PHY 248 Lecture 16 Gary Shiu 3/5/07

$k = 8.98755 \times 10^9 \ Nm^2/c^2$

e^-

$V = -\frac{ke^2}{r}$ just like gravity

p

We'll solve this problem 4 in Phy 448 (Junior year)

Energy $E = \frac{p^2}{2m} + V(r)$

$$= \frac{p^2}{2m} - \frac{ke^2}{r}$$

Estimate the ground state energy using the uncertainty principle.

$$\overline{p^2} \sim (\Delta p)^2 \geq \frac{\hbar^2}{(\Delta x)^2} \sim \frac{\hbar^2}{r^2}$$

$$\Rightarrow \quad E = \frac{\hbar^2}{2mr^2} - \frac{ke^2}{r}$$

Minimize $E \Rightarrow \frac{dE}{dr} = 0 \Rightarrow -\frac{\hbar^2}{mr^3} + \frac{ke^2}{r^2} = 0$

$$\Rightarrow \boxed{r_m = \frac{\hbar^2}{ke^2m}}$$

$$\boxed{E_m = -\frac{k^2e^4m}{2\hbar^2} = -13.6\,eV}$$

Exactly the right answer $\Rightarrow$ dimensional analysis

Not the most convenient units for atomic physics ....

Define

$$\boxed{\alpha = \frac{ke^2}{\hbar c}} \simeq \frac{1}{137}$$

small
$\Rightarrow$ perturbation theory

$$\boxed{a_0 = r_{min} = \frac{\hbar}{mc}\frac{\hbar c}{ke^2} = \frac{\hbar}{mc}\frac{1}{\alpha}}$$

Bohr radius

$$\boxed{E_n = -\frac{mk^2e^4}{2\hbar^2 n^2} = -\frac{mc^2}{2}\alpha^2\frac{1}{n^2}}$$

Wave function (Ground state) of e^-

$$\psi = C\, e^{-Zr/a_0}$$

Although ψ = max at $r=0$, probability per unit r is

$$4\pi r^2 |\psi|^2 dr = P(r)\,dr$$

Can show that max of $P(r)$ is at $r = a_0/Z$

$$\frac{d}{dr}P(r) = 0 \Rightarrow r^2\left(-\frac{2Z}{a_0}\right) + 2r = 0$$

$$\Rightarrow r = a_0/Z$$

Keeping track of the factors of Z

$$E = \frac{p^2}{2m} + V(r) = \frac{p^2}{2m} - \frac{Zke^2}{r}$$

Uncertainty principle

$$\Rightarrow \quad E = \frac{\hbar^2}{2mr^2} - \frac{Zke^2}{r}$$

$$\frac{dE}{dr} = 0 \Rightarrow -\frac{\hbar^2}{mr^3} + \frac{Zke^2}{r^2} = 0$$

$$\Rightarrow \boxed{r_m = \frac{\hbar^2}{Zke^2m} = \frac{a_0}{Z}}$$

$$E_m = \frac{\hbar^2 Z^2}{2m a_0^2} - \frac{Zke^2 Z}{a_0}$$

$$= \frac{Z^2}{a_0^2}\left[\frac{\hbar^2}{2m} - ke^2 a_0\right]$$

$$\boxed{E_n = -\frac{mc^2}{2}\frac{Z^2\alpha^2}{n^2}}$$

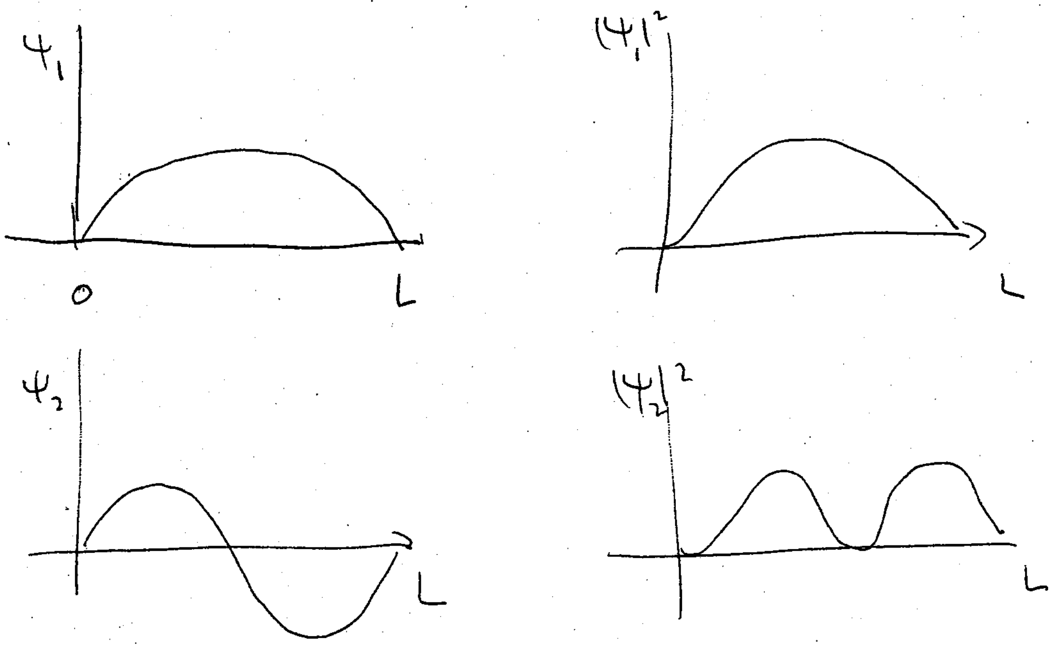
Transition from Quantum to Classical occur when n (quantum number) becomes large

For example

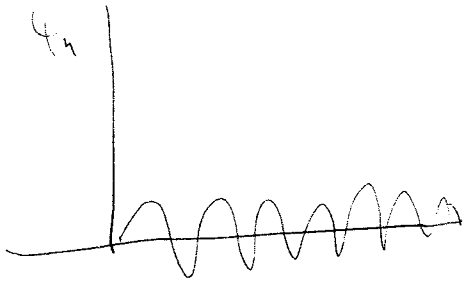
Infinite well

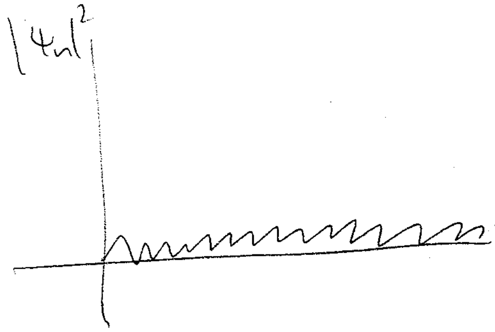
$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L} \qquad n = 1, 2, 3, \ldots$$

$$E_n = n^2 \frac{\pi^2 \hbar^2}{2mL^2}$$



As $n \to \infty$





$|\psi_n|^2 \simeq$ constant (couldn't tell the probability is changing)

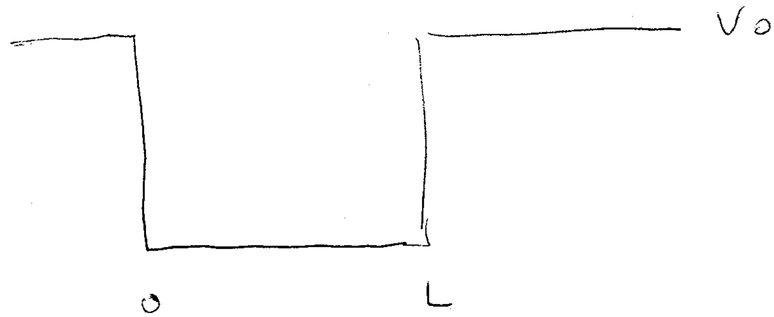
$$|\psi_n|^2 = \frac{2}{L} \sin^2 \frac{n\pi x}{L} \xrightarrow[\text{time average}]{} \frac{2}{L} \times \frac{1}{2} = \frac{1}{L}$$

Does it make sense?

$$P(x)dx \propto \frac{dx}{\underset{\approx \text{ constant}}{v}}$$

Properly normalized $\Rightarrow P(x) = \frac{1}{L}$

Finite Well



We argued that $\psi(0) = \psi(L) = 0$ because $V = \infty$ at $x = 0, L$

For V_0 = finite, the wavefunction are not vanishing at $x = 0, L$

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

For $0 < x < L$ $\quad V = 0 \Rightarrow \psi'' = \underbrace{-\frac{2mE}{\hbar^2}}_{\text{negative}}\psi(x)$

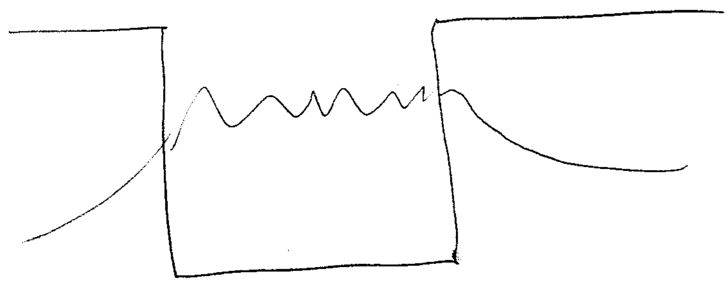
$$\Rightarrow \psi = A\sin kx + B\cos kx$$
or $A'e^{ikx} + B'e^{-ikx}$

For x outside the well

$$\psi'' = \underbrace{\frac{2m}{\hbar^2}(V_0 - E)}_{\text{positive}}\psi(x) \qquad \alpha^2 = \frac{2m}{\hbar^2}(V_0 - E)$$

$$\psi(x) = Ce^{\alpha x} + De^{-\alpha x}$$

Hence qualitatively



How could this be possible ?

Outside the well "kinetic energy" is -ve

Answer : Uncertainty principle

$$\psi(x) \sim e^{-\alpha x} \quad \Rightarrow \quad \Delta x \sim \frac{1}{\alpha}$$

$$\Rightarrow \quad \Delta p > \frac{\hbar}{\Delta x} \sim \hbar \alpha$$

Large uncertainty in kinetic energy

$$\frac{(\Delta p)^2}{2m} = \frac{\hbar^2 \alpha^2}{2m} = V_0 - E \quad \leftarrow$$

prevent us from measuring -ve kinetic energy