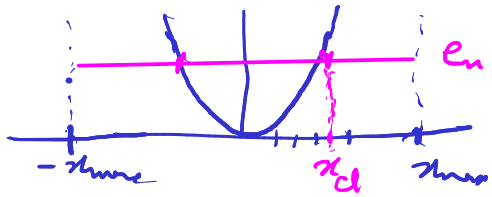
Algorithm we discussed till now:

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



$u_n(x)$ to be determined from x_0 to $x_0 + x_{max}$

For HO, $x_0 = 0$

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

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

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

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

1. Input $x_0 = 0$ (center of potential, take default value to zero), x_{max}, N (no of intervals, no of grid pts $= N+1$), max nodes (highest wavefn to be determined; if this is 5 then first six wavefns $u_0, u_1, \ldots, u_5$ will be determined), n_iter (max no of iter), tol

x_0, x_{max}, vpot are floats; N, n_nodes → integers

2. $dx = \frac{x_{max}}{N}$

3. $ddx12 = \frac{dx * dx}{12}$ $\quad \frac{(\Delta x)^2}{12}$

4. Make the array of x-values (size $N+1$) s.t

$x_i = x_0 + i * dx \qquad i = 0, \ldots, N$

5. Define vpot array by calling potential for $V(x)$

$vpot_i = V(x_i)$

→ must be even fn $vpot(x_0 - x) = vpot(x_0 + x)$

6. Give name of the file where data will be stored

7. n_nodes = 0

→ 8. if n_nodes > max nodes → stop

9. emax = max(vpot)
   emin = min(vpot)

} Trial energy range $e_{max} = \frac{1}{2} x_{max}^2$, emin = 0

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

iterations → for shooting

11. For k = 1, n_iter

a) icl = -1

b) for i = 0 to N

i) Construct the f-array
   $f_i = 2(vpot_i - e)$

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 $(f_i * f_{i-1})$
   x_{cl} is bet x_{i-1} & x_i
   approx x_{cl}

c) if icl ≥ N - 10 → stop → need to change x_{max}
   else if icl < 1 → stop → No turning pt → something wrong

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

Set up the f required in Numerov
f < 0 → classically allowed region
f > 0 → classically forbidden
f_0 should be +ve

d) Start with numerov

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

we are integrating in half the region

if n_nodes is even there are 2*hnodes no of nodes

if n is odd there are 2*hnodes + 1 nodes (as one node is at x=0)

$c_i = 1 + delx12 * f_i$

e) if 2*hnodes = n_nodes → even

$u_0 = 1$

$u_1 = (6 - 5c_0)/c_1$

else

$u_0 = 0$

$u_1 = dx$

end if

} Check for even & odd

(f) Start integrating from 0 to xmax counting the no of times for crosses zero

$ncross = 0$

For $i = 1, N-1$

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

it separate for all Numerov

write a separate fn numerov

if u_{i+1} & u_i have diff signs — 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 → if $n\_cross = h_{nodes}$

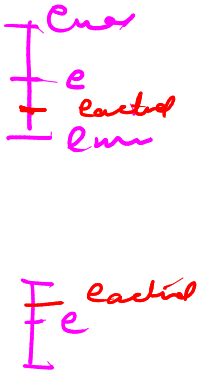
if $(n\_cross > h_{nodes})$ then — means $e > e_{actual}$

$e_{max} = e$

else — means $e < e_{actual}$

$e_{min} = e$

end if



New trial value

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

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

end if

$k\_iter = k$

end k-for Loop (go to 11)

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

norm = 0

a) $p_i = u_i^2$ for i = 0 to icl
$p_i = 0$ otherwise

b) A = integral (p)

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

d) compare with classical prob for
pcl

The wavefn obtained is not normalised

Calculate the prob density

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

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

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

$$\int_0^{xcl} p \, dx = 0.5$$

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

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

14 Defn wavefn from $[-x_{max} : 0]$ using parity

15 Write x_i, u_i, p_i in a file

16) Plot u_i using pts & u anal as continuous curve

↳ remember to use the dimensionless form

17) Plot p_i and p_{cl}