Numerical methods
Bachelor in Physics

Practicum 11: The time-independent Schrödinger equation

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In this last practical, we will study the time-independent Schrödinger equation for some simple problems. There are many ways to solve the Schrödinger equation numerically. We will discuss two methods, which both give the answer to the same question: how can we translate the Schrödinger eigenvalue problem into a matrix eigenvalue problem?

1 'Finite-difference' method

The one-dimensional time-independent Schrödinger equation is given by

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) + V(x)\psi(x) = E\psi(x). \tag{1}$$

Analogously to practical 4, we can find the solution by discretizing the differential equation:

$$-\frac{\hbar^2}{2m}\frac{\psi_{i+1}+\psi_{i-1}-2\psi_i}{h^2} + V(x_i)\psi_i = E\psi_i.$$

This yields the following eigenvalue problem:

$$H\tilde{\psi} = E\tilde{\psi}$$

with

$$\tilde{\psi} = (\psi_1\psi_2\dots\psi_N),$$

for N grid points. The matrix **H** is a tridiagonal matrix for one-dimensional problems. The eigenvalues and eigenvectors can be found by diagonalizing matrix **H**. In MATLAB, one could use the commands `eig` and `eigs`.

A script, which solves such an eigenvalue problem, will perform the following steps:

- Initialize the parameters (number of grid points, number of eigenvalues, ...)
- Implement the Hamiltonian (sparse) matrix H
- Solve the eigenvalue problem using `eigs`
- Plot the eigenvalues and eigenfunctions

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1. Find the eigenvalues and eigenstates of a particle in an infinite potential well with width L. Note that the wave function $\tilde{\psi}$ is only defined at the grid points, and is considered to be zero outside the well. Take the ground energy as the unit of energy $E' = \hbar^2\pi^2/2mL^2$, and the width as length unit $x' = L$. The Hamiltonian is now given by

$$\mathcal{H} = -\frac{1}{\pi^2}\frac{d^2}{dx^2} + V(x) \tag{2}$$

   with

$$V(x) = \begin{cases} 0, & |x| \leq 1/2 \\ \infty, & |x| > 1/2 \end{cases} \tag{3}$$

2. Use the same method to compute the energy levels of a one-dimensional harmonic oscillator. What is the expression for the Hamiltonian when you use the units $E' = \hbar\omega_0$ en $x' = \sqrt{\hbar/m\omega_0}$. Plot the eigenvalues and eigenfunctions.

3. Consider a finite potential well. Study the energy spectrum and the wave functions for different depths.

2 Two-dimensional problems

This method can also be used for multi-dimensional problems. As an example, we will study a two-dimensional harmonic oscillator:

$$-\frac{\hbar^2}{2m}\left(\frac{d^2}{dx^2}+\frac{d^2}{dy^2}\right)\psi(x,y)+V(x,y)\psi(x,y)=E\psi(x,y), \tag{4}$$

with $V(x,y)=\frac{1}{2}m\omega_0^2(x^2+y^2)$. After discretizing, we get

$$-\frac{\hbar^2}{2m}\frac{\psi_{i+1,j}+\psi_{i-1,j}+\psi_{i,j+1}+\psi_{i,j-1}-4\psi_{i,j}}{h^2}+V(x_i,y_j)\psi_{i,j}=E\psi_{i,j}. \tag{5}$$

The discretized wave function depends on two indices. Because we need to represent the wave function as a column vector, we will use the following ordering $\psi_1 \equiv \psi_{1,1}, \psi_2 \equiv \psi_{1,2}, \ldots, \psi_{N_y} \equiv \psi_{1,N_y}, \psi_{N_y+1} \equiv \psi_{2,1}, \ldots, \psi_n \equiv \psi_{\mathrm{floor}((n-1)/N_y)+1,n-(i-1)N_y}, \cdots$ The matrix $\mathbf{H}$, which need to be diagonalized, is no longer tridiagonal (why?), but it is still sparse.

Extra:

Try to find the wave functions and the corresponding energy levels of a 2D harmonic oscillator. (You can also solve this problem analytically.)