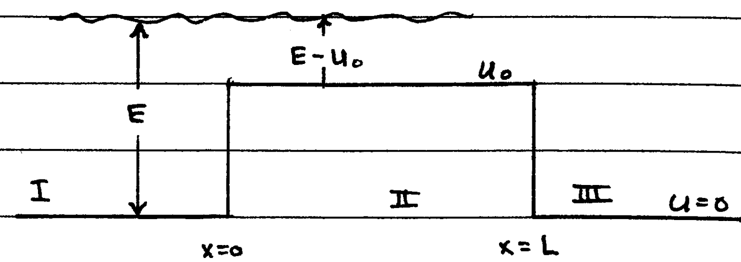
The Schrödinger Equation

Constant Potential Energy (a "free" particle)

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + U_0\psi = E\psi$$



$$\frac{d^2\psi}{dx^2} + (E-U_0)\frac{2m}{\hbar^2}\psi = 0$$

Looks like $\frac{d^2\psi}{dx^2} + k^2\psi = 0$ whose solution $\Rightarrow \psi(x) = A\sin kx + B\cos kx$

and $k = \sqrt{\frac{2m}{\hbar^2}(E-U_0)}$ in region II

In regions I and III $k = \sqrt{\frac{2mE}{\hbar^2}}$ because $U_0 = 0$

What happens when $E < U_0$?

Then, the Schrödinger Equation becomes:

Regions I & III $-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi \Rightarrow \frac{d^2\psi}{dx^2} + \underbrace{\frac{2mE}{\hbar^2}}_{k^2}\psi = 0$

$k^2 = \frac{2mE}{\hbar^2}$ $\qquad \psi_{I,III} \sim A\cos kx + B\sin kx$

$\qquad\qquad\qquad\qquad E\cos kx + F\sin kx$

Region II $-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + U_0\psi = E\psi \qquad \frac{d^2\psi}{dx^2} - (U_0-E)\frac{2m}{\hbar^2}\psi = 0$

$$\frac{d^2\psi}{dx^2} - K^2\psi = 0 \qquad K^2 = \frac{2m}{\hbar^2}(U_0-E) > 0$$

$$\psi_{II} \sim Ce^{-Kx} + De^{+Kx}$$

Free Particle Let $U_0 = 0$ $\qquad -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi \Rightarrow \frac{d^2\psi}{dx^2} + \overbrace{\frac{2mE}{\hbar^2}}^{k^2}\psi = 0$

$\frac{d^2\psi}{dx^2} + k^2\psi = 0 \qquad \psi = A\sin kx + B\cos kx = \frac{A}{2i}\left(e^{ikx} - e^{-ikx}\right) + \frac{B}{2}\left(e^{ikx} + e^{-ikx}\right)$

The Schrödinger Equation

Free Particle cont'd

$$\psi(x) = \left(\frac{A}{2i} + \frac{B}{2}\right) e^{ikx} + \left(\frac{B}{2} - \frac{A}{2i}\right) e^{-ikx} = A' e^{ikx} + B' e^{-ikx}$$

$$\psi(x,t) = \psi(x)\, e^{-i\omega t}$$ $\Rightarrow$ time-evolution of the wave function

$$\psi(x,t) = \underset{(L \to R)}{A' e^{i(kx-\omega t)}} + \underset{(R \to L)}{B' e^{-i(kx+\omega t)}}$$

Eigenfunction Equation

$$P_{op}\left(A' e^{i(kx-\omega t)}\right) = \frac{\hbar}{i}\frac{d}{dx}\left(A' e^{i(kx-\omega t)}\right) = \frac{\hbar}{i}(ik)\left(A' e^{i(kx-\omega t)}\right)$$

$$P_{op}\left(A' e^{i(kx-\omega t)}\right) = \underbrace{\hbar k}_{\substack{\text{momentum} \\ \text{eigenvalue}}}\left(A' e^{i(kx-\omega t)}\right)$$

$$A'\left(e^{i(kx-\omega t)}\right) \Rightarrow A' e^{\frac{i}{\hbar}(\hbar k x - \hbar\omega t)} = A' e^{\frac{i}{\hbar}(px - Et)}$$

The wave can be seen to have $\boxed{\text{momentum} \to p = \hbar k}$ and $\boxed{\text{energy} \to E = \hbar\omega}$

$$P(x) = \psi^*(x)\,\psi(x)$$

$$P(x,t) = \psi^*(x)\,\psi(x)\, e^{i\omega t} e^{-i\omega t} = \psi^*(x)\,\psi(x)\, e^{0} = \underbrace{\psi^*(x)\,\psi(x)}_{\text{probability/length}}$$

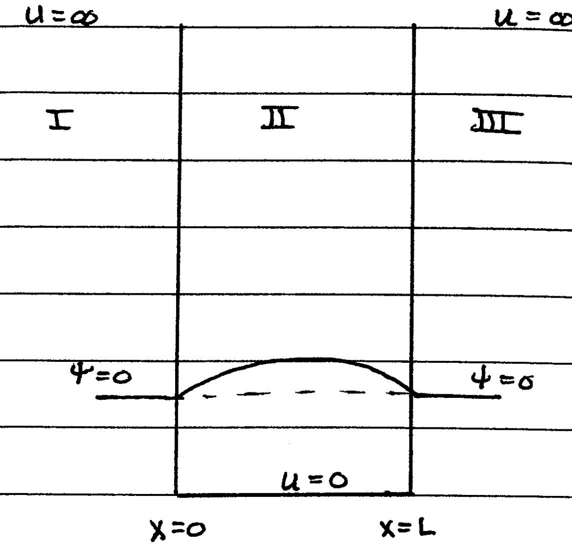
Probability density is a constant. (constant in time)

This is consistent with the Heissenberg Uncertainty Principle.

$k \to$ is precisely defined $\Delta k = 0 \Rightarrow \Delta p = \hbar \Delta k = 0 \quad \Delta x \to \infty$

The Schrödinger Equation

Infinite Potential Energy Well



Regions I & III
$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \infty\psi = E\psi$$

$\psi=0$ is the only solution.

Region II
$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + 0\psi = E\psi$$

$$\psi(x) = A\sin kx + B\cos kx$$

where $k^2 = \frac{2mE}{\hbar^2}$

Apply the Boundary Conditions:

@ $x=0$ $\quad \psi_I(0) = \psi_{II}(0) \Rightarrow 0 = A\sin(0) + B\cos(0) = B$

$\boxed{\text{So, } B=0}$

@ $x=L$ $\quad \psi_{II}(L) = \psi_{III}(L) \Rightarrow A\sin(kL) = 0$

This occurs when $k = \frac{n\pi}{L}$ So, $\boxed{\psi_{II}(x) = A\sin k_n x}$

How do you find A? Use the normalization requirement.

$$1 = \int_{-\infty}^{\infty}\psi^*(x)\psi(x)\,dx = \int_{-\infty}^{0}\underbrace{\psi_I^*(x)\psi_I(x)\,dx}_{=0} + A^2\underbrace{\int_0^L \sin^2\left(\frac{n\pi x}{L}\right)dx}_{L/2} + \int_L^{\infty}\underbrace{\psi_{III}^*(x)\psi_{III}(x)\,dx}_{=0}$$

$A^2 = \frac{2}{L}$ or $A = \sqrt{\frac{2}{L}}$ $\quad \boxed{\psi_{II}(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right)} = \psi_n(x)$

$$E_n = \frac{p_n^2}{2m} = \frac{(\hbar k_n)^2}{2m} = \frac{\left(\hbar\left(\frac{n\pi}{L}\right)\right)^2}{2m} \quad \boxed{E_n = \frac{n^2\pi^2\hbar^2}{2mL^2}} = n^2E_1$$

Schrödinger Equation

one dimensional infinitely deep potential well

Example 3.2 Electron trapped in a one-dimensional well of length $L = 0.10$ nm.

a.) Find E_1, E_2, E_3

$$E_n = \frac{n^2 \pi^2 \hbar^2}{2m L^2} \Rightarrow E_1 = \frac{\pi^2 (\hbar c)^2}{2 m_e c^2 L^2} = \frac{\pi^2 (197 \text{ eV} \cdot \text{nm})^2}{2(511{,}000 \text{ eV})(.01 \text{ nm}^2)}$$

$E_1 = 37.6$ eV

$E_2 = 150.4$ eV

$E_3 = 338.4$ eV

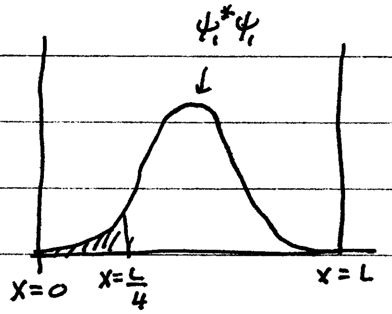
b.) How much energy is required to excite the electron from $n=1 \rightarrow n=3$

$$\boxed{\Delta E = E_3 - E_1 = 300.8 \text{ eV}}$$

c.) The electron drops down from $n=3 \rightarrow n=2$.

How much energy is released in the process.

$$E^* + E_2 = E_3 \qquad \boxed{E^* = E_3 - E_2 = 188.0 \text{ eV}}$$



Find the probability of locating a particle between $0 \le x \le L/4$ in an infinitely deep potential well. in the $n=1$ state.

$$\frac{2}{L}\int_0^{L/4} \sin^2\left(\frac{\pi x}{L}\right) dx = \frac{2}{L}\frac{1}{2}\int_0^{L/4}\left(1 - \cos\frac{2\pi x}{L}\right) dx$$

$$\text{Prob} = \frac{1}{L}\left[\int_0^{L/4} dx - \int_0^{L/4} \cos\frac{2\pi x}{L}\, dx\right] = \frac{1}{L}\left[\frac{L}{4} - \frac{L}{2\pi}\sin\frac{2\pi x}{L}\Big|_0^{L/4}\right]$$

$$\text{Prob} = \left[\frac{1}{4} - \frac{1}{2\pi}(1-0)\right] = \underline{0.0909}$$

$= 0.090845$ (Mathematica)

$0.25 - 0.1591$

Schrödinger Equation

$$\sigma = \sqrt{\overline{x^2} - \bar{x}^2} \qquad \bar{x} = \int_0^L x\, \psi^* \psi \, dx = \frac{2}{L}\int_0^L x \sin^2\!\left(\frac{\pi x}{L}\right) dx$$

$$\bar{x} = \frac{L}{2} \qquad \overline{x^2} = \int_0^L x^2 \psi^* \psi\, dx = \frac{2}{L}\int_0^L x^2 \sin^2\!\left(\frac{\pi x}{L}\right) dx$$

$$\overline{x^2} = \frac{1}{6}\left(2 - \frac{3}{\pi^2}\right) L^2$$

$$\sigma^2 = \overline{x^2} - \bar{x}^2 = \left(\frac{1}{3} - \frac{1}{2\pi^2}\right) L^2 - \frac{L^2}{4} = L^2\left[\frac{1}{12} - \frac{1}{2\pi^2}\right] = 0.03267\, L^2$$

$$\sigma = 0.18076\, L$$

Correspondence Principle $\quad n \to$ large

$\overline{x^2} \quad \langle x^2 \rangle = L^2\left(\frac{1}{3} - \frac{1}{2\pi^2 n^2}\right) \qquad \bar{x}^2 = \frac{L^2}{4} \qquad \sigma^2 = \overline{x^2} - \bar{x}^2 = L^2\left(\frac{1}{12} - \frac{1}{2\pi^2 n^2}\right)$

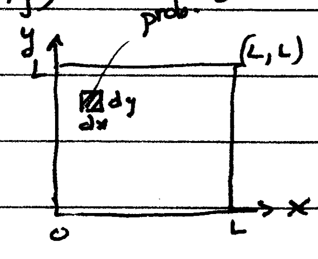
$\psi^*\psi$ is uniformly distributed between $0 \to L$ for large n.

Two Dimensional Infinite Potential Well. (Degeneracy)

Start with the Schrödinger Equation. $\to \psi(x,y)$

$$-\frac{\hbar^2}{2m}\left(\frac{d^2\psi}{dx^2} + \frac{d^2\psi}{dy^2}\right) + U(x,y)\,\psi(x,y) = E\,\psi(x,y)$$

prob. density = ??



$U(x,y) = 0 \qquad 0 \le x \le L \qquad 0 \le y \le L$

$U(x,y) = \infty \qquad$ otherwise

Assume the solutions are separable.