Lecture 18 Review

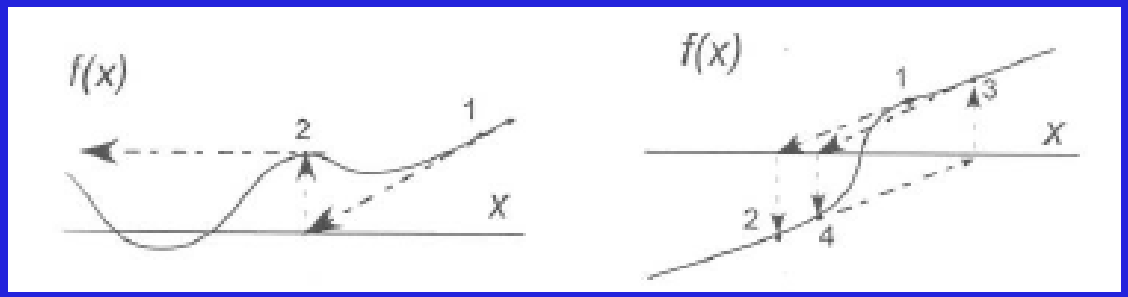
Numerov technique for ODE solution.

Sketched numerical solution of square well potential.

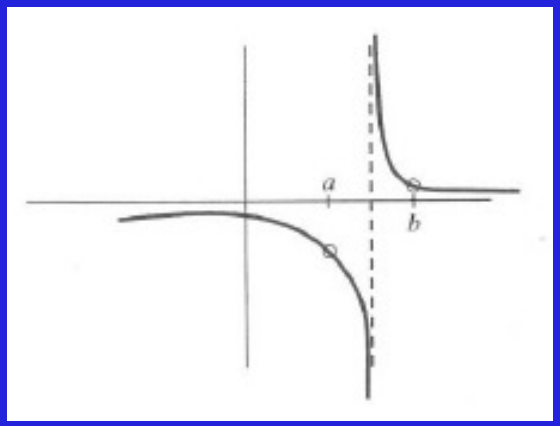
Newton-Raphson Beware

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.)

numerov.cc discussion

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

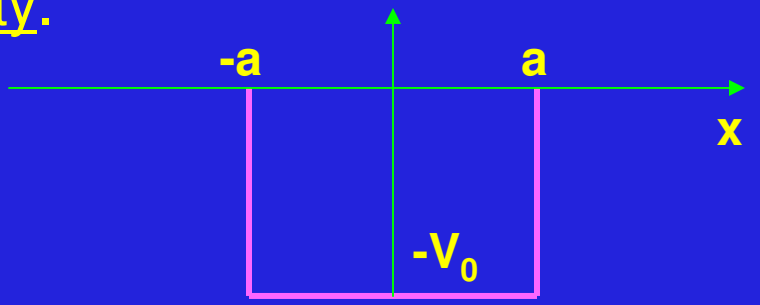
Basic algorithm.

Start w/ ψ_0 and ψ_1 specified.

Symmetric QM wells have ψ's of definite parity.

Recall, ψ(-x) = ψ(x) , "even" parity

ψ(-x) = -ψ(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.)

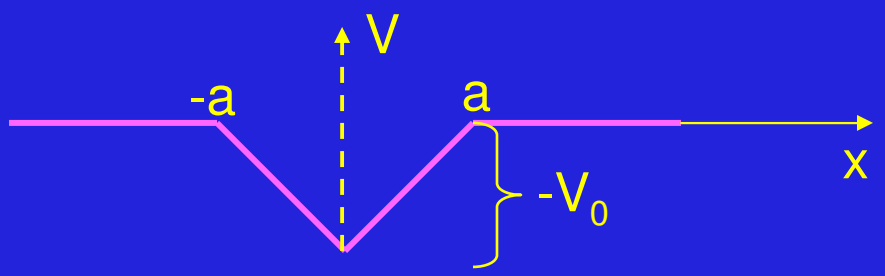
`numerov.cc` as coded does not check for continuity of ψ' .

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

Newton-Raphson warnings.

`numerov.cc` discussion.

Solution of triangular well via `numerov.cc`

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