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Exercise class in HCI J7.

General note: It is highly recommended to try and write the covered algorithms from scratch, using any programming language you like. This way, you can design the algorithms as you see fit. We also provide jupyter notebooks as "gap texts", with function stumps that you can use.

Exercise 1. ***1D Numerov algorithm 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

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

and zero everywhere else, with $c \geq 0$ a positive constant. We choose our unit system such that $\hbar = m = 1$.

Use the Numerov algorithm, the bidirectional shooting method (section 3.1.3 in the lecture notes) and a root solver (e.g. the bisection method in `scipy.optimize.bisect`) as discussed in the lecture. In particular, note that bound-state solutions exist only for discrete negative energy eigenvalues.

1. Plot the number of bound states as a function of the parameter c for some values inside the interval (0, 1000].

   *Hint. H*ow many nodes has the first bound state? How many the second, the third, ...? How can you use this information to find the number of bound states?

2. Plot the bound-state spectrum and the wavefunctions for the value $c = 400$.

   *Hint. F*or possible bound state energies, look at the log-derivative difference obtained by the bidirectional shooting method at these energies. Are the log-derivative differences as a function of the energy continuous? How many roots do you find? How can you find all the roots and know to which solution they belong?

Exercise 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

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

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 $\int dx\, |\Psi(x)|^2 = 1$.

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. Plot the position, velocity, spread (FWHM) and norm of the wavepacket as a function of time. Do this for the following methods:

(a) Spectral method.

(b) Unitary direct numerical integration.

(c) Split operator method.

Work in units such that $\hbar = m = 1$.

Hint. Compare your results with the exact solution:

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

Hint. The velocity of the wave packet is given by:

$$v(t) = -\int_{-\infty}^{\infty} dx \mathrm{Im}\Psi\nabla\Psi^{\star} \tag{4}$$

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

$$V(x) = \begin{cases} 0, & x < 0 \\ x\tan\theta & x \geq 0 \end{cases} \tag{5}$$

where θ is the tilting angle. The solution cannot be found analytically. Investigate the behavior of the wave packet numerically as it hits the wall: use any of the above evolution methods to study its position and velocity.