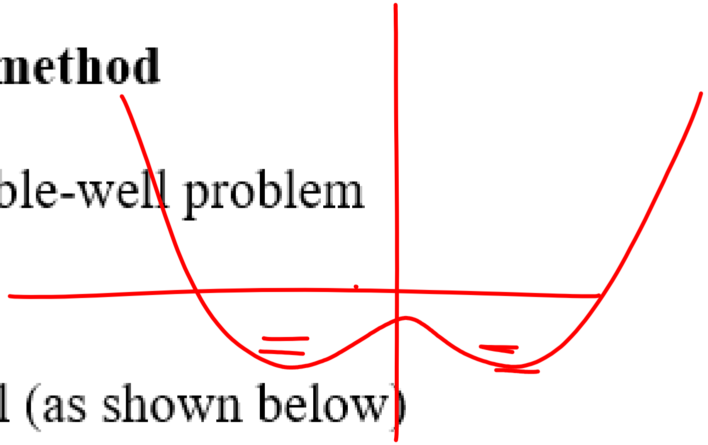
Final project

Math-III

Due on Aug. 12, 2021, at the class time

(presentation)

Solving 1-d Schrödinger equation by the shooting method



Use Runge-Kutta (4th order) method to solve a one-dimensional double-well problem

$$[-\frac{1}{2}\frac{d^2}{dx^2}+V(x)]\psi(x)=\varepsilon\psi(x)$$

where the atomic unit (a.u.) is used. The potential V is a double-well (as shown below)

$$V(x)=ax^4-bx^2$$

with $\boldsymbol{a=2}$ **and** $\boldsymbol{b=8}$.

a) Find all the energy eigenvalues below zero ($\varepsilon < 0$). (at least 4 significant figures)

b) plot the lowest two states (orthonormal wave functions) together with $V(x)$ in ($-2.5<x<2.5$).

c) Discuss that if V(x) is approximated as a simple harmonic oscillator around x0, where x0 is one of the two bottoms, what kind of structures for the energy eigenvalues and wavefunctions will be. Compared (qualitatively) with your results from a) and b).

Potential well

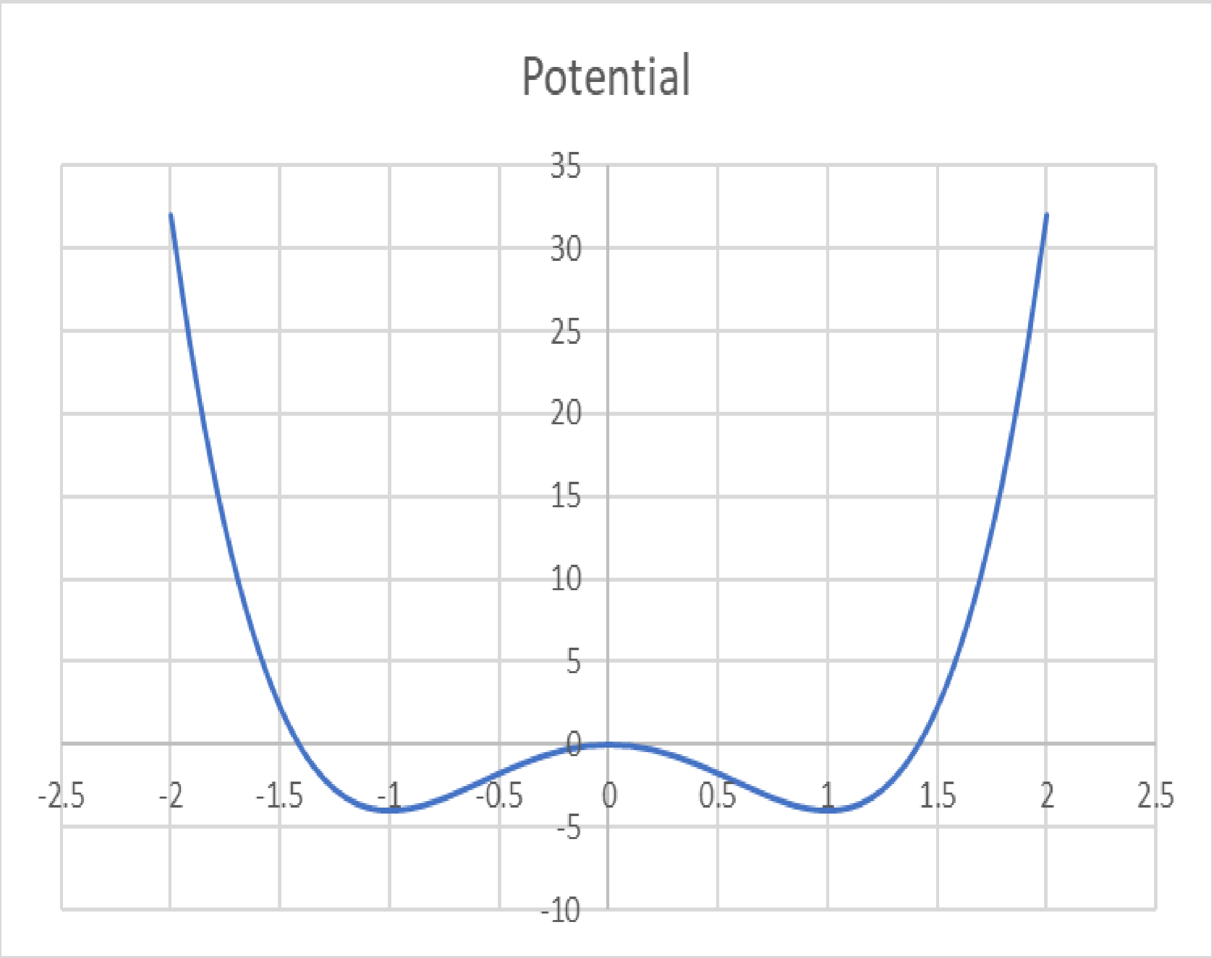
node

ψ_1 0

ψ_2 1

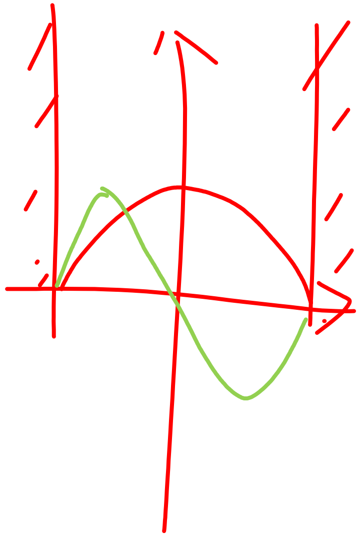
ψ_3 2

⋮



real

$\psi \xrightarrow[x \to \pm\infty]{} 0$



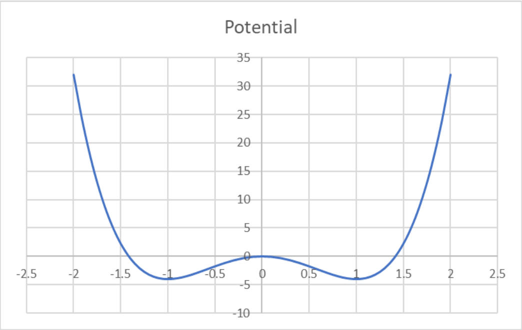
RK method

$$\frac{\psi'}{\psi} = (\ln \psi)'$$

$h < 0$

$\boxed{h = 0.1}$

$N = 501$



$$[-\frac{1}{2}\frac{d^2}{dx^2} + V(x)]\psi(x) = \varepsilon\psi(x)$$

Shooting method

This method finds the solutions to a differential equation when the value of a parameter as well as the solution to the differential equation must be found at the same time.

ψ, ψ'

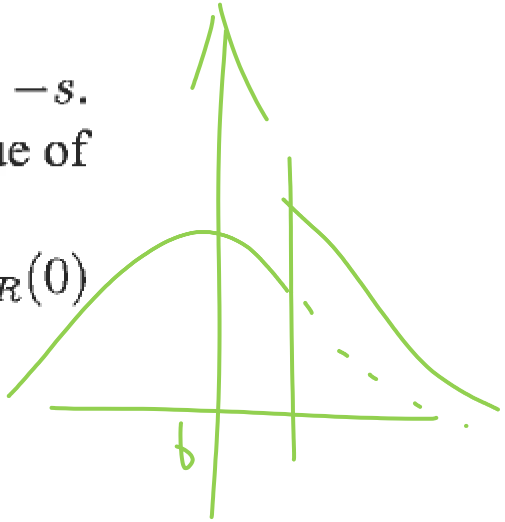
For a trial value ε, integrate the initial wavefunction (and its 1st order derivative) from left ($\psi_L(x; E)$) and right ($\psi_R(x; E)$) using the Runge-Kutta method.

Boundary conditions: $\psi_{L,R}(x \to \infty) = 0$; $d\psi_L(x \to \infty)/dx = s$, $d\psi_R(x \to \infty)/dx = -s$. (hint: you can choose $s = 1$; if your box is very large, you may want to reduce the value of s)

Since both $\psi(x)$ and $\alpha\psi(x)$ are solutions of the SE, the matching conditions $z_{1L}(0) = z_{1R}(0)$ and $z_{2L}(0) = z_{2R}(0)$ reduce to a single condition

ψ_L

$$\frac{z_{2L}(0)}{z_{1L}(0)} = \frac{z_{2R}(0)}{z_{1R}(0)},$$



ψ'

i.e. the derivative of the logarithm of the solution (DLS) must match at the centre.

The matching happen only at an eigenvalue ε !