Physics 5403: Computational Physics – Project 4b

due date: Oct 4, 2022

Quantum eigenstates in a potential well

Consider the one-dimensional Schrödinger equation

$$-\frac{1}{2}\frac{d^2}{dx^2}\ \phi(x) + u(x)\ \phi(x) = \epsilon\ \phi(x)$$

with the potential given by

$$u(x) = \frac{1}{2}\ \alpha^2\ \lambda(\lambda-1)\ \left(\frac{1}{2} - \frac{1}{\cosh^2(\alpha x)}\right)\ .$$

Solve this quantum eigenstate problem numerically by transforming it into a matrix eigenvalue problem.

a) Write a program which does the following: Transform the above problem into a matrix eigenvalue problem by discretizing space and replacing the derivative by a finite-difference expression. (Use an x-interval from x_{min} to x_{max} divided into N_x steps.) Solve the resulting matrix eigenvalue problem. Output all eigenvalues and the eigenvectors for the lowest N_{state} states.

b) Perform the simulation for potential parameters $\alpha = 1$ and $\lambda = 4$. What are reasonable values for x_{min}, x_{max}, N_x? Discuss why? Study the lowest 6 eigenvalues and eigenstates in detail. Plot the eigenstates together with the potential.

c) Consider again the first 6 eigenstates. How do they depend on the box sizes? (Change x_{min} and x_{max})? Explain this dependence.

d) Investigate the influence of the boundary conditions on the solution. To do so, change from open boundary conditions to periodic boundary conditions (identifying x_{min} and x_{max}). How are the first 6 eigenstates influenced? Why?