Numerov's Method

BVP: $$\frac{d^2y}{dx^2} = F(x) - k^2(x)y \qquad y(a)=\alpha \quad y(b)=\beta$$

$$y(x\pm h) = y(x) \pm hy' + \frac{h^2}{2!}y'' \pm \frac{h^3}{3!}y''' + \frac{h^4}{4!}y'''' + \cdots$$

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

$$\Rightarrow \quad y'' = \frac{y(x+h)+y(x-h)-2y(x)}{h^2} - \frac{h^2}{12}y''''$$

$$\Rightarrow \quad F(x) - k^2(x)y(x) = \frac{y(x+h)+y(x-h)-2y(x)}{h^2} - \frac{h^2}{12}\frac{d^2}{dx^2}\left[F(x)-k^2(x)y(x)\right]$$

Discretize:

$$\frac{y(n+1)+y(n-1)-2y(n)}{h^2} - \frac{h^2}{12}\cdot\frac{1}{h^2}\left[F(n+1)+F(n-1)-2F(n)\right]$$
$$+\frac{h^2}{12}\cdot\frac{1}{h^2}\left[k^2(n+1)y(n+1)+k^2(n-1)y(n-1)-2k(n)y(n)\right]$$
$$= F(n) - k^2(n)y(n)$$

$$y(n+1)\left[1+\frac{h^2}{12}k^2(n+1)\right] + y(n-1)\left[1+\frac{h^2}{12}k^2(n-1)\right]$$
$$-2y(n)\left[1+\frac{h^2}{12}k^2(n)-\frac{h^2}{2}k^2(n)\right]$$
$$-h^2F(n) - \frac{h^2}{12}\left[F(n+1)+F(n-1)-2F(n)\right] = 0$$

$$y(n+1)\left[1+\frac{h^2}{12}k^2(n+1)\right] = 2y(n)\left[1-\frac{5}{12}h^2k^2(n)\right]$$
$$-y(n-1)\left[1+\frac{h^2}{12}k^2(n-1)\right]$$
$$+h^2F(n) + \frac{h^2}{12}\left[F(n+1)+F(n-1)-2F(n)\right]$$

1-d Schrödinger Eqn:

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

- $\psi(x) \to 0$, $x \to \infty$ Bounded
- $\int_{-\infty}^{\infty} |\psi(x)|^2 dx = 1$ Normalized
- $\psi(x), \psi'(x) \to$ continuous

Set, $m=1$ $e^2=1$ $\hbar=1$ in Hartree units:

$$\frac{d^2\psi(x)}{dx^2} - 2\left[V(x) - E\right]\psi(x) = 0$$

$$\frac{d^2\psi(x)}{dx^2} + \underbrace{2\left[E - V(x)\right]}_{k^2(x)}\psi(x) = 0$$

Numerov's Method is applicable:

$$\left\{\begin{array}{l} x \Rightarrow n \\ y \Rightarrow \psi \\ F(n) = 0 \\ 2\left[E - V(n)\right] = k^2(n) \end{array}\right\}$$

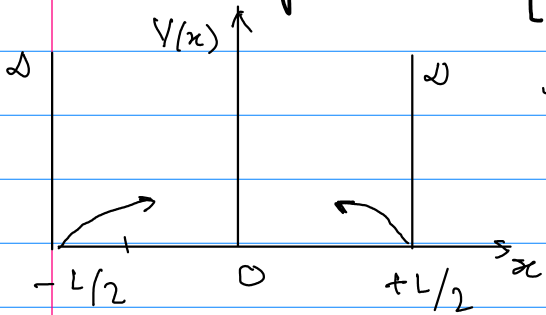
$$\psi(n+1)\left[1 + \frac{h^2}{12}k^2(n+1)\right] = \psi(n)\left[2 - \frac{5}{6}h^2k^2(n)\right] - \psi(n-1)\left[1 + \frac{h^2}{12}k^2(n-1)\right]$$

Let, $\phi(n) = 1 + \frac{h^2}{12}k^2(n)$

$$\phi(n) = 1 + 2\left[E - V(n)\right]h^2/12$$

$$\psi(n+1) = \frac{\psi(n)\left[12 - 10\phi(n)\right] - \psi(n-1)\phi(n-1)}{\phi(n+1)}$$

Numerically Estimate $[E_k, \psi_k]$ $\quad k=0$, ground state



Discretize space : $[-L/2 : L/2] \rightarrow [0, n]$

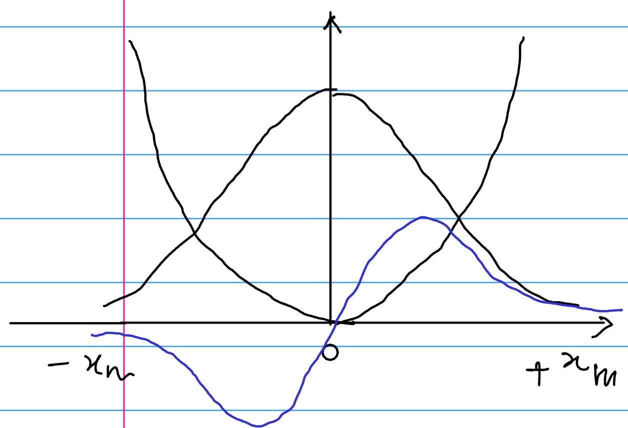
$$\Delta x \equiv h = L/n$$

$$\psi(0) = 0 \qquad \psi(1) = \epsilon$$

$$\psi(n) = 0 \qquad \psi(n-1) = \epsilon$$

Vary E to find $\{E_0, \psi_0\}$

- shoot & match $\psi(x = L/2) = \delta \approx 0$
- •• shoot & match $\left|\psi_L(x=0) - \psi_R(x=0)\right| = \delta \approx 0$



$$x \in [-\infty, \infty] \longrightarrow x \in [-x_m, x_m]$$

Compare logarithmic derivatives $\gamma = \dfrac{\psi'}{\psi}$

$$|\gamma_L - \gamma_R| = \delta \approx 0$$

For odd parity match $1/\gamma$

Check for nodes