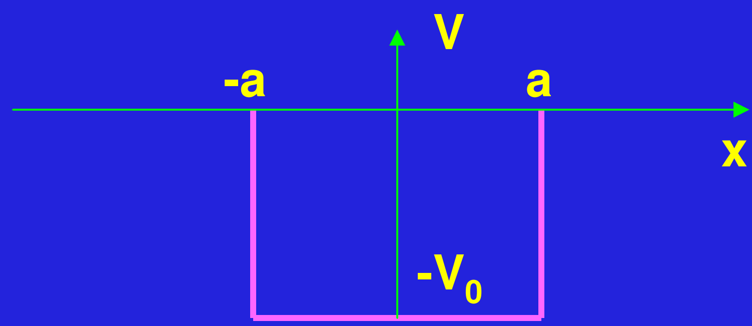
Lecture 17 Review

Tree hugging (fractally speaking).

Root finding: Newton-Raphson & bisection algorithms.

Application of root finding to particle in a quantum box

Particle in a Quantum Box



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

$$\mathcal{P} = |\psi(x)|^2 dx$$

$$\int_{-\infty}^{\infty} dx\, |\psi(x)|^2 = 1$$

$$V(x) = \begin{cases} -V_0 = -83\,\mathrm{MeV}, & \text{for } |x| \leq a = 2\,\mathrm{fm} \\ 0, & \text{for } |x| > a = 2\,\mathrm{fm} \end{cases}$$

$$\frac{d^2\psi(x)}{dx^2} + \frac{2m}{\hbar^2}(E + V_0)\psi(x) = 0$$ for $|x| \leq a$

$$\frac{d^2\psi(x)}{dx^2} + \frac{2m}{\hbar^2}E\psi(x) = 0$$ for $|x| > a$

$$\frac{2m}{\hbar^2} = \frac{2mc^2}{(\hbar c)^2} = \frac{2\times 940\ \mathrm{MeV}}{(197\ \mathrm{Mev-fm})^2} = 0.483\,\mathrm{MeV}^{-1}\mathrm{fm}^{-2}$$

Particle in a Quantum Box

$$\psi(x) = \begin{cases} Ce^{\beta x}, & \text{for } -\infty < x < -a \\ B\cos\alpha x, & \text{for } -a < x < a \\ Ce^{-\beta x}, & \text{for } a < x < +\infty \end{cases}$$

$$\alpha = \sqrt{\frac{2m(E+V_0)}{\hbar^2}} = \sqrt{0.483(E+83)}$$

$$\beta = \sqrt{\frac{-2mE}{\hbar^2}} = \sqrt{-0.483E}$$

$$B\cos\alpha a = Ce^{-\beta a}$$ ψ continuity

$$-\alpha B\sin\alpha a = -\beta Ce^{-\beta a}$$ ψ' continuity

$$\Rightarrow \quad \alpha a\tan\alpha a - \beta a = 0$$

$$\sqrt{2m(E+V_0)}\tan\sqrt{\frac{2m(E+V_0)}{\hbar^2}}\,a - \sqrt{-2mE} = 0$$

$$\xi\tan\xi - \eta = 0$$ with $\xi = \alpha a$ $\quad \eta = \beta a$

$$\xi^2 + \eta^2 = \frac{2mV_0a^2}{\hbar^2} = 16.08$$

$$f(\xi) = \xi\tan\xi - \eta = 0 \quad \longleftarrow$$

Numerov Algorithm for ODE Solution

NUMEROV TECHNIQUE

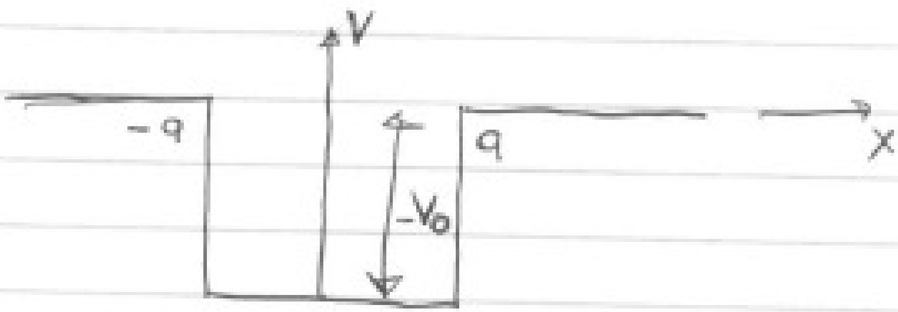
$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x)$$

$$\frac{d^2\psi(x)}{dx^2} + k^2(x)\psi = 0$$

$$k^2(x) \equiv (2m/\hbar^2)\begin{cases} E - V_0 & |x| < a \\ E & |x| > a \end{cases}$$

RECALL THAT $E < 0$ FOR BOUND STATES

$$(2m/\hbar^2) = 0.4829\ \mathrm{MeV}^{-1}\mathrm{fm}^{-2}$$



$$\psi(x+h) = \psi(x) + h\psi' + \frac{h^2}{2}\psi'' + \frac{h^3}{3!}\psi''' + \frac{h^4}{4!}\psi^{iv}$$

$$\psi(x-h) = \psi(x) - h\psi' + \frac{h^2}{2}\psi'' - \frac{h^3}{3!}\psi''' + \frac{h^4}{4!}\psi^{iv} + \dots$$

$$\Rightarrow \psi(x+h) + \psi(x-h) \simeq 2\psi(x) + h^2\psi'' + \frac{h^4}{12}\psi^{iv} + \mathcal{O}(h^6)$$

$$\psi''(x) \simeq \frac{\psi(x+h) + \psi(x-h) - 2\psi(x)}{h^2} - \frac{h^2}{12}\psi^{iv}(x) + \mathcal{O}(h^6)$$

TRICK: APPLY $1 + \frac{h^2}{12}\frac{d^2}{dx^2}$ TO TISE

$$\left(1 + \frac{h^2}{12}\frac{d^2}{dx^2}\right)\left(\frac{d^2\psi}{dx^2} + k^2(x)\psi\right) = 0$$

courage…

$$\psi''(x) + \frac{h^2}{12}\psi^{IV}(x) + k^2\psi + \frac{h^2}{12}\frac{d^2}{dx^2}\left[k^2(x)\psi\right] = 0$$

SUB FOR $\psi''(x) \simeq \dfrac{\psi(x+h) + \psi(x-h) - 2\psi}{h^2} - \dfrac{h^2}{12}\psi^{IV}$

SO,

$$\frac{\psi(x+h) + \psi(x-h) - 2\psi(x)}{h^2}$$

$$- \frac{h^2}{12}\psi^{IV} + \frac{h^2}{12}\psi^{IV} + k^2(x)\psi$$

$$+ \frac{h^2}{12}\frac{d^2}{dx^2}\left[k^2(x)\psi(x)\right] \simeq 0$$

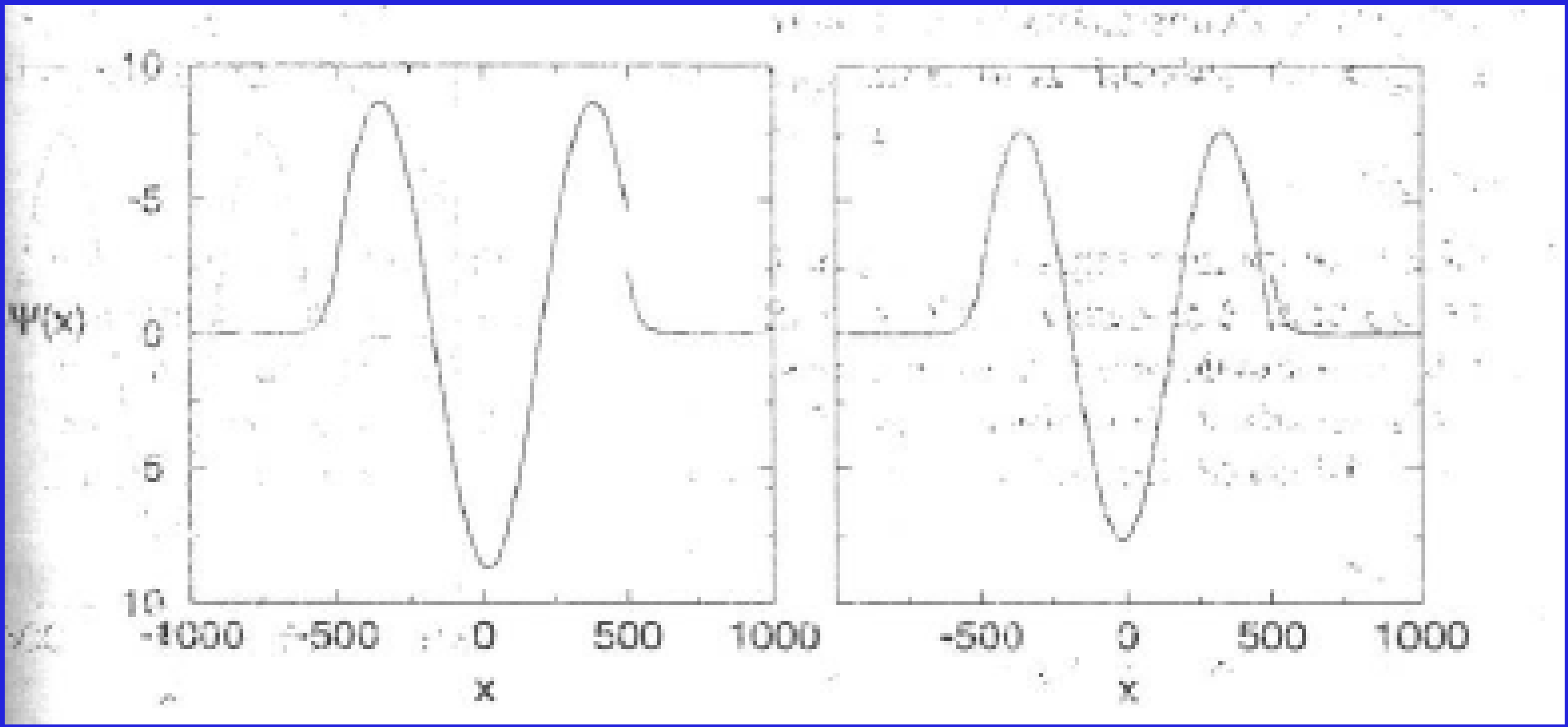
NOW, $\dfrac{d^2\left[k^2\psi\right]}{dx^2} \simeq$

$$\frac{\left[k^2(x+h)\psi(x+h) - k^2(x)\psi(x)\right]}{h^2} + \frac{\left[k^2(x-h)\psi(x-h) - k^2(x)\psi(x)\right]}{h^2}$$

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

$$\psi_{i+1} \simeq \frac{2(1 - \frac{5}{12} h^2 k_i^2)\psi_i - (1 + \frac{h^2}{12} k_{i-1}^2)\psi_{i-1}}{1 + \frac{h^2}{12} k_{i+1}^2}$$

See `numerov.cc`



10
5
Ψ(x)
0
5
10
-1000
-500
0
500
1000
x
-500
0
500
1000
x

Summary

Numerov technique for ODE solution.

Numerical solution of square well potential.

Don’t suffer in silence. Scream for help!!!