Final Project

Path to source code: `/home/d/dx/dxj4360/Final`

File list:

`final.f90` : scan method to find the lowest 4 eigenvalues
`final2.f90` : bisection method with advancing E to find the lowest 4 eigenvalues
`manual.f90` : use bisection method to find eigenvalue between user input e1,e2
`psive.f90` : loop over E to find the tendency of $\psi(x_0)$ for eigenvalues

The Problem

The one-dimensional double-well problem:

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

with potential $V(x) = ax^4 - bx^2$, where $a = 2, b = 8$

The ODE

It can be reformulated to:

$$\psi'' = 2(V(x) - E)\psi = (4x^4 - 16x^2 - 2E)\psi$$

which doesn't include ψ'. Thus,

$$\frac{d\psi}{dx} = \psi'$$

$$\frac{d\psi'}{dx} = (4x^4 - 16x^2 - 2E)\psi$$

The boundary condition & initial parameters

It is impossible to integrate the wave function over $[-\infty, \infty]$ and archive unity. But the potential grows very fast outside $|x| > x_0$, where x_0 is set to 2.5 in my calculation. Thus, the problem is approximately solved as a double-well potential within infinite potential box.

- lower bound energy level: $E = \min(V(x)) = -8$

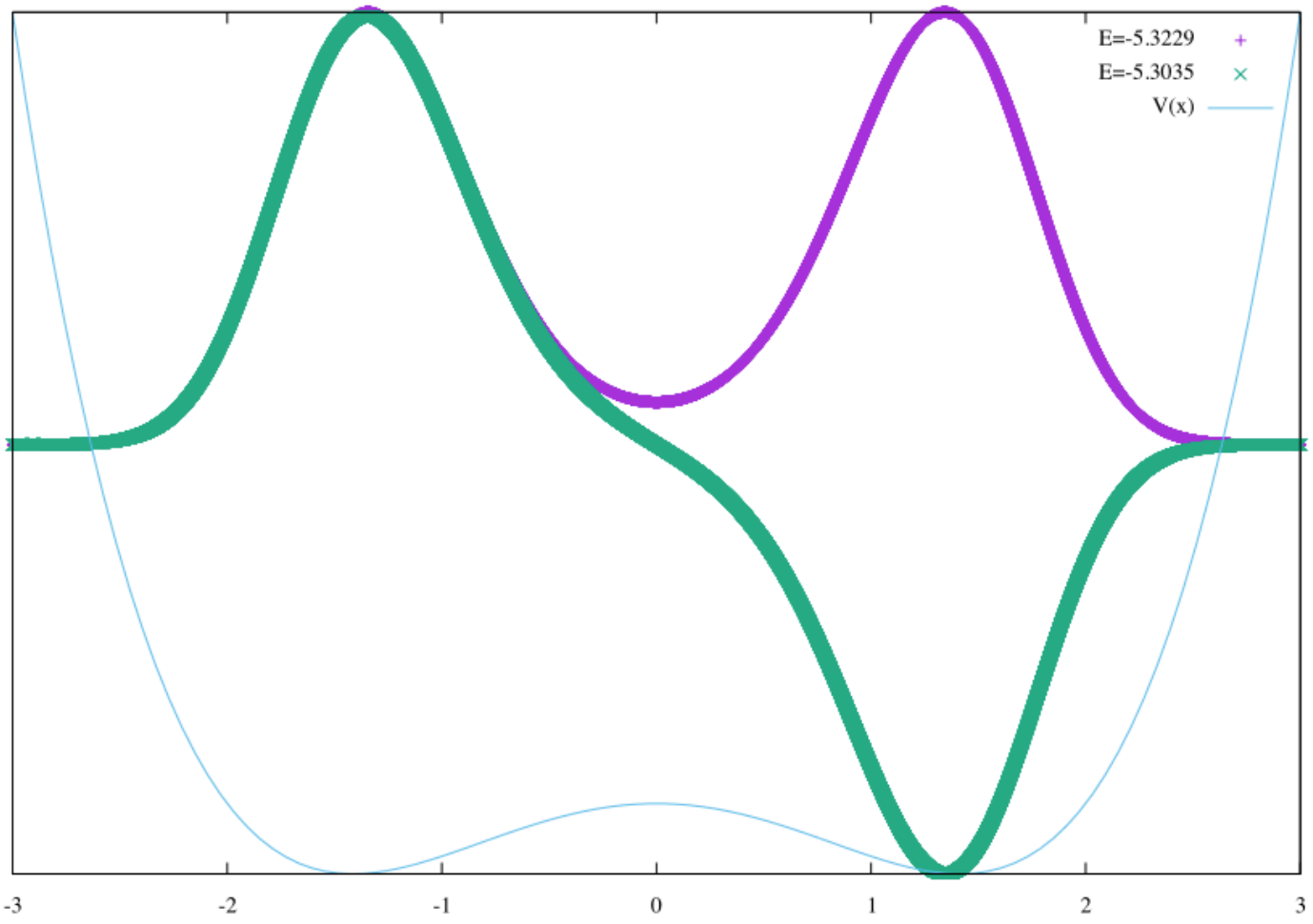
- infinity assumption: $x_0 = 2.5$ such that $\lim_{|x|\geq x_0} \psi(x) \to \epsilon; \psi'(x_0) \sim \epsilon$
- resolution: $dE = 1e-4, dx = 1e-3$
- $\psi(-x_0) = \psi'(-x_0) = \epsilon$
- converge condition: $\psi(x_0) \leq \epsilon$

Pseudocode

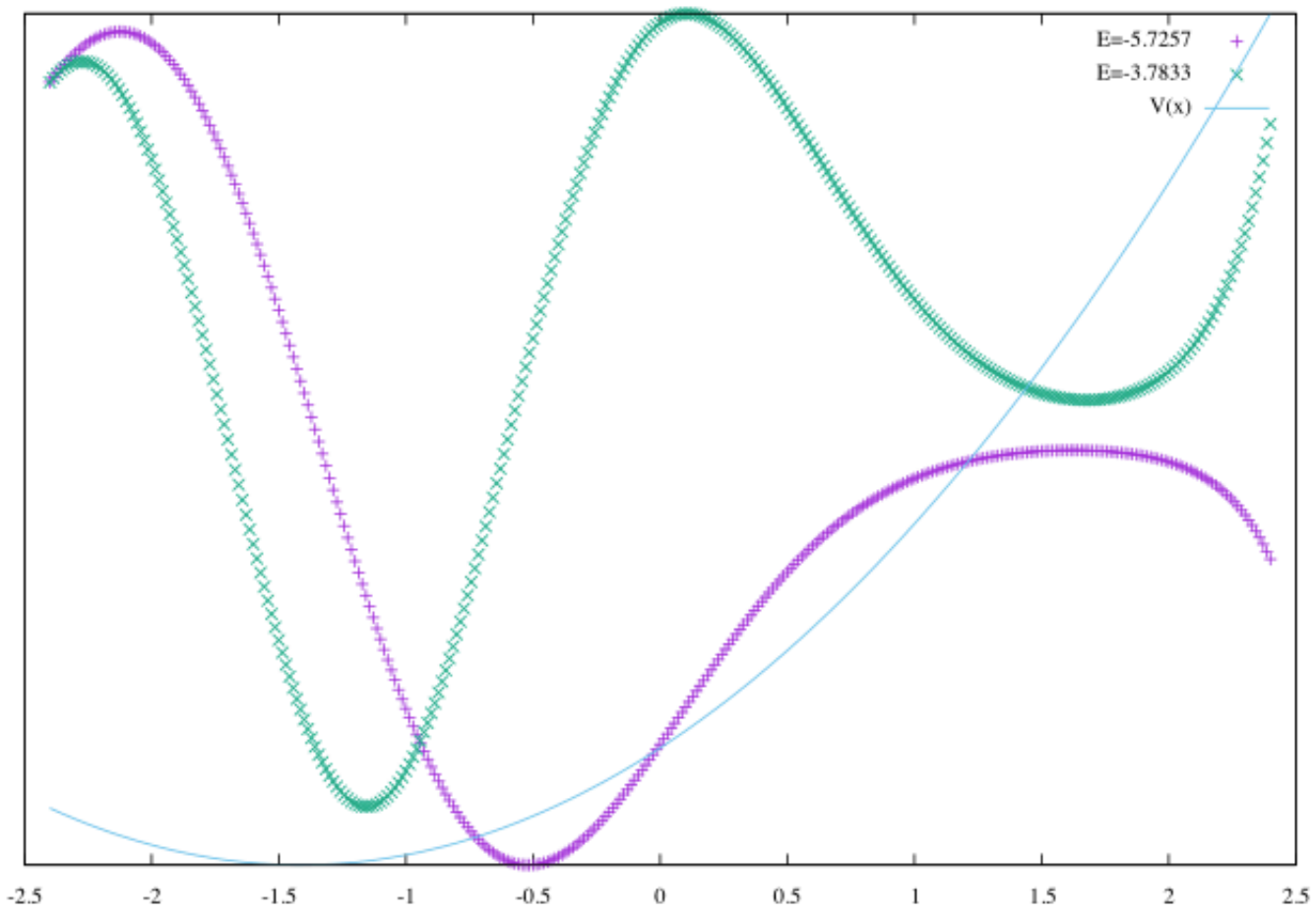
```
initialize parameters
do loop over E
    runge kutta integration from -x_0 to x_0
    if psi(x_0) -> 0 then
        record all psi(x)
        print E
    E increase by some steps
```

Result

- (a) energy eigenvalue below 0 when $x_0 = 2.5$:
    - -5.3229
    - -5.3035
    - -1.0206
    - -0.3616
- (b) lowest two states with $V(x)$



- (c) if $V(x)$ is approximated as SHO at $x_0 = \pm\sqrt{2}$, the wave function will be symmetric at $x = x_0$, the energy eigenvalue will change depend on the shape of SHO potential. If the minimum potential is the same, the wider potential, the higher the energy eigenstate.



Discussion

Manually guessing the energy eigenvalue is very inefficient, so I used do-loop to scan from $E = [-8, 0]$ with some small steps. I found the eigenstates are highly dependent on the shooting interval. If $x_0 = \pm 3$ is assumed as the cut-off boundary, the ground state energy will be extremely hard to find, even with a more efficient bisection method and adapting dx resolution. So I checked the $\psi(x_0)$ vs E. The eigenvalues are extremely narrow and easy to miss. If dx is too small, ψ will accumulate a lot at the beginning and hard to cross 0.