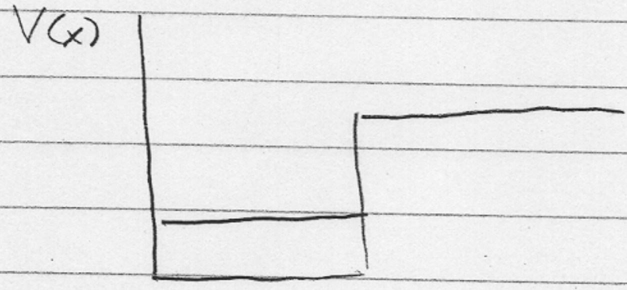
Last Time

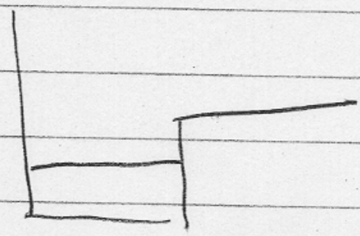
Particle in Half Box:



Solved the Schrödinger Equation:

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

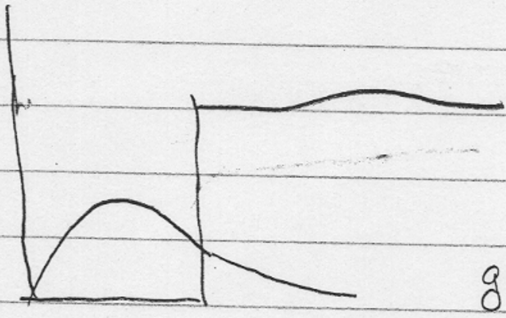
① $E<V$ classical orbits, bouncing back and forth



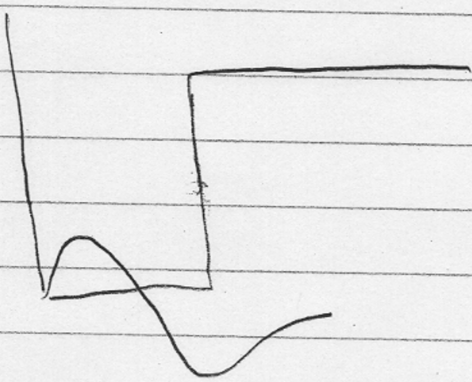
- QM; becomes standing waves with definite frequencies

Then we looked at the props of wave fcns

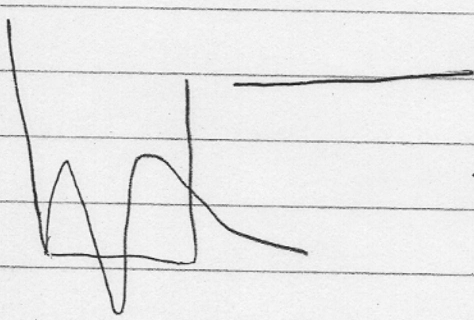
I.



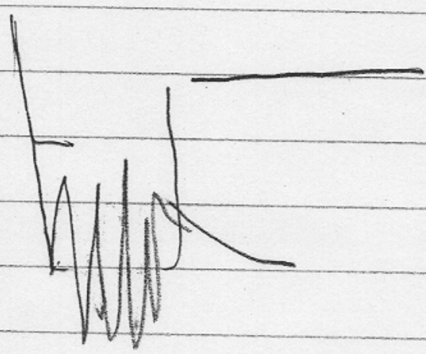
ground



first



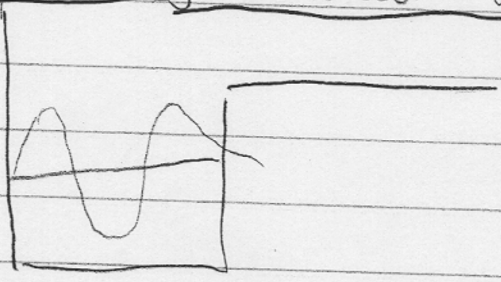
third



many

the number of bound states may terminate

III. Classically allowed region $E > V$

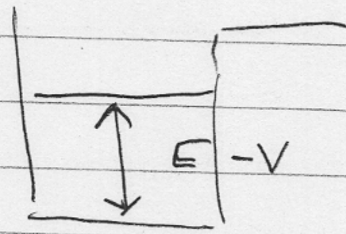


As $K = E - V$ increases the wavelength gets shorter

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx} = E - V\,\psi$$

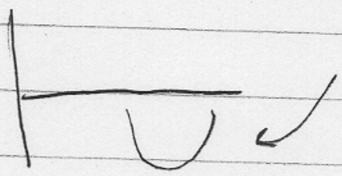
$$\frac{d^2\psi}{dx^2} = -\left[\frac{2m}{\hbar^2}(E-V)\right]\psi$$

concavity

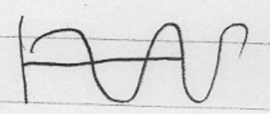


- So if ψ is positive and $E-V$ large >0 expect a strong negative concavity

- If ψ is negative get a strong positive concavity

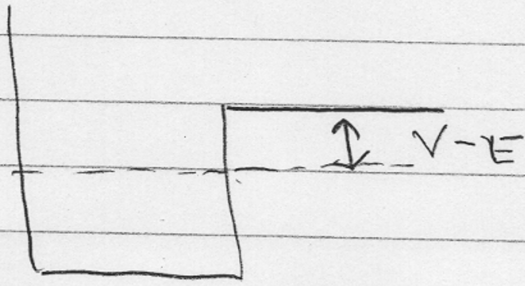


- Together find oscillations with



$$\frac{\hbar^2 k^2}{2m} \sim E - V \quad \text{or} \quad k = \left(\frac{2m(E-V)}{\hbar^2}\right)^{1/2}$$

IV. Classically Forbidden Region $E<V$



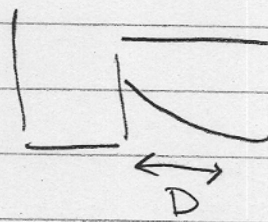
- Expon

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

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

Says is ψ is positive the concavity is also positive and vice-versa

Find exponential decay:



$$\psi \sim Ce^{-kx} \qquad k \sim \sqrt{\frac{2m}{\hbar^2}(V-E)}$$

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

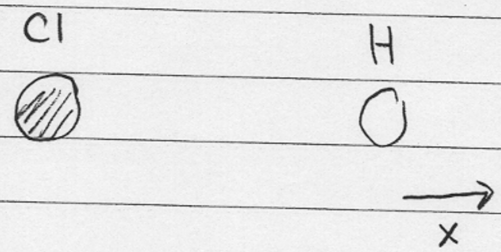
- So suppose you localize the wave in a region D, the uncertainty is

$$\Delta p \sim \frac{\hbar}{D} \qquad \Delta K \sim \frac{\Delta p^2}{2m} \sim \frac{\hbar^2}{2mD^2} \sim (V-E)$$

So when you localize in the electron in

Example: Simple Harmonic Oscillator

Example: Vibrations of a diatomic moleclue



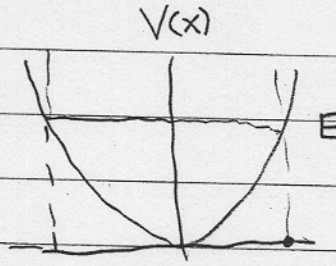
$$V(x) = \frac{1}{2} k x^2$$

$$F = -kx$$

Classically the hydrogen vibrates at a frequency of

$$\omega_0 = \sqrt{\frac{k}{m}} \qquad x(t) = A \cos(\omega_0 t)$$

Classical Picture



Classical turning point

$$\frac{1}{2} k x_{max}^2 = E$$

$$x_{max} = \sqrt{\frac{2E}{k}}$$

To Find the Allowed energies need to solve

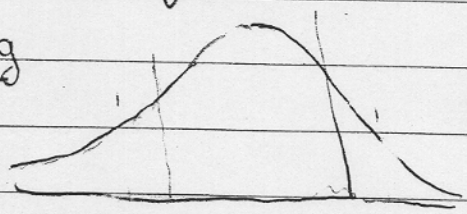
$$-\frac{\hbar^2}{2m} \frac{d^2 \psi_n(x)}{dx^2} + \frac{1}{2} k x^2 \psi_n(x) = E_n \psi_n(x)$$

See handout

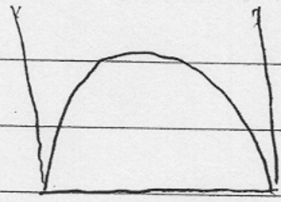
Wave functions and Energy Levels

$\psi_0(x)$ Box

Spring

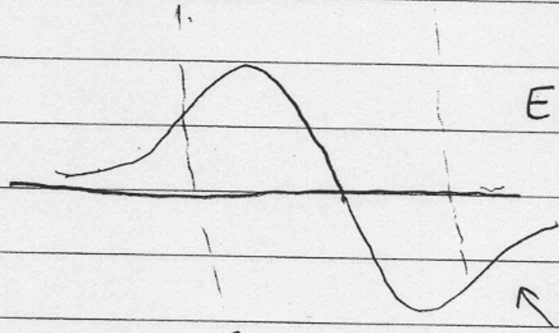


$E_0 = \frac{1}{2}\hbar\omega_0$

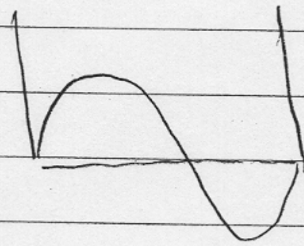


$\sqrt{\frac{2E_0}{k}}$

$\psi(x)$



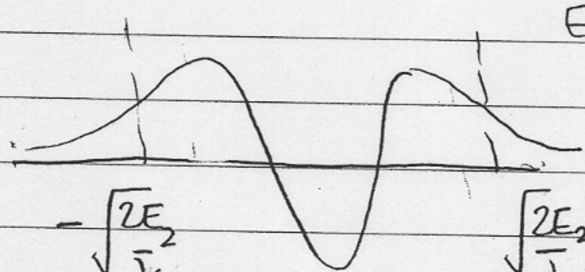
$E_1 = \frac{3}{2}\hbar\omega_0$

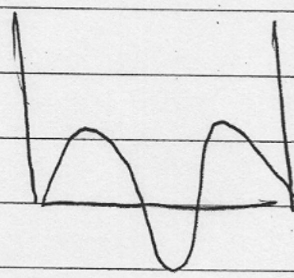


$\sqrt{\frac{2E_1}{k}}$

$\psi_3(x)$

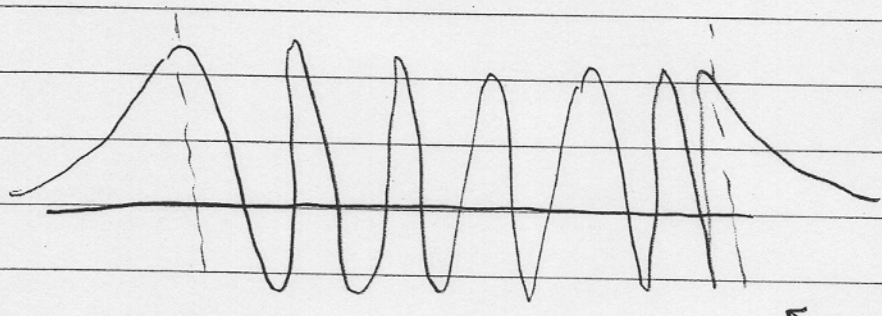
$E_2 = \frac{5}{2}\hbar\omega_0$

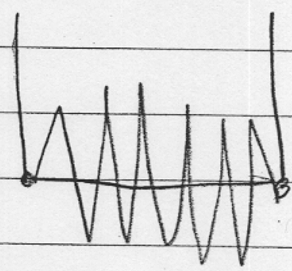




$-\sqrt{\frac{2E_2}{k}}$ $\sqrt{\frac{2E_2}{k}}$

A Highly excited state: Box

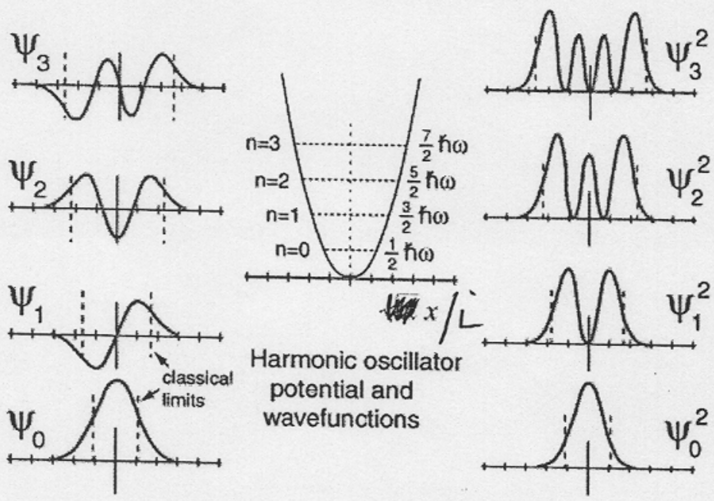




$E_n = \left(n + \frac{1}{2}\right)\hbar\omega_0$ $12 = n$, one half wave length per state

Quantum Harmonic Oscillator: Wavefunctions

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



Harmonic oscillator potential and wavefunctions

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

$$V = \frac{1}{2}kx^2 \tag{1}$$

and the classical oscillation frequency is

$$\omega_o = \sqrt{\frac{k}{m}} \qquad \omega_o = 2\pi f \tag{2}$$

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

$$L = \left(\frac{\hbar^2}{mk}\right)^{1/4} \tag{3}$$

The lowest energies are

$$E_n = \left(\frac{1}{2} + n\right)\hbar\omega_o \qquad n = 0, 1, 2, 3 \ldots \tag{4}$$

The lowest wave functions are

$$\Psi_0 = \left(\frac{1}{\sqrt{\pi}L}\right)^{1/2} e^{-y^2/2} \tag{5}$$

$$\Psi_1 = \left(\frac{1}{\sqrt{\pi}L}\right)^{1/2} \sqrt{2}ye^{-y^2/2} \tag{6}$$

$$\Psi_2 = \left(\frac{1}{\sqrt{\pi}L}\right)^{1/2} \frac{1}{\sqrt{2}}(2y^2 - 1)e^{-y^2/2} \tag{7}$$

where

$$y \equiv \frac{x}{L} \tag{8}$$

Numerical Solution of Simple Harmonic Oscillator

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

First Change to dimension less variables $\frac{x}{L} = \bar{x}$

Free to choose a system of units for fundaments

mass, time, pos

Find

$$\left[\frac{\hbar^2}{2mL^2} \frac{d^2}{d\bar{x}^2} + \frac{1}{2} k L^2 \bar{x}^2 \right] \psi = E \psi$$

Yesterday showed that if take

$L = \left(\frac{\hbar^2}{mk} \right)^{1/4}$, then $\frac{\hbar^2}{2mL^2} = \frac{1}{2} k L^2 = \frac{\hbar\omega_0}{2}$

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

So want to solve

$$\left[-\frac{1}{2} \frac{d^2}{d\bar{x}^2} + \underbrace{\frac{1}{2} \bar{x}^2}_{\equiv V(\bar{x})} \right] \psi = \bar{E} \psi \qquad \bar{E} \equiv \frac{E}{\hbar\omega_0}$$

We can do this numerically

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

and

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

Or

$$\frac{d\psi'}{dx} = -2\,(E - \underset{2}{V(x)})\,\psi \qquad (*)$$

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

Or

$$\psi(x+\Delta x) \simeq \psi(x) + \Delta x\,\psi'(x)$$

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

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

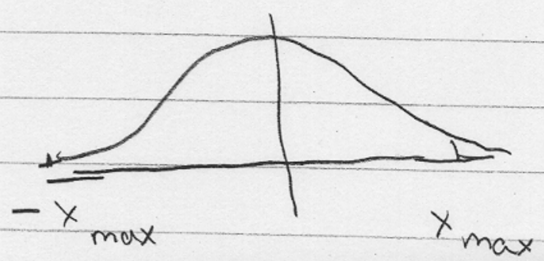
Program:

① Start at $x = -x_{max}$,

- Choose $E/\varepsilon_0 \simeq 0.3$ say.
- $\psi(-x_{max}) \simeq$ small $\simeq 10^{-6}$

and

$\psi'(-x_{max}) \simeq$ small $\sim 10^{-6}$



The function must be small at $x = -x_{max}$

(2) Find $\psi(x+dx)$ and $\psi'(x+dx)$

$$\psi(x+dx) = \psi(x) + \Delta x\, \psi'(x)$$

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

where

$$\frac{d\psi'}{dx} = -2\left(\varepsilon - \frac{1}{2}\bar{x}^2\right)\psi(x)$$

repeat, until we reach $x = \overbrace{+\text{(a large number)}}^{x_{max}}$

(3) ∘ Most choices of $\frac{E}{\varepsilon_0}$ we will find

$\psi(x_{max})$ is $\pm\infty$

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

fcn will apprach 0 as $x \to \infty$

(4) Change E/ε_0 and repeat until $\psi(x_{max})$ is small,