COMPUTATIONAL PHYSICS
Third assignment WS 2022/2023

Deadline: 7th of January 2023 23:00
Final date for the mini-exam: 9th/10th of January

The aim of this assignment is to get familiar with the numerical solution of the time-independent and time-dependent one-dimensional Schrödinger equation.

Note: The assignments contain questions and tasks, labeled (a), (b), etc. For some of these tasks, you are supposed to create and hand in one of the following:

- 💻 a script or a part of a script written in the computer language of your choice;
- 📈 a figure with legends and axis titles.

Other questions primarily serve to guide you through the exercises; you do not need to submit the answers in writing. However, you may be asked these or similar questions during the assessment discussions.

Note: Many tasks in the exercises can be performed using an existing library or toolbox. In line with the aim of the course, however, programming your own analysis tools is encouraged. If libraries or toolboxes are used, you are expected to be able to explain in detail how these algorithms work.

Note: When collaborating in groups of up to 3 students, you are allowed to hand in identical code. Please list all collaborators, for example in the header.

Note: The scripts in the programming exercises should be considered to be intended for general use, and a corresponding coding style will be appreciated. For example, using input parameters as variables, clear presentation of input and output, naming of variables and/or comprehensive comments in the script are among the grading criteria.

1 The time-independent Schrödinger equation

The single-particle time-independent Schrödinger equation in one spatial dimension reads:

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right]\psi(x) = E\psi(x), \tag{1}$$

where m and E are the mass and energy of the particle and $V(x)$ is a space-dependent potential. We want to solve the Schrödinger equation on a finite domain with length L which is bounded on both sides by two infinitely high potential walls. The appropriate boundary conditions are therefore:

$$\begin{aligned}\psi(-L/2) &= 0,\\ \psi(L/2) &= 0.\end{aligned}$$

In order to use the RK-4 solver developed in the first project, we rewrite this problem as an initial value problem. For convenience we make the Schrödinger equation dimensionless:

$$\left[-\frac{1}{2}\frac{d^2}{ds^2} + \tilde{v}(s)\right]\psi(s) = \varepsilon\psi(s) \tag{2}$$

with $s = x/L$, $\varepsilon = (mL^2/\hbar^2)E$ and $\tilde{v}(s) = (mL^2/\hbar^2)V(x/L)$.[1] Then we can transform the second order differential equation into a system of two coupled first order ODE's:

$$\frac{d}{ds}\begin{pmatrix}\psi\\ \psi'\end{pmatrix} = \vec{f}(\psi, \psi', s). \tag{3}$$

As initial value for the derivative you may use $\psi'(s = -1/2) = 1$. The algorithm presented in the lecture can then be implemented in the following way:

[1] This means that we express the Schrödinger equation in different units, for example $s = 0.1$ means 1/10th of our domain.

Pseudocode for our algorithm

1. Choose 2 trial energies ε_1 and ε_2 and define the required accuracy η.
2. If $\psi_{\varepsilon_1}(L/2)\psi_{\varepsilon_2}(L/2) > 0$, choose new values for ε_1 and ε_2 and go to step 1.
3. Otherwise choose $\bar{\varepsilon} = \dfrac{\varepsilon_1 + \varepsilon_2}{2}$
4. $$\begin{aligned} &\text{If } \psi_{\varepsilon_1}(L/2)\psi_{\bar{\varepsilon}}(L/2) < 0 \qquad &&\text{set } \varepsilon_2 \leftarrow \bar{\varepsilon} \\ &\text{If } \psi_{\varepsilon_2}(L/2)\psi_{\bar{\varepsilon}}(L/2) < 0 \qquad &&\text{set } \varepsilon_1 \leftarrow \bar{\varepsilon} \end{aligned}$$
5. if $|\varepsilon_1 - \varepsilon_2| < \eta$, where η is the required accuracy terminate, otherwise go to 3.

(a) Remember your general explicit Runge-Kutta solver from the first assignment and its functionality. If you have no working explicit Runge-Kutta solver, write a routine for a RK-4 solver which accepts an arbitrary system of ordinary differential equations as input.

(b) 💻 Use the RK-4 method to solve equation 2 numerically for a particle in a box, i.e. $\tilde{v}(s) = 0$ for $-1/2 \leq s \leq 1/2$ and ∞ otherwise. The infinite potential is implemented via the boundary condition on $\psi(s)$. Find the first 5 eigenvalues ε and compare with their analytical values.

(c) 📈 Plot the eigenfunctions from (b) and compare with their analytical form. [2]

(d) 💻 Now include potentials of the form

- $\tilde{v}(s) = \tilde{v}_0 \exp\left(\frac{s^2}{0.08}\right)$
- $\tilde{v}(s) = \tilde{v}_0\, \theta(s - 0.3)\, \theta(0.35 - s)$
- $\tilde{v}(s) = -\tilde{v}_0 \theta(0.25 - s)\, \theta(s + 0.25)$,

[2] Do not forget about normalization!(Remember how wave function and probability are related)

with appropriately chosen values of $\tilde{v}_0$. Determine the first five eigenvalues and eigenfunctions of the corresponding Schrödinger equation.

(e) 📈 Create a plot displaying the eigenfunctions of the Schrödinger equation with the non-zero potentials of the previous task. What do you conclude about the roots of these wave-functions?

(f) 💻 Calculate $\langle s \rangle$ and $\langle s^2 \rangle - \langle s \rangle^2$, and interpret your results, by using the plots created in the previous tasks.

2 The time-dependent Schrödinger equation in one dimension with Crank-Nicolson

The time-dependent Schrödinger equation in one spatial dimension reads:

$$i\hbar \frac{\partial}{\partial t}\psi(x,t) = \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right)\psi(x,t) \tag{4}$$

In the lecture the solution of the time-dependent Schrödinger equation with Crank-Nicolson was introduced. The wave function $\psi(x,t)$ is thereby discretized in space and time. The evolution in time is achieved by the Crank-Nicolson scheme, and the discretation of the second spatial derivative is done with finite differences of order Δx^2. Crank-Nicolson is an implicit scheme for the numerical solution of ordinary differential equations. In the case of the time-dependent Schrödinger equation it is particularly useful, as it ensures the unitarity of the time evolution operator. In the following, ψ_k^n refers to $\psi(x_k, t_n)$ and you can set $\hbar = 1$. The Crank-Nicolson scheme for the Schrödinger equation works in the following way:[3]

1. Choose the initial conditions ψ_k^0, $k = 0, 1, ..., N$ which satisfy the boundary conditions $\psi_0^0 = \psi_N^0 = 0$.

2. Set

$$a_1 = 2\left(1 + \frac{m\Delta x^2}{\hbar^2}V_1 - \frac{i2m\Delta x^2}{\hbar\Delta t}\right) \tag{5}$$

and calculate for $k = 2, ..., N-1$

$$a_k = 2\left(1 + \frac{m\Delta x^2}{\hbar^2}V_k - \frac{i2m\Delta x^2}{\hbar\Delta t}\right) - \frac{1}{a_{k-1}} \tag{6}$$

[3]For an explicit derivation of the algorithm see Reinhard Alkofer's lecture notes or the book: Basic Concepts in Computational Physics, by Ewald Schachinger and Benjamin Stickler, chapter 11.5

3. Start the time loop: $n = 1, ...M$, with M being the maximum number of steps

4. Calculate for $k = 1, 2, ..., N-1$

$$\Omega_k^n = -\psi_{k-1}^n + 2\left(\frac{i2m\Delta x^2}{\hbar\Delta t} + 1 + \frac{m\Delta x^2}{\hbar^2}V_k\right)\psi_k^n - \psi_{k+1}^n \tag{7}$$

5. Set

$$b_1^n = \Omega_1^n \tag{8}$$

and calculate for $k = 2, ..., N-1$

$$b_k^n = \frac{b_{k-1}^n}{a_{k-1}} + \Omega_k^n \tag{9}$$

6. Calculate for $k = N-1, N-2, ...1$

$$\psi_k^{n+1} = \frac{1}{a_k}(\psi_{k+1}^{n+1} - b_k^n) \tag{10}$$

with $\psi_0^{n+1} = \psi_N^{n+1} = 0$.

7. Set $n = n + 1$ and go to step 4.

(a) 💻 Write a routine for the solution of the time-dependent Schrödinger equation by using the algorithm described above,[4] which accepts as inputs:

- `Nx`: number of spatial grid points
- `dx`: distance Δx between two adjacent grid points
- `Nt`: maximum number of time steps
- `dt`: the time step Δt
- `psi0`: the wave function at $t = 0$ as the initial condition
- `V`: a function or a function handle of the potential

and gives as outputs

- `psi`: an array containing the values of $\psi(x, t)$ as a function of space and time.

[4]Choose the spacing between adjacent grid-points Δt and Δx carefully. You are allowed to set $\hbar = 1$ for convenience.

(b) 💻 Use the routine from above to solve the Schrödinger equation to study the time evolution for a freely propagating Gaussian wave packet:

$$\psi(x,0) = \frac{1}{\sqrt{\sigma\sqrt{\pi}}} \exp\left(\frac{-(x-x_0)^2}{2\sigma^2}\right) \exp\left(\tfrac{i}{\hbar} q x\right), \tag{11}$$

which describes a wave packet propagating in positive x direction with momentum q [5]. As parameters use $\sigma = 10$, $q = 2$, and $x_0 = 0$ and $m = 1$. Verify that the velocity of the maximum of the wave packet is $v = \frac{q}{m}$ and that the width of the wave packet is given by $d(t) = \sigma\sqrt{1+\Delta^2}$ with $\Delta = t/(2m\sigma^2)$.

(c) 📈 Plot $|\psi(x,t)|^2$ as a function of time (snapshots or animation) and check in an additional plot whether the total probability is conserved.

(d) 💻 We now want to study the scattering of the Gaussian wave packet ($\sigma = 20$, $q = 2$, $x_0 = 0$ and $m = 1$) on two different potentials:

$$V_1(x) = V_0[\theta(x-a) - \theta(x-(a+d))] \tag{12}$$

$$V_2(x) = V_1(x) + V_0[\theta(x-b) - \theta(x-(b+d))] \tag{13}$$

Calculate the time evolution of ψ for $V_0 = 1.5, 2.0, 2.5$ with $a = 100$, $b = 200$ and $d = 10$.

(e) 📈 Create 10 plots which display the essential parts of the time evolution of $|\psi(x,t)|^2$ and interpret your results. Do they look plausible?[6]

3 The split operator method

Finite difference schemes are only one possible way to solve partial differential equations. Faster and easier to implement methods exist, e.g. so-called pseudo-spectral methods. In the case of the time-dependent Schrödinger equation, a very interesting approach is the split-operator method. We start with the time-dependent Schrödinger equation and split the Hamilton operator H in 2 parts. The kinetic part T, which is diagonal in a momentum space basis, and a space dependent potential $V(x)$ diagonal in position space.

[5] Remember that a similar situation was considered in the *Electrodynamics* exercise 7.4.

[6] As alternative to the 10 plots you may show an animation

$$i\hbar\frac{\partial}{\partial t}\psi(x,t) = H\psi(x,t) = (T + V(x))\psi(x,t) \tag{14}$$

with

$$T = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}. \tag{15}$$

The formal time evolution of the system would now be described by

$$\psi(x, t + dt) = U\psi(x,t) = \exp(-\tfrac{i}{\hbar}Hdt)\psi(x,t). \tag{16}$$

with the time evolution operator U

$$U = \exp(-\tfrac{i}{\hbar}Hdt) = \exp(-\tfrac{i}{\hbar}(T + V(x))dt) \tag{17}$$

With the help of the Baker-Campbell-Hausdorff formula we can now split

$$\exp(-\tfrac{i}{\hbar}(T + V(x))dt) = \exp(-\tfrac{i}{\hbar}V(x)dt)\exp(-\tfrac{i}{\hbar}Tdt)\exp(-\tfrac{i}{2\hbar}[V(x), T]dt^2) \tag{18}$$

$$= \exp(-\tfrac{i}{\hbar}V(x)dt)\exp(-\tfrac{i}{\hbar}Tdt) + \mathcal{O}(dt^2) \tag{19}$$

This approximation however does not preserve unitarity. In order to improve the approximation and make sure that U is unitary, a process called Strang-splitting is used:

$$U = \exp(-\tfrac{i}{2\hbar}(V(x))dt)\exp(-\tfrac{i}{\hbar}Tdt)\exp(-\tfrac{i}{2\hbar}V(x)dt) + \mathcal{O}(dt^3) \tag{20}$$

If we introduce a Fourier-transform $\mathcal{F}$ by

$$\phi(q,t) = \mathcal{F}\{\psi(x,t)\} = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty}\exp(-\tfrac{i}{\hbar}qx)\psi(x,t)dx, \tag{21}$$

as well as its inverse $\mathcal{F}^{-1}$, we obtain

$$\psi(x, t + dt) \approx \exp(-\tfrac{i}{2\hbar}V(x)dt)\mathcal{F}^{-1}\{\exp(-\tfrac{i}{\hbar}T_q dt)\mathcal{F}\{\exp(-\tfrac{i}{2\hbar}V(x)dt)\psi(x,t)\}\} \tag{22}$$

with $T_q = q^2/2m$, the representation of T with respect to momentum eigenstates. As no analytical form of the Fourier transform exists, the so-called discrete Fourier transformation is used. A particular fast implementation of this discrete Fourier transform is called FFT(fast Fourier transform). For detailed information on the discrete and fast Fourier transform, please read Chapter 2.3 of last year's lecture notes, which can be found on the teach center.

(a) 💻 Solve the free particle ($V(x) = 0$) time-dependent Schrödinger equation with the split operator method.[7] As initial wave function choose Gaussian wave packets with $\sigma = 20$, $q = 2, 20$ and $x_0 = 0$.

[7] You may use some library for the fft function

(b) 📈 Make a plot of $|\psi|^2$ at $t = 400$ and compare it with $|\psi|^2$ at $t = 400$ from the Crank-Nicolson method. Which of these two deviates less from the analytical evolution of the Gaussian wave packet?

(c) 📈 Solve the Schrödinger equation for the potentials V_1 and V_2 and the corresponding parameters from the previous task and compare your results graphically. Which algorithm is in your implementation more efficient?

4 Bonus: The harmonic oscillator

(a) 📈 Consider the potential of a harmonic oscillator $V(x) = \frac{1}{2}x^2$. As initial wave function use a Gaussian wave packet with $\sigma = 1$, $q = 0$ and $x_0 = -1$. Create an animation of the "motion" of this Gaussian wave packet.

(b) 💻 If the system is evolved in imaginary time, all higher energy states decay, until the wave function reaches its ground state. Use this fact to determine the ground state wavefunction and the corresponding energy eigenvalue of the harmonic oscillator. [8]

(c) 💻 Use the evolution in imaginary time to obtain the Eigenvalues and corresponding wave functions of the first three excited states of the harmonic oscillator.

[8] Think about normalization. What does $|\psi|^2$ explain.