Lecture 15 Review

Fractal dimension of Sierpinski's gasket .

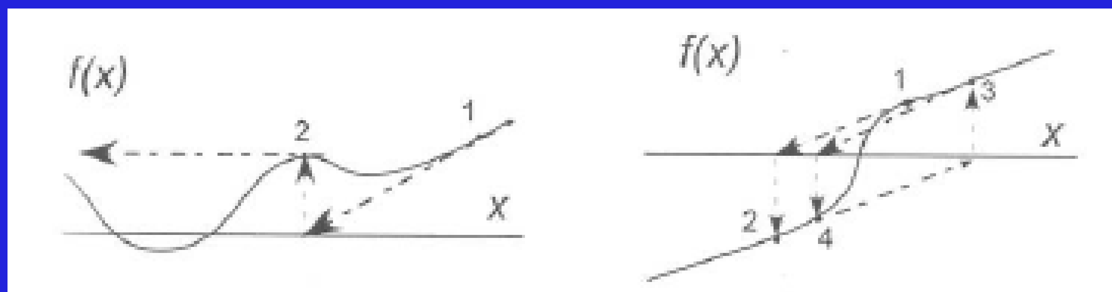
Affine transformations and fractal examples.

Root finding: N-R and bi-section algorithm.

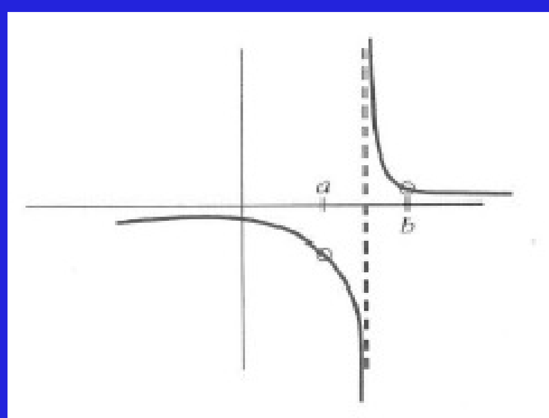
HW aside: Newton-Raphson Beware

Software ain't magic...

Potential pathologies using N-R root finding technique



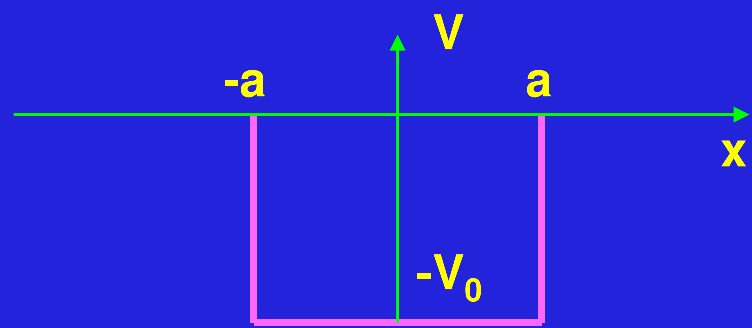
df(x)/dx = 0 "S"-shaped curves



…nasty…

NR solution potentially sensitive to initial guess. Beware. (Graph, too.)

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 $|x| > a$

$$\frac{2m}{\hbar^2} = \frac{2mc^2}{(\hbar c)^2} = \frac{2\times 940\,\mathrm{MeV}}{(197\,\mathrm{Mev-fm})^2} = 0.0483\,\mathrm{MeV}^{-1}\mathrm{fm}^{-2}$$

Particle in a Quantum Box

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

$$\alpha = \sqrt{\frac{2m(E+V_0)}{\hbar^2}} = \sqrt{0.0483(E+83)}$$

$$\beta = \sqrt{\frac{-2mE}{\hbar^2}} = \sqrt{-0.0483E}$$

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

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

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

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

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

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

$$\boxed{f(E) = \xi\tan\xi - \eta = 0}$$ ← Even parity solutions only.

Particle in a Quantum Box (2)

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

$$\alpha = \sqrt{\frac{2m(E+V_0)}{\hbar^2}} = \sqrt{0.0483(E+83)}$$

$$\beta = \sqrt{\frac{-2mE}{\hbar^2}} = \sqrt{-0.0483E}$$

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

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

$\Rightarrow$ $\alpha a\cot\alpha a + \beta a = 0$

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

$\xi\cot\xi + \eta = 0$ with $\xi = \alpha a$ $\eta = \beta a$

$$\xi^2 + \eta^2 = \frac{2mV_0 a^2}{\hbar^2} = 16.08$$

$\boxed{f(E) = \xi\cot\xi + \eta = 0}$ $\longleftarrow$ Odd parity solutions only.

Numerov Method for ODE Solution

Runge-Kutta (4^{th} order) is our preferred solver for ODEs.

Why not use it to solve Schrödinger equation?

For special case of dy/dx missing (e.g., Schrödinger eqn)

Use Numerov's method:

More accurate than RK-4^{th} order AND w/ fewer steps.

When applied to potential wells, Numerov's method is an example of solving ODE w/ boundary conditions (as opposed to ICs).

Numerov Method for ODE Solution (2)

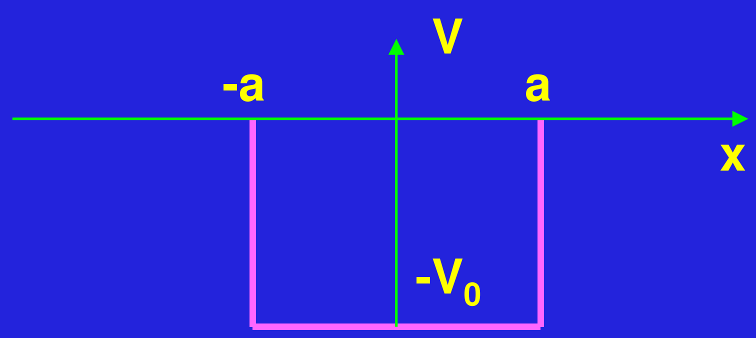
$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x)$$

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

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

Recall that E < 0 for bound states

$$(\frac{2m}{\hbar^2}) = 0.04829\,\mathrm{Mev}^{-1}\,\mathrm{fm}^{-2}$$



Numerov Method for ODE Solution (3)

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

$$\psi(x-h) = \psi(x) - h\psi' + \frac{h^2}{2}\psi'' - \frac{h^3}{3!}\psi''' + \frac{h^4}{4!}\psi^{\mathrm{IV}} + \ldots$$

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

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

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

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

Numerov Method for ODE Solution (5)

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

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

See `numerov.cc`

numerov.cc discussion

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

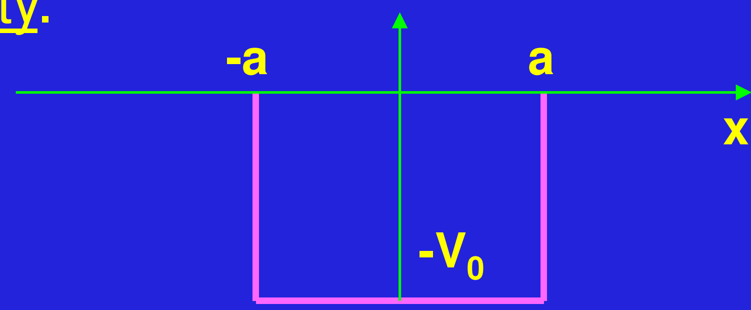
Basic algorithm.

Start w/ ψ_0 and ψ_1 specified.

Symmetric QM wells have ψ's of definite parity.

Recall, $\psi(-x) = \psi(x)$, "even" parity

$\psi(-x) = -\psi(x)$, "odd" parity



$|\psi(x)|^2$ and $|\psi(-x)|^2$ have physical significance.

ψ and ψ' must be continuous.

`numerov.cc` lets you pick parity. (By selecting sign of ψ_1.)

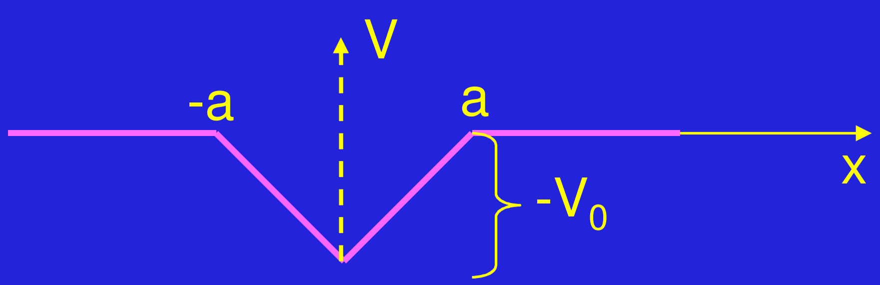
`numerov.cc` as coded does not check for continuity of ψ' .

Numerov Technique Lab Exercise

Modify `numerov.cc`

- Limit number of possible iterations to, say, 1000.
  Modification should tell you if you reached this limit.

- Alter potential from a square well to a V-shaped well.



Find energy eigenvalues and eigenstates
(i.e., find permissible energy levels & corresponding wavefunctions.)

Summary

Application of root finding to particle in a quantum box

Numerov technique for ODE solution.

Numerical solution of square well potential.

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