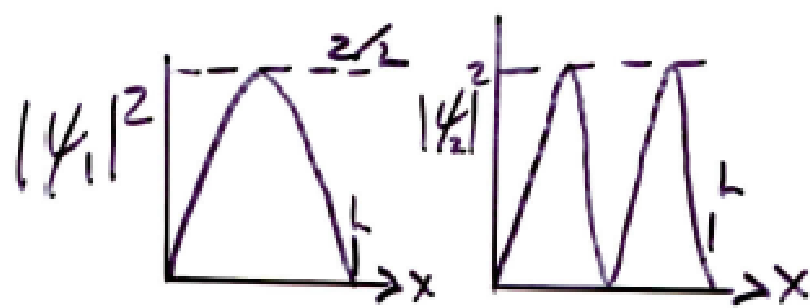
so $\frac{2mE}{\hbar^2} = \frac{n^2\pi^2}{L^2}$

$\frac{\pi^2\hbar^2}{2m_0} = 38\,\text{eV-Å}$

For each allowable n, particle energy is quantized

E_n = quantum state (energy)





etc.

These quantized levels appear in a variety of small geometry structures encountered in semiconductor devices. Also known as "particle-in-a-box".

$n=1$ $\quad \psi_1(x)=\sqrt{\frac{2}{L}}\sin\left(\frac{\pi x}{L}\right)$ $\quad E_1=$

$n=2$ $\quad \psi_2(x)=\sqrt{\frac{2}{L}}\sin\left(\frac{2\pi x}{L}\right)$ $\quad E_2=$

$n=3$ $\quad \psi_3(x)=\sqrt{\frac{2}{L}}\sin\left(\frac{3\pi x}{L}\right)$ $\quad E_3=$

$\vdots$

n $\quad \psi_n(x)=\sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right)$ $\quad E_n=$

For finite V, allowed n limited by $E_n < V$.

Contrary to classical world, where continuum of energies allowed.

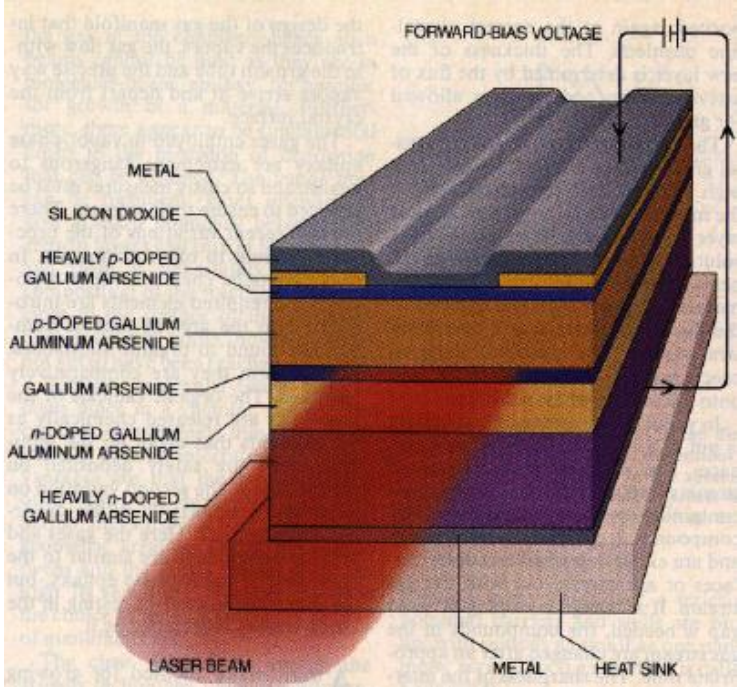
Example: Calculate first 3 levels of an electron in an infinite potential well. Well width = 5 Å

$$E_n = \frac{\hbar^2 n^2 \pi^2}{2mL^2} = \frac{n^2 (1.054\times10^{-34}\,J\text{-}s)^2 \pi^2}{2(9.11\times10^{-31}\,kg)(5\times10^{-10}\,m)^2}$$

$$= n^2 (2.407\times10^{-19})\,J$$

or $E_n = n^2 \frac{(2.407\times10^{-19})}{1.602\times10^{-19}} = n^2 (1.504)\,eV$

$n=1$: $E_1 = 1.504\,eV$; $n=2$: $E_2 = 6.018\,eV$, $n=3$: $E_3 = 13.54\,eV$



Laser Diode

Multi-Quantum Well Laser

25Å Quantum Well

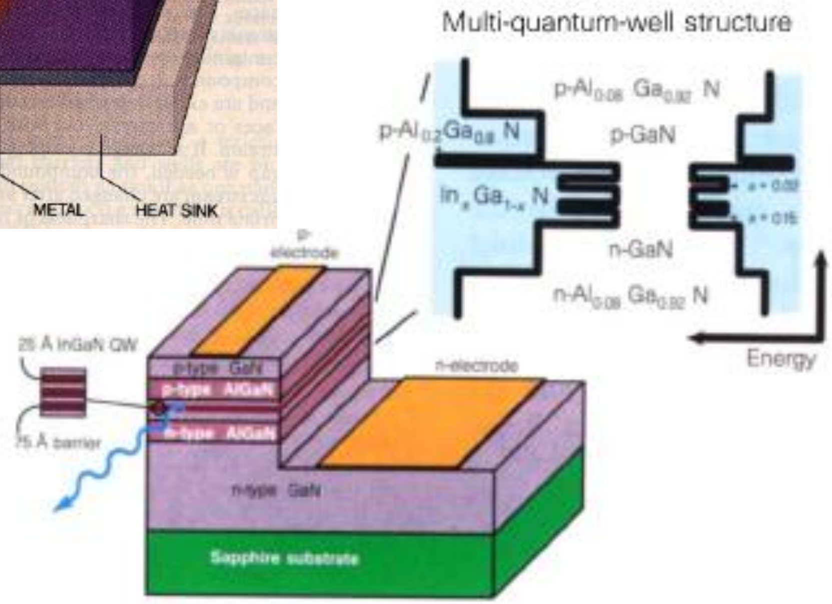
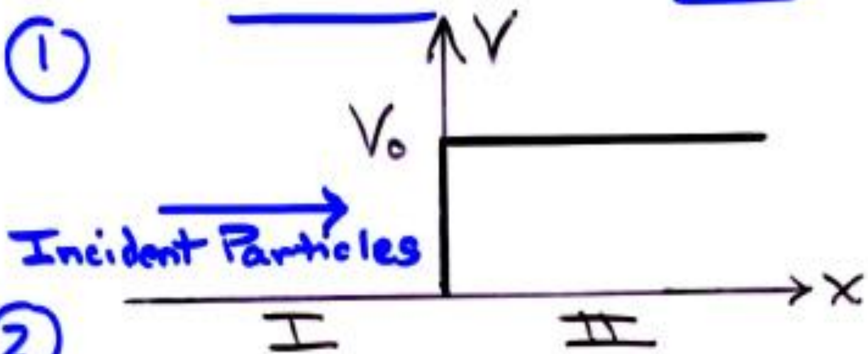


Figure 7 Diagram of the structure of InGaN multiple quantum well (MQW) diode laser[47]. Inset shows the energy band diagram associated with the MQW structure. Carrier confinement is achieved by the adjacent layers of wider bandgap GaN and the AlGaN cladding layers. In addition, the p-type $Al_{0.2}Ga_{0.8}N$ layer immediately above the MQW may play a critical role in carrier confinement.

Example: Step Potential

(1)



Assume $E < V_o$

(2)

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{2m}{\hbar^2}\left(E - V(x)\right)\psi(x) = 0$$

Time-independent Schroedinger equation

(3) General solution: $\psi_I(x) = A_1 e^{jk_1 x} + B_1 e^{-jk_1 x}$
for $x \leq 0$ (region I)

where $k_1 = \sqrt{\frac{2mE}{\hbar^2}}$

note: since not a standing wave, exponential form for ψ is easier

In region II, $V = V_0$ and $\frac{\partial^2 \psi_2(x)}{\partial x^2} + \frac{2m}{\hbar^2}(E - V_0)\,\psi_2(x) = 0$

$\psi_2(x) =$

Since E< V_0 and (E-V) → (-1)(V-E)

where $k_2 =$ for $x > 0$

④ • Since ψ must be finite at all x, $B_2 = 0$

Therefore, $\psi_2(x) = A_2 e^{-k_2 x}$

• At $x = 0$, $\psi_1(0) = \psi_2(0)$ so $A_1 + B_1 = A_2$

• Since 1st derivative at boundary continuous $\left.\frac{\partial \psi_1}{\partial x}\right|_{x=0} = \left.\frac{\partial \psi_2}{\partial x}\right|_{x=0}$