

Problem 1. 1D Numerov for a Finite Harmonic Well

The goal of this exercise is to find bound-state solutions ($E < 0$) to the 1D time-independent Schrödinger equation for a finite harmonic well, i.e. for a potential $V(x)$ satisfying

$$V(x) = c(x^2 - x), 0 \leq x \leq 1, \quad (1)$$

and zero everywhere else, where $c > 0$ is a positive constant.

Use the Numerov algorithm and a root solver as described in section 3.1.3 of the lecture notes. In particular, note that bound-state solutions exist only for discrete energy eigenvalues.

1. Plot the number of bound states as a function of the parameter c for some values inside the interval $(0, 1000]$.
2. Plot the bound-state spectrum and the wavefunctions for the value $c = 400$.

Start with finding the ground state energy (which has zero nodes) and proceed further with 1, 2, 3... nodes.

Hint: Check the number of zeros (nodes) in the solution. For your guessed energy, if you find more nodes in your solution than the desired number of nodes, decrease the trial energy and vice versa.

Problem 2. Stopping light

Here, we will study the dynamics of a quantum particle in one dimension being reflected off a tilted wall. As initial state at $t = 0$, we choose a Gaussian wave packet going in x -direction

$$\Psi(x) = \mathcal{N} e^{ik_0 x} e^{-(x-x_0)^2/a^2}, \quad (2)$$

with center $x_0 = -10$, spread $a = 1$ and $k_0 = 5$. The normalization constant $\mathcal{N} = (\pi a^2/2)^{-1/4}$ is chosen such that $\int_{-\infty}^{\infty} dx |\Psi(x)|^2 = 1$.

1. Show that the operator $(1 + \frac{i\Delta_t}{2\hbar} H)^{-1} (1 - \frac{i\Delta_t}{2\hbar} H)$ is unitary.
2. Numerically compute the free time evolution of the particle in the absence of any potential.
 - a) Plot $\text{Re}\Psi(x, t)$, $\text{Im}\Psi(x, t)$ and the density $|\Psi(x, t)|^2$ at different times t .
 - b) Elaborate on the spread, amplitude, velocity and local kinetic energy across the wave packet.

Hint: Compare your results with the exact solution ($\hbar = m = 1$):

$$\Psi(x, t) = \mathcal{N} \left(\frac{a^2}{a^2 + 2it} \right) e^{i(k_0 x - k_0^2 t/2)} e^{-(x-x_0 - k_0 t)^2 / (a^2 + 2it)}. \quad (3)$$

3. Modify your code to include a tilted wall at $x = 0$, as described by the following potential:

$$V(x) = \begin{cases} 0, & x < 0 \\ \tan \theta, & x \geq 0 \end{cases}, \quad (4)$$

where θ is the tilting angles. The solution cannot be found analytically. Investigate the behavior of the wave packet numerically as it hits the wall. In particular, study the time evolution of the velocity of the wave packet

$$v(t) = - \int_{-\infty}^{\infty} dx \operatorname{Im} \Psi \nabla \Psi^*, \quad (5)$$

for different tilting angles.