Last Time

Particle in Half Box:

\[ V(x) \]

Solved the Schrödinger Equation:

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

1. \( E < V \) classical orbits, bouncing back and forth

- QM; becomes standing waves with definite frequencies

Then we looked at the props on wave lenses
I. The number of bound states may terminate

ground

first

third

many
III. Classically allowed region $E > V$

As $k = E - V$ increases, the wavelength gets shorter.

\[-\frac{\hbar^2}{2m} \frac{d^2 \psi}{dx^2} = (E - V) \psi\]

\[\frac{d^2 \psi}{dx^2} = -\left[\frac{2m}{\hbar^2} (E - V)\right] \psi\]

\[\uparrow \text{concavity}\]

\[\downarrow \text{convergence}\]

- So if $\psi$ is positive and $E - V$ large $\gg 0$ expect a strong negative concavity.

- If $\psi$ is negative get a strong positive concavity.

- Together find oscillations with

\[\frac{\hbar^2 k^2}{2m} \sim E - V \text{ or } k = \left(\frac{2m(E - V)}{\hbar^2}\right)^{\frac{1}{2}}\]
IV. Classically Forbidden Region $E < V$

\[ \Delta x^2 \uparrow \quad \text{V-E} \]

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

Says is $\psi$ is positive

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

\[ \psi \sim e^{-\frac{r}{\lambda}} \quad k \sim \sqrt{\frac{2m(V-E)}{\hbar^2}} \]

Find exponential decay:

\[ D \sim \frac{1}{k} \sim \sqrt{\frac{\hbar^2}{2m(V-E)}} \]

\[ \frac{1}{D^2} \sim \frac{2m(V-E)}{\hbar^2} \]

So suppose you localize the wave in a region $D$, the uncertainty is

\[ \Delta p \sim \frac{\hbar}{D} \quad \Delta k \sim \frac{\Delta p^2}{2m} \sim \frac{k^2}{2mD^2} \sim (V-E) \]

So when you localize in the electron in
Example: Simple Harmonic Oscillator

Example: Vibrations of a diatomic molecule

\[ V(x) = \frac{1}{2} k x^2 \]

\[ F = -kx \]

Classically, the hydrogen vibrates at a frequency of

\[ \omega_0 = \sqrt{\frac{k}{m}} \]

\[ x(t) = A \cos (\omega_0 t) \]

Classical Picture

\[ \frac{1}{2} k x_{\text{max}}^2 = E \]

\[ x_{\text{max}} = \sqrt{\frac{2E}{k}} \]

Classical turning point

To Find the Allowed energies need to solve

\[ -\frac{\hbar^2}{2m} \frac{d^2 \psi_n(x)}{dx^2} + \frac{1}{2} k x^2 \psi_n(x) = E_n \psi_n(x) \]

See handout
Wave functions and Energy Levels

**Spring**

$\psi_0(x)$

$E_0 = \frac{1}{2} \hbar \omega_0$

$2\psi_0(x)$

$E_1 = \frac{3}{2} \hbar \omega_0$

$2\psi_1(x)$

$E_2 = \frac{5}{2} \hbar \omega_0$

$2\psi_2(x)$

$A\text{ Highly excited state:}$

$E_n = \left( n + \frac{1}{2} \right) \hbar \omega_0$

$2 = n$, one half wave length per state
Quantum Harmonic Oscillator: Wavefunctions

The Schrödinger equation for a harmonic oscillator may be solved to give the wavefunctions illustrated below.

\[ \Psi_{n}^{2} \]

For the simple harmonic oscillator (the spring) the potential is

\[ V = \frac{1}{2} kx^2 \]  \hspace{1cm} (1)

and the classical oscillation frequency is

\[ \omega_{o} = \sqrt{\frac{k}{m}} \quad \omega_{o} = 2\pi f \]  \hspace{1cm} (2)

We used the uncertainty principle to estimate that the particle at the bottom of the well oscillates over a length scale

\[ L = \left( \frac{\hbar}{mk} \right)^{1/4} \]  \hspace{1cm} (3)

The lowest energies are

\[ E_{n} = \left( \frac{1}{2} + n \right) \hbar \omega_{o} \quad n = 0, 1, 2, 3 \ldots \]  \hspace{1cm} (4)

The lowest wave functions are

\[ \Psi_{0} = \left( \frac{1}{\sqrt{\pi L}} \right)^{1/2} e^{-y^2/2} \]  \hspace{1cm} (5)

\[ \Psi_{1} = \left( \frac{1}{\sqrt{\pi L}} \right)^{1/2} \sqrt{2y} e^{-y^2/2} \]  \hspace{1cm} (6)

\[ \Psi_{2} = \left( \frac{1}{\sqrt{\pi L}} \right)^{1/2} \frac{1}{\sqrt{2}} (2y^2 - 1) e^{-y^2/2} \]  \hspace{1cm} (7)

where

\[ y = \frac{x}{L} \]  \hspace{1cm} (8)
Numerical Solution of Simple Harmonic Oscillator

\[
\left[ -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2} kx^2 \right] \psi = E \psi
\]

First change to dimension less variables \( \frac{x}{L} \)

Free to choose a system of units for: fundamentals
 mass, time, pos

Find

\[
\left[ -\frac{\hbar^2}{2mL^2} \frac{d^2}{dx^2} + \frac{1}{2} kL^2 \frac{x^2}{L^2} \right] \psi = E \psi
\]

Yesterday showed that if take

\( L = \left( \frac{\hbar}{mk} \right)^{\frac{1}{4}} \) then \( \frac{\hbar^2}{2mL^2} = \frac{1}{2} kL^2 = \frac{\hbar \omega_0}{2} \)

\( \hbar \omega_0 \left[ -\frac{1}{2} \frac{d^2}{dx^2} + \frac{1}{2} x^2 \right] \psi = E \psi \)

So want to solve

\[
\left[ -\frac{1}{2} \frac{d^2}{dx^2} + \frac{1}{2} x^2 \right] \psi = \frac{E}{\hbar \omega_0} \]

\( E = \hbar \omega_0 \psi(\bar{x}) \)
We can do this numerically

$$\psi'(x) = \frac{d\psi}{dx}$$

and

$$-\frac{1}{2} \frac{d^2\psi'}{dx^2} + \frac{1}{2} x^2 \psi = E \psi$$

Or

$$\frac{d^2\psi'}{dx^2} = -2(E - \frac{1}{2} x^2) \psi$$  \(\text{(*)}\)

So given \(\psi(x)\) and \(\psi'(x)\) we determine \(\psi(x+\Delta x), \psi'(x+\Delta x)\)

Or

$$\psi(x+\Delta x) \approx \psi(x) + \Delta x \psi'(x)$$

$$\psi'(x+\Delta x) \approx \psi'(x) + \Delta x \left( \frac{d\psi'}{dx} \right)$$

where \(d\psi'/dx\) is given by the Schrödinger Eq: \(\text{(*)}\)

**Program:**

1. Start at \(x = -x_{\text{max}}\)

   - Choose \(E/E_0 \approx 0.3\) say,
   - \(\psi(x_{\text{max}}) \approx \text{small} \approx 10^{-6}\)
   - \(\psi'(-x_{\text{max}}) \approx \text{small} \approx 10^{-6}\)

   \(\text{The function must be small at } x = -x_{\text{max}}\)
2) Find \( \psi(x+dx) \) and \( \psi'(x+dx) \)

\[
\psi(x+dx) = \psi(x) + dx \psi'(x)
\]

\[
\psi'(x+dx) = \psi'(x) + dx \frac{d\psi'}{dx}
\]

where

\[
\frac{d\psi'}{dx} = -2 \left( \frac{3}{2} - \frac{1}{2}x^2 \right) \psi(x)
\]

Repeat until we reach \( x = \pm \text{(a large number)} \)

3) Most choices of \( \frac{E}{\varepsilon_0} \), we will find \( \psi(x_{\text{max}}) \) is \( \pm \infty \)

For certain values of \( \frac{E}{\varepsilon_0} \) the wave

sce will approach 0 as \( x \rightarrow \infty \)

4) Change \( E/\varepsilon_0 \) and repeat until \( \psi(x_{\text{max}}) \) is small.