

# Verification of Uncertainty Principle

$(\Delta x)$  &  $(\Delta p)$

$\psi_n(x)$

$x_{\text{max}}$

$$\int_{x_{\text{min}}}^{x_{\text{max}}} |\psi_n(x)|^2 dx = I$$

Redefine

$$\frac{\psi_n(x)}{\sqrt{I}}$$

$\leftarrow$

$\psi_n(x)$

$\rightarrow$

Normalisation

$$(\Delta x)^2 = \langle x^2 \rangle - \langle x \rangle^2 = - \langle (x - \langle x \rangle)^2 \rangle$$

$$(\Delta p)^2 = \langle \hat{p}^2 \rangle - \langle \hat{p} \rangle^2 = \langle (\hat{p} - \langle \hat{p} \rangle)^2 \rangle$$

where  $\langle x^n \rangle = \int_0^L x^n |u(x)|^2 dx$  for infinite pot well

$$= \int_0^L x^n \rho(x) dx$$

$$\rho(x) = |u(x)|^2 \\ = (u(x))^2$$

→ Prob density

Also for a real wave fn

$$\langle \hat{p} \rangle = \int_{-\infty}^{\infty} u^* \left( -i\hbar \frac{d}{dx} \right) u dx$$

$$u^* = u$$

$$= -i\hbar \int_0^L u u' dx = -i\frac{\hbar}{2} \int_0^L \frac{d}{dx} (u^2) dx$$

$$= -i\frac{\hbar}{2} [u^2]_0^L = 0$$

## Uncertainty Relation

$$(\Delta X)(\Delta P) \geq \frac{\hbar}{2}$$

In dimensionless units

$$x \rightarrow \frac{\xi}{L},$$

$$\hat{p} \equiv -i\hbar \frac{d}{dx} \rightarrow -i\frac{\hbar}{L} \frac{d}{d\xi}$$

Define  $\zeta = \frac{L}{\hbar} \hat{p}$

$\frac{\hbar}{L}$  have dimensions  
of momentum

$$\therefore \hat{p} \rightarrow \zeta = -i \frac{d}{d\xi}$$

In program, use  $x$  &  $p$  in place of  $\xi$  &  $\zeta$   
respectively

Thus, in  $n$ th state

$$\langle x \rangle_n = \int_0^L x \psi_n^2(x) dx$$

$$\langle x^2 \rangle_n = \int_0^L x^2 \psi_n^2(x) dx$$

$$\langle \hat{p} \rangle_n = \int \psi_n(x) \left( -i \underbrace{\frac{d}{dx}}_{\text{dimensionless}} \right) \psi_n(x) dx = 0$$

$$\langle \hat{p} \rangle_n^2 = \int_0^L \psi_n \left( -\frac{d^2}{dx^2} \right) \psi_n dx$$

Approximate  $u''$  by

$$\left. \frac{d^2 u_n}{dx^2} \right|_{x=x_j} = \frac{u_n(x_{j+1}) - 2u_n(x_j) + u_n(x_{j-1}))}{h^2}$$

$$h = \frac{x_N - x_0}{N} = \frac{1-0}{N}$$

Use Simpson<sub>1/3</sub> to compute these integrals  
for the discrete data  $\{u_n(x)\}$  for each state

Define  $D_n = (\Delta x)_n (\Delta \hat{p})_n$

and print the table

$n$	$D_n$	$D_n(\text{analytical})$
1		
2		
...		
...		

$D_1$  will be minimum  
but  $D_1 > \frac{1}{2}$

Compare with analytical values

## Numerov Method

Special Problem -- Without the first order derivative term  $y'$  -- appear in various physical problems

Such problems can be solved by a better algorithm -- the Numerov Method

$$y'' + [k(x)]^2 y = F(x) \quad a \leq x \leq b$$

*(Note: An arrow points from the handwritten  $k^2(x)$  to the  $[k(x)]^2$  term in the equation.)*

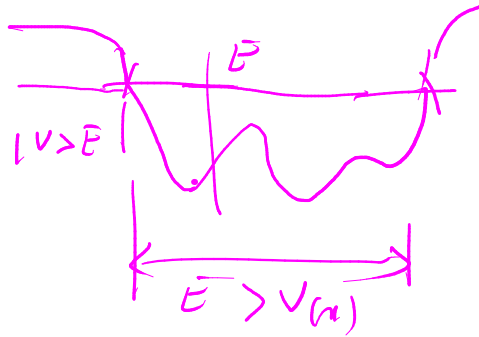
$$y(a) = \alpha, \quad y(b) = \beta$$

We can interpret  $F(x)$  as an inhomogenous driving force

$k(x)$  is a real function.

If it is positive the solutions  $y(x)$  will be oscillatory functions, and if negative they are exponentially growing or decaying functions.

Schrodinger Equation is this kind of equation - no first order derivative



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

$$F(x) = 0$$

$$\& \quad k^2(x) = \frac{2m}{\hbar^2} [E - V(x)]$$

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

Taylor's series

$$y(x+h) = y(x) + h y^{(1)}(x) + \frac{h^2}{2!} y^{(2)}(x) + \frac{h^3}{3!} y^{(3)}(x) \\ + \frac{h^4}{4!} y^{(4)}(x) + \frac{h^5}{5!} y^{(5)}(x) + \dots$$

$$y^{(n)}(x) \equiv \frac{d^n y}{dx^n}$$

$$y(x-h) = y(x) - h y^{(1)}(x) + \frac{h^2}{2} y^{(2)}(x) \\ - \frac{h^3}{3!} y^{(3)}(x) + \frac{h^4}{4!} y^{(4)}(x) - \frac{h^5}{5!} y^{(5)}(x) + \dots$$

$$y(x+h) - y(x-h) = 2y(x) + h^2 y^{(2)}(x) + \frac{h^4}{12} y^{(4)}(x) + O(h^6)$$



$$y^{(2)}(x) = \frac{y(x+h) + y(x-h) - 2y(x)}{h^2} - \frac{h^2}{12} y^{(4)}(x) + O(h^4)$$

$$y^{(2)} + \frac{h^2}{12} y^{(4)}(x) = \left(1 + \frac{h^2}{12} \frac{d^2}{dx^2}\right) y^{(2)}(x)$$

To eliminate the fourth-derivative term we apply the operator  $\left(1 + \frac{h^2}{12} \frac{d^2}{dx^2}\right)$

on the differential equation  $y'' + k^2(x) y = 0$

$$\underbrace{y^{(2)}(x) + \frac{h^2}{12} y^{(4)}(x)} + k^2(x) y(x) + \frac{h^2}{12} \frac{d^2}{dx^2} [k^2 y] = 0$$

$$\Rightarrow y(x+h) + y(x-h) - 2y(x) + h^2 k^2 y(x) + \frac{h^4}{12} \frac{d^2}{dx^2} (k^2 y) \approx 0$$

approximate the second derivative of  $k^2 y(x)$

$$\frac{d^2}{dx^2}(k^2 y) = \frac{1}{h^2} \left[ (k^2 y)|_{x+h} + (k^2 y)|_{x-h} - 2(k^2 y)|_x + \mathcal{O}(h^2) \right]$$

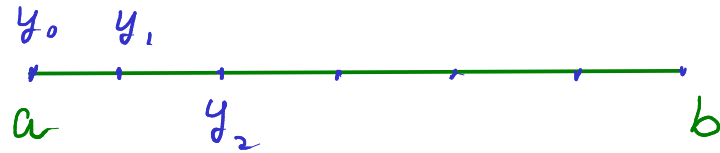
$$\frac{d^2}{dx^2}(k^2 y) \approx \frac{1}{h^2} \left[ \left\{ k^2(x+h) y(x+h) - k^2(x) y(x) \right\} \right. \\ \left. + \left\{ k^2(x-h) y(x-h) - k^2(x) y(x) \right\} \right]$$

Writing  $x = x_i$ ,  $x+h = x_{i+1}$ ,  $x-h = x_{i-1}$ ,

$y(x) = y_i$ ,  $y(x+h) = y_{i+1}$ ,  $y(x-h) = y_{i-1}$

$$y_{i+1} = \frac{1}{\left[ 1 + \frac{h^2}{12} k_{i+1}^2 \right]} \left[ 2 \left( 1 - \frac{5}{12} h^2 k_i^2 \right) y_i \right. \\ \left. - \left( 1 + \frac{1}{12} h^2 k_{i-1}^2 \right) y_{i-1} \right] + \mathcal{O}(h^6)$$

The Numerov method can be used to determine  $y_p$  for  $p = 2, 3, 4, \dots$ , given two initial values,  $y_0$  &  $y_1$ . We need two initial values because we are solving a second order differential equation.



$$\underline{f(x) \neq 0}$$

$$y_{i+1} = \frac{1}{\left[1 + \frac{h^2}{12} k_{i+1}^2\right]} \left[ 2\left(1 - \frac{5}{12} h^2 k_i^2\right) y_i - \left(1 + \frac{1}{12} h^2 k_{i-1}^2\right) y_{i-1} \right]$$

$$+ \frac{h^2}{12} \left( f_{i+1} + f_{i-1} - 2 f_i \right) + \mathcal{O}(h^6)$$

The error in one x-step is  $\mathcal{O}(h^6)$

However, the number of steps needed to integrate over a fixed range of x, from a to b is

$$\frac{b-a}{h} \propto \frac{1}{h}$$

One might expect that the errors at each step would be roughly comparable so so the total error in the Numerov method would be  $\mathcal{O}(h^5)$ .

Thus it is a 5-th order method, one higher than RK4.

Local Truncation Error  $\sim \mathcal{O}(h^6)$

Global Error  $\sim \mathcal{O}(h^5)$

We shall see that the Global error actually turns out to be  $\sim \mathcal{O}(h^4)$  same as RK

there can be problems with roundoff errors in using algorithm so make sure you use double precision arithmetic

## Solution of 1-d Time independent Schrodinger Equation

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

$$\Rightarrow \frac{d^2\psi(x)}{dx^2} + \frac{2m}{\hbar^2} [E - V(x)] \psi(x) = 0$$

of the form  $y'' + k^2(x)y = 0$  with  $k^2(x) = \frac{2m}{\hbar^2} [E - V(x)]$

Thus we can solve by Numerov method

write  $f(x) = k^2(x)$

Two additional Complexities

(i) Solution does not exist for all E. For Bound states, only certain discrete values of E give valid solution

Valid means -- satisfying the conditions of continuity of  $\psi$  and  $\psi'$  and wave function should approach zero at  $|x| \rightarrow \infty$

SO the numerical algorithm or code should be able to identify the valid values of E

(ii) In the classically forbidden regions the wavefunction should be exponentially decaying

# Simple Harmonic Oscillator Using Numerov Method

Sch eq'

$$u'' + k(x) u = 0$$

x is dimensionless

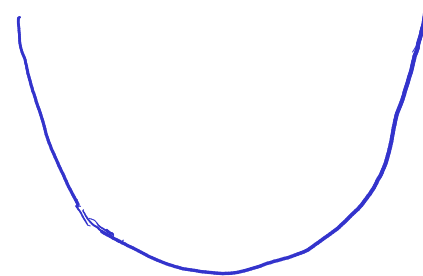
$$k^2(x) = E - V(x) = f(x)$$

$$f_i = f(x_i)$$

$$u_i = u(x_i)$$

$$x \equiv x_0, \dots, x_N$$

$\uparrow$   
 $x_{\min}$ 
 $\leftarrow$   $x_{\max}$



$$u_{i+1} = \frac{1}{\left[1 + \frac{(\Delta x)^2}{12} f_{i+1}\right]} \left[ 2 \left(1 - \frac{5}{12} (\Delta x)^2 f_i\right) u_i - \left(1 + \frac{1}{12} (\Delta x)^2 f_{i-1}\right) u_{i-1} \right] + \mathcal{O}(\Delta x^6)$$

Define

$$C(x) = 1 + \frac{(\Delta x)^2}{12} f(x)$$

$$C_i = C(x_i)$$

$$\left| \begin{array}{l} C_i = 1 + \frac{(\Delta x)^2}{12} f_i \\ f_i = \frac{12C_i - 12}{(\Delta x)^2} \end{array} \right.$$

$$-\frac{5}{12} = \frac{1-6}{12} = \frac{1}{12} - \frac{1}{2}$$

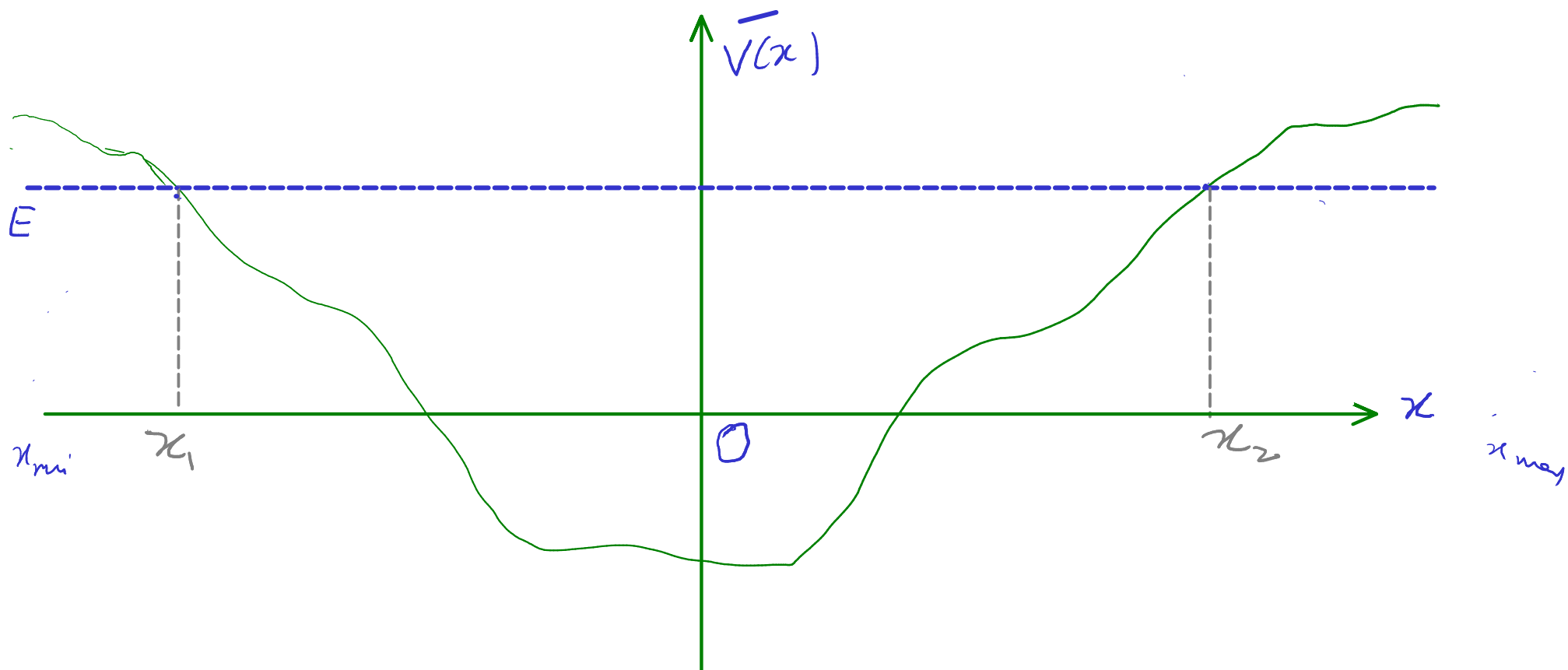
$$\begin{aligned} 2 \left( 1 - \frac{5}{12} (\Delta x)^2 f_i \right) &= 2 \left( 1 + \frac{(\Delta x)^2}{12} f_i \right) - (\Delta x)^2 f_i \\ &= 2 \left( 1 + \frac{(\Delta x)^2}{12} f_i \right) - (\Delta x)^2 \left( \frac{12 C_i - 12}{(\Delta x)^2} \right) \\ &= 2 C_i - 12 C_i + 12 \\ &= -10 C_i + 12 \end{aligned}$$

$$u_{i+1} = \frac{1}{C_{i+1}} \left[ (12 - 10 C_i) u_i - C_{i-1} u_{i-1} \right]$$

$$C_{i+1} = 1 + \frac{\Delta x^2}{12} f_{i+1}$$

$$C_{i-1} = 1 + \frac{1}{12} (\Delta x)^2 f_{i-1}$$





$\pm \infty$  ?

$[x_{\min}, x_{\max}]$

classically forbidden

$x < x_1$  &  $x > x_2$

$V(x) \rightarrow 0$  as  $x \rightarrow \pm \infty$

## Lab 5

### Harmonic Oscillator

$$-\frac{\hbar^2}{2m} \frac{d^2 u}{dx^2} + \frac{1}{2} m \omega^2 x^2 u = E u$$

classical turning pt  
for  $0^{\text{th}}$  state  $\rightarrow x_{cl} = \sqrt{\frac{\hbar}{m\omega}}$

Define

$$\xi = \sqrt{\frac{m\omega}{\hbar}} x \quad \& \quad \xi_{cl} = \sqrt{\frac{m\omega}{\hbar}} x_{cl} = 1$$

$$\frac{d}{dx} = \sqrt{\frac{m\omega}{\hbar}} \frac{d}{d\xi}, \quad \frac{d^2}{dx^2} = \frac{m\omega}{\hbar} \frac{d^2}{d\xi^2}$$

$$-\frac{\hbar^2}{2m} \cdot \frac{m\omega}{\hbar} \frac{d^2 u}{d\xi^2} + \frac{1}{2} m \omega^2 \left( \frac{\hbar}{m\omega} \right) \xi^2 = E u$$

$$-\frac{\hbar\omega}{2} \frac{d^2 u}{d\xi^2} + \frac{\hbar\omega}{2} \xi^2 = E u$$

$$u''(\xi) - \xi^2 u = -\frac{2E}{\hbar\omega} u$$

$$E = \frac{E}{\hbar\omega}$$

$$u''(\xi) + f(\xi) u(\xi) = 0$$

$$f(\xi) = (2E - \xi^2) = 2(E - V)$$

$$V = \frac{1}{2} \xi^2$$

For prog call  $\xi$  as  $x$  only &  $E$  as  $E$

$$\text{i.e. } u''(x) + f(x) u(x) = 0 \quad ; \quad f(x) = 2(E - V(x)); \quad V(x) = \frac{1}{2} x^2$$

Potential is even function of  $x$

Wave functions are of definite parity - so we determine the wavefunction for only  $x > 0$  and use parity property to find wavefunction for  $x < 0$

Discrete non-degenerate energy eigenvalues

Wavefunctions have a fixed number of nodes

$u_0$  - 0 nodes - even fn

$u_1$  - 1 node - odd fn

$u_n(x)$  has  $n-1$  number of nodes

The probability to find particle in classically forbidden region is expected to decrease exponentially

The classical turning points determine the classically allowed region:  $-x_{cl} < x < x_{cl}$

$x_{cl}$  depends upon energy of particle

$$\frac{1}{2} m \omega^2 x_{cl}^2 = E_n$$

The classical turning point for ground state  $n=0$  is

$$\frac{1}{2} m \omega^2 x_{cl}^2 = E_0 = \frac{1}{2} \hbar \omega$$
$$x_{cl} = \sqrt{\frac{\hbar}{m \omega}} \Rightarrow x_{cl} = 1 \quad \text{for } \text{gd state}$$

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

for  $n$ th state,  $\frac{1}{2} m \omega^2 x_{cl}^2 = E_n = \left( n + \frac{1}{2} \right) \hbar \omega$  or  $x_{cl}(n) = \sqrt{2n+1} \cdot \sqrt{\frac{\hbar}{m \omega}}$

Choose the range of integration  $[-x_{max}, x_{max}]$

s.t.  $x_{max} \gg x_{cl}(n_{max})$  if interested in finding eigenstates  
for  $n=0, 1, 2, \dots, n_{max}$

## Determination of Energy Eigen values

use shooting method with Bisection

Search for solutions  $\psi_n(x)$  for a given number of nodes  $n_{\text{nodes}} = n-1$

Start with a range  $[E_{\min}, E_{\max}]$

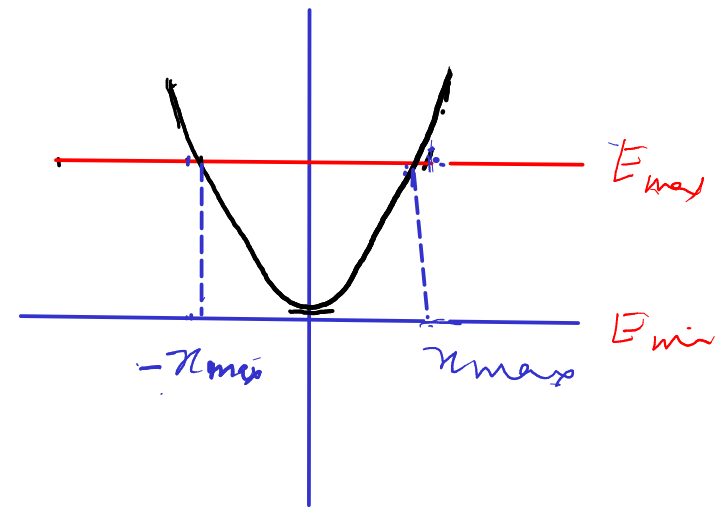
→ should include the actual energy  $E_{\text{actual}}$

For HO.

$$E_{\min} = 0$$

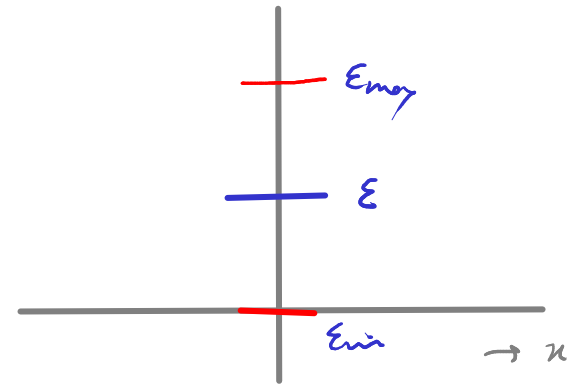
$$E_{\max} = \frac{1}{2} m \omega^2 x_{\max}^2$$

$$\Rightarrow E_{\min} = 0, \quad E_{\max} = \frac{1}{2} m \omega^2 x_{\max}^2$$



Start with guess value

$$\varepsilon = \frac{E_{\min} + E_{\max}}{2}$$



Use this  $\varepsilon$  and integrate from  $n=0$

towards right to find  $U_n(n)$

with  $n = n_{\text{nodes}} - 1$

While integrating count no of nodes, say  $n_c$

if  $n_c = n_{\text{nodes}} -$  we get the energy

In general  $n_c < n_{\text{nodes}}$

or  $n_c > n_{\text{nodes}}$

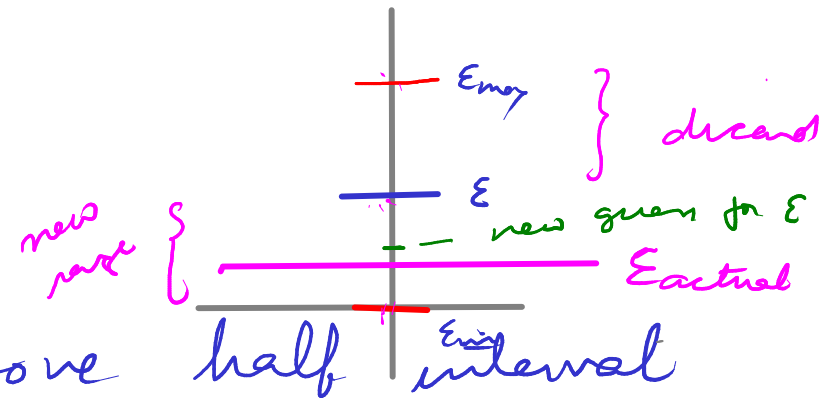
1) If  $n_c > n\_nodes$

$$\Rightarrow \varepsilon > E_{actual}$$

$\therefore$  discard the above half interval  
of energy

$\Rightarrow$  new range is  $[\varepsilon_{min}, \varepsilon]$

i.e. replace  $\varepsilon \leftarrow \varepsilon_{max}$

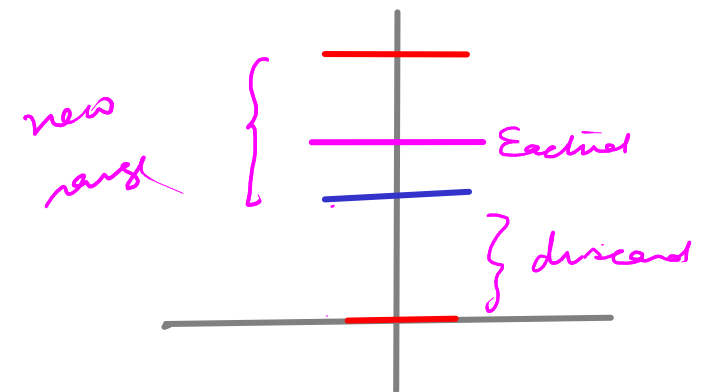


2) If  $n_c < n\_nodes$

$$\Rightarrow \varepsilon < E_{actual}$$

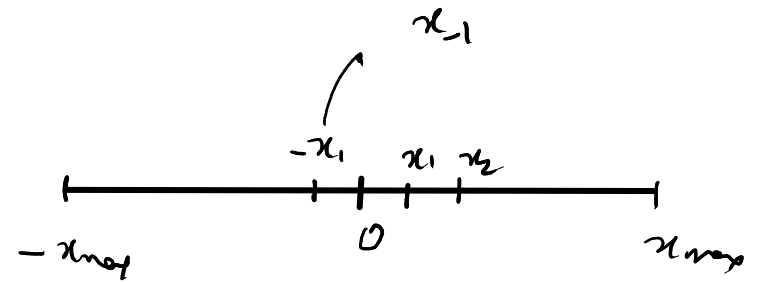
$$\varepsilon \leftarrow \varepsilon_{min}$$

new range  $[\varepsilon, \varepsilon_{max}]$



Thus energy range reduces

Again 
$$\varepsilon = \frac{E_{\min} + E_{\max}}{2}$$



determine  $u_n(x)$  by integration (call numerical fn)  
compare  $n_c$  with  $n\_nodes$

Repeat  $|E_{\max} - E_{\min}| < \text{tolerance}$   
 $\sim 10^{-8}$

$\Rightarrow$  the energy eigen value is  $\varepsilon$  for  $n\_nodes$  no  
of nodes and  $u_n(x)$  is corresponding  
wavefn. for  $x > 0$

use 
$$u_n(-x) = (-1)^n u_n(x)$$

$$u_{-i} = \begin{cases} u_i & n \text{ is even} \\ -u_i & n \text{ is odd} \end{cases}$$

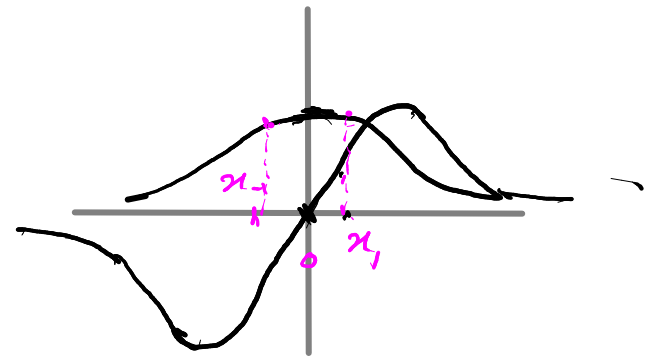
$$n = n\_nodes$$

$$u_{-i} = u(-x_i)$$

normalize  $u_n(x)$  and plot along with the analytical sol<sup>n</sup>



Initial Conditions  $u_0$  &  $u_1$   
use parity



If  $n$  is odd

$$\underline{u_{ni} = u_n(x_i)}$$

$$u'_0 = 1$$

$$u_1 = u_0 + \Delta x u'_0$$

$$u_{n0} = u_n(x=0) = \underline{0}$$

$$u_{n1} = -u_n(x = \Delta x) = \text{arbitrary finite value}$$

If  $n$  is even

$$u_{n0} = \text{arbitrary finite value}$$

and

$$u_{n1} = \frac{1}{c_1} \left[ (12 - 10c_0) u_0 - c_{-1} u_{-1} \right]$$

$$c_{-1} = c_1 \quad \& \quad u_{n-1} = u_{n1} \quad \text{as } u_n \text{ is even fn.}$$

$$\therefore u_{n1} = \left( \frac{6 - 5c_0}{c_1} \right) u_{n0}$$

# Input parameters

-  $x_{\max}$

- No of grid points  $N$

$$\Delta x = \frac{x_{\max}}{N}$$

-  $n$  for  $n$ th wave fn  $\Rightarrow$   $n_{\text{nodes}} = n$   $n=0, 1, 2, \dots$

- Total energy range  $E_{\min} = 0$   
 $E_{\max} = \frac{1}{2} x_{\max}^2$

- File name to store the wavefn

- Potential fn  $V_{\text{pot}}(x) \rightarrow$

$n=0 \rightarrow$   
 $n=1 \rightarrow$  }  $\rightarrow$  obtain  $E$  &  $u(x)$   
Plot  $u(x)$  along with actual wave fn

HW

might not lead to correct asymptotic  
behaviour

$$-\frac{\hbar^2}{2m} u'' + V(x)u = E u \Rightarrow u'' + \frac{2m}{\hbar^2} (E - V(x)) u = 0$$

$$u''(x) + f(x) u(x) = 0$$

$$f(x) = 2(E - V(x)) = 2\left(E - \frac{1}{2} x^2\right)$$

$$x \leftarrow \sqrt{\frac{m\omega}{\hbar}} x$$

$$e = \frac{E}{\hbar\omega}$$

$$v = \frac{1}{2} x^2$$

Numerove algorithm

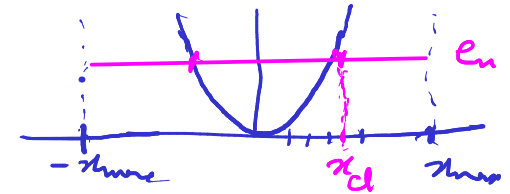
$$u_{i+1} = \frac{1}{C_{i+1}} \left[ (12 - 10 C_i) u_i - C_{i-1} u_{i-1} \right]$$

$$C_{i+1} = 1 + \frac{\Delta x^2}{12} f_{i+1}$$

$$C_{i-1} = 1 + \frac{1}{12} (\Delta x)^2 f_{i-1}$$

Algorithm we discussed till now:

$$E_n = n + \frac{1}{2}$$



For HO,  $x_0 = 0$

$$x_{max} \gg x_{cl}$$

$$tol = 0.5 \times 10^{-8}$$

Use Parity to find  $u(x)$  in  $[x_0 - x_{max}, x_0]$

$$u_n(x_0 - x) = (-1)^n u_n(x_0 + x)$$

center of potential  
Take default value to zero

1. Input  $x_0=0$ ,  $x_{max}$ ,  $N$ ,  $maxnodes$ ,  $n\_iter$ ,  $tol$   
 ↳ no of intervals  $\rightarrow$  highest wavefn to be determined  
 ↳ max no of iter  
 ↳ no of grid pts  $= N+1$   
 if this is 5 then first five wavefn  $u_0, u_1, \dots, u_5$  will be determined
2.  $dx = \frac{x_{max}}{N}$   
 $x_0, x_{max}, v_{pot}$  are floats  
 $N, n\_nodes \rightarrow$  integers

$$3. \quad dd x_{12} = \frac{dx * dx}{12}$$

$$\frac{(\Delta x)^2}{12}$$

4. Make the array of  $x$ -values s.t.  
 $x_i = x_0 + i * dx$   
 $i = 0, \dots, N$   
 size  $(N+1)$



5. Define  $v_{pot}$  array by calling potential fn  $V(x)$   
 $v_{pot}_i = v(x_i)$   
 ↳ must be even fn  $v_{pot}(x_0 - x) = v_{pot}(x_0 + x)$
6. Give name of the file where data will be stored

7.  $n\_nodes = 0$

→ 8. if  $n\_nodes > max\_nodes \rightarrow stop$

9.  $e_{max} = \max(v_{pot})$   
 $e_{min} = \min(v_{pot})$

} Trial energy range  $e_{max} = \frac{1}{2} \pi_{max}^2$   
 $e_{min} = 0$

10.  $e = \frac{e_{min} + e_{max}}{2}$

If you want your code to run for a single trial energy add an optional guess value here  
 → here  $n\_iter = 1$

iterations  
for shooting →

11. For  $k = 1, n\_iter$

a)  $icl = -1$

b) for  $i = 0$  to  $N$

c) Construct the  $f$ -array  
 $f_i = 2(e - v_{pot}i)$

(ii) if  $f_i = 0$ ,  $f_i = 1 \times 10^{-20}$

(iii) if  $f_i$  has sign opposite to  $f_{i-1}$ ,  $icl = i$  check sign of  $(f_i \neq f_{i-1})$   
 $n_{cl}$  is bet  $\underline{n_{i-1}}$  &  $\underline{n_i}$   
 approx  $n_{cl}$

c) if  $icl \geq N - 10 \rightarrow stop \rightarrow$  need to change  $\pi_{max}$

elseif  $icl < 1 \rightarrow stop \rightarrow$  No turning pt → something wrong

Set up the  $f$  required in Numerov

$f > 0 \rightarrow$  classically allowed regions

$f < 0 \rightarrow$  classically forbidden

$f_0$  should be +ve

d) Start with numerov

$$h\_nodes = \text{int}\left(\frac{n\_nodes}{2}\right)$$

$$C_i = 1 + dx^2 * f_i$$

we are integrating in half the region  
if  $n\_nodes$  is even there are

$2 * h\_nodes$  no of nodes

if  $n$  is odd there are  $2 * h\_nodes + 1$   
nodes (as one node is at  $n=0$ )

e) if  $2 * h\_nodes = n\_nodes \rightarrow$  even

$$u_0 = 1$$

$$u_1 = (6 - 5c_0) / C_1$$

else

$$u_0 = 0$$

$$u_1 = dx$$

endif

} Check for even & odd

if separate  
fn  
call Numerov

(f) Start integrating from 0 to  $n_{max}$  counting the no of  
times fn crosses zero

$$n_{cross} = 0$$

For  $i = 1, N-1$

$$u_{i+1} = -\left((12 - 10C_i)u_i - C_{i-1}u_{i-1}\right) / C_{i+1}$$

write a separate  
fn numerov

if  $u_{i+1} \in u_i$  have diff sign

check the sign of  $(u_i * u_{i+1})$

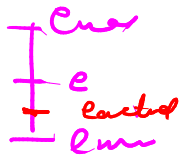
$$n_{cross} = n_{cross} + 1$$

end for loop

g) print  $k, e, n_{cross}, h_{nodes}$ .

h) if  $n_{iter} > 1$  then  $\rightarrow$  if  $n_{cross} = h_{nodes}$   
if  $(n_{cross} > h_{nodes})$  then  
 $e_{max} = e$

means  $e > e_{actual}$



else  
 $e_{min} = e$

means  $e < e_{actual}$



end if

New trial value

$$e = 0.5 * (e_{min} + e_{max})$$

if  $(e_{max} - e_{min}) < e_{tol}$  exit the  $k$ -loop

end if

$$k_{iter} = k$$

end  $k$ -for loop (go to ")

12 if  $k_{iter} = n_{iter}$   
print "Required tolerance could not be achieved in max no of iterations"

else  
print "Reqd tolerance achieved in " k\_iter "no of iterations"

### 13 Normalisation

$$\text{norm} = 0$$

a)  $p_i = u_i^2$  for  $i = 0$  to  $i_{cl}$   
 $p_i = 0$  otherwise

b)  $A = \text{integral}(p)$

c)  $u_i = \frac{u_i}{\sqrt{2A}}$  for each  $i$

d) compare with classical prob for  $p_{cl}$

14 Define wavefn from  $[-x_{max}; 0]$  using parity

15 Write  $x_i, u_i, p_i$  in a file

16) Plot  $u_i$  using pts & lines as continuous curve

17) Plot  $p_i$  and  $p_{cl}$

The wavefn obtained is not normalised

Calculate the prob density

$$p(x_i) = [u(x_i)]^2$$

$$\int_{-x_{max}}^{+x_{max}} p_i dx = 1$$

$$u(-x_i) = \pm u(x_i)$$

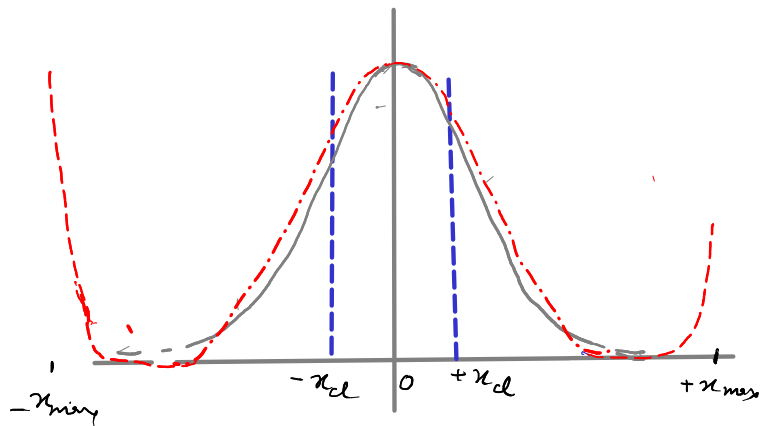
$$\int_0^{x_{cl}} p dx = 0.5$$

$$\text{If } \int_0^{x_{max}} p dx = A$$

$$u \leftarrow \frac{u}{\sqrt{2A}}$$

remember to use the dimensionless form





$$x_{max} = 10 \quad N = 100$$

For ground state  $e = \frac{1}{2}$

$$\frac{1}{2} x_d^2 = \frac{1}{2} \Rightarrow x_d = \pm 1$$

$x_i$        $u_i$        $P_i$        $P_d$        $V_i$



#### Assignment 4a

- Take a fixed value of  $e$  (say  $e = 1/2$  for ground state) and solve the Schrodinger equation with Numerov method

#### Assignment 4b

- Implement the above algorithm and get the eigenvalues and eigenfunctions for first five ( $n=0,1,2,3,4$ ) eigenstates
- Plot the wavefunctions and show that though the eigenvalues obtained are quite accurate the wavefunctions do not show the correct asymptotic behaviour.