NTNU
Institutt for Fysikk

Numerical exercise
FY2045 Quantum Mechanics

Tutorials: 18, 19, 25, 26 October, 16.15 - 18.00
Hand in: Friday October 27, 12.00

Introduction

The goal of this exercise is to study some aspects of quantum mechanics:

- Numerical integration of the Schrödinger equation
- Propagation of wave packets
- Scattering by a barrier
- Tunneling

You will hand in a report (on Blackboard), containing your results. You should describe briefly how you have proceeded, include the answers to all questions posed in the problems, as well as any plots that are asked for. The bonus problems are optional. Include your source code as an attachement. You will probably modify your source code to answer the different questions, and you don't have to include all versions. You should state briefly what the included code does, for example "Running the included program will produce the plot and numbers asked for in Problem 3".

Two students may work together on one report. I recommend using python, but you may use any other language if you prefer. This exercise is based on a similar exercise by David Roundy at Oregon State University[1]. It may be helpful to consult that webpage as well as this assigment.

Theory

The Schrödinger equation reads

$$\mathrm{i}\hbar\frac{\partial}{\partial t}\Psi(x,t) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\Psi(x,t) + V(x)\Psi(x,t). \tag{1}$$

In order to numerically integrate[2] this equation, we need a procedure that allows us to calculate $\Psi(x, t + \Delta t)$, if $\Psi(x, t)$ is known, where Δt is a short time interval.

We will begin by writing the wave function as a sum of a real and an imaginary part,

$$\Psi(x,t) = \Psi_R(x,t) + \mathrm{i}\Psi_I(x,t). \tag{2}$$

[1] http://physics.oregonstate.edu/~roundyd/COURSES/ph365x/366.html

[2] The word "integrate" here means to find solutions of a differential equation, not to calculate an integral.

You should verify that this leads to the following two coupled equations:

$$-\hbar\frac{\partial}{\partial t}\Psi_I(x,t) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\Psi_R(x,t) + V(x)\Psi_R(x,t), \tag{3a}$$

$$\hbar\frac{\partial}{\partial t}\Psi_R(x,t) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\Psi_I(x,t) + V(x)\Psi_I(x,t). \tag{3b}$$

Next, we will approximate the derivatives using central finite differences, i.e., by using

$$\frac{\partial}{\partial x}f(x) \approx \frac{f(x+\Delta x/2) - f(x-\Delta x/2)}{\Delta x}. \tag{4}$$

Using Eq. (4), and the fact that

$$\frac{\partial^2}{\partial x^2}f(x) = \frac{\partial}{\partial x}\left(\frac{\partial}{\partial x}f(x)\right) \tag{5}$$

we find that

$$\frac{\partial^2}{\partial x^2}f(x) \approx \frac{f(x+\Delta x) - 2f(x,t) + f(x-\Delta x)}{(\Delta x)^2}. \tag{6}$$

Finally, using Eqs. (4) and (6), we find that Eq. (3a) can be rewritten into

$$\begin{aligned}\Psi_I(x,t+\frac{\Delta t}{2}) = \Psi_I(x,t-\frac{\Delta t}{2}) - \Delta t\Bigg[&\frac{V(x)}{\hbar}\Psi_R(x,t) \\ &-\frac{\hbar}{2m}\frac{\Psi_R(x+\Delta x,t) - 2\Psi_R(x,t) + \Psi_R(x-\Delta x,t)}{(\Delta x)^2}\Bigg].\end{aligned} \tag{7a}$$

Since Eq. (7a) allows us to calculate Ψ_I at times $t = (n+\frac{1}{2})\Delta t$, if Ψ_R is known at times $t = n\Delta t$, where n is an integer, we rewrite Eq. (3b) into

$$\begin{aligned}\Psi_R(x,t+\Delta t) = \Psi_R(x,t) + \Delta t\Bigg[&\frac{V(x)}{\hbar}\Psi_I(x,t+\frac{\Delta t}{2}) \\ &-\frac{\hbar}{2m}\frac{\Psi_I(x+\Delta x,t+\frac{\Delta t}{2}) - 2\Psi_I(x,t+\frac{\Delta t}{2}) + \Psi_I(x-\Delta x,t+\frac{\Delta t}{2})}{(\Delta x)^2}\Bigg].\end{aligned} \tag{7b}$$

We now have a procedure for finding $\Psi_I(x,t+\frac{\Delta t}{2})$, if $\Psi_I(x,t-\frac{\Delta t}{2})$ and $\Psi_R(x,t)$ is known, and similarly finding $\Psi_R(x,t+\Delta t)$, if $\Psi_R(x,t)$ and $\Psi_I(x,t-\frac{\Delta t}{2})$ is known.

The aim of the exercise is to study the propagation of a wave packet, which we will represent as a plane wave multiplied with a Gaussian:

$$\Psi(x,t) = C\mathrm{e}^{-\frac{(x-x_s)^2}{2\sigma_x^2}}\mathrm{e}^{\mathrm{i}(k_0 x-\omega t)}, \tag{8}$$

where C is a normalisation constant. The wave packet will start out centered at x_s at $t=0$, and will have a width (in x-space) determined by σ_x.

Numerical implementation

In order to calculate the spatial derivatives numerically, we will need to evaluate $\Psi(x,t)$ at discrete points along the x-axis. We will look at the interval from $x = 0$ to $x = L$, at N_x discrete points with constant spacing $\Delta x = \frac{L}{N_x - 1}$.

We will need to create three arrays of length N_x:

- A real array to hold all the values of x, from $x = 0$ to $x = L$.
- A real array to hold the values of $V(x)$ for each x.
- A complex array to hold the values of Ψ.

In order to calculate the value of $\Psi(x_i, t)$, you will need the values at x_{i-1} and x_{i+1} at the previous timestep. Hence, special treatment is required for the first and the last point in our domain. One option is to simply set $\Psi(x_0 = 0, t) = 0$ and $\Psi(x_{N_x} = L, t) = 0$ from the beginning, and then never update these values. In other words, calculate $\Psi(x_1, t)$ using the values at x_0 and x_2, but never change the value of $\Psi(x_0, t)$, and similarly at the other end. This is essentially the same as saying the potential is infinite outside the domain, since that would also force the wave function to be zero at the boundary.

For the various constants[3], we will use the values $\hbar = 1$, $m = 1$, $k_0 = 20$ and $L = 20$. From these, calculate ω and E, using k_0 to represent the wave number of the packet.

Numerical stability

By numerically evaluating the derivatives at discretely spaced points, both in space and time, we are approximating the true solution of the Schrödinger equation. In order to maintain accuracy, it is necessary to consider the relationship between Δt and Δx. If we make a poor choice for these parameters, we will get results where small errors grow exponentially with each iteration.

The Schrödinger equation gives the value of the time derivative of the wave function, which we use to calculate how much it will change during a short interval Δt. If we write equations (7a) and (7b) in a simplified manner, they essentially say

$$\Psi(x, t + \Delta t) - \Psi(x,t) = \Delta t \frac{\partial}{\partial t} \Psi(x,t). \tag{9}$$

We know that this is only an approximation, since in reality $\frac{\partial}{\partial t}\Psi(x,t)$ is a function of time, while here we implicitly assume it to be constant for the duration Δt. Hence, if the wave function changes by a significant fraction during a time step Δt, we are likely to get incorrect results. The fraction by which the wave function

[3] Setting $\hbar = 1$ and $m_e = 1$ (where m_e is the mass of the electron) is known as using atomic units.

changes during an interval Δt is given by

$$\frac{\Delta\Psi}{\Psi(x,t)} = \frac{\Psi(x,t+\Delta t) - \Psi(x,t)}{\Psi(x,t)} = \Delta t \frac{\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\Psi(x,t) + V(x)\Psi(x,t)\right)}{\mathrm{i}\hbar\Psi(x,t)}. \tag{10}$$

To proceed, we need an estimate of the magnitude of $\frac{\partial^2}{\partial x^2}\Psi(x,t)$. In our discrete system, the largest possible spatial rate of change for the wave function is if it changes from a positive peak to a negative peak across a distance Δx, and the largest possible curvature for the wave function would be if it changed from a positive peak to a negative peak and back across a distance $2\Delta x$. It is worth pointing out that if this is the case, the spatial resolution is too low to accurately represent the wave function, but we can still use these estimates to say that

$$\left|\frac{\partial^2}{\partial x^2}\Psi(x,t)\right| < \left|\frac{\Psi(x,t)}{\Delta x^2}\right|. \tag{11}$$

As an estimate for $V(x)$, we will simply use $V_{max} = \max|V(x)|$, i.e., the highest absolute value of $V(x)$ on our interval from $x = 0$ to $x = L$. Hence, if we want to make sure that the fraction by which Ψ changes during an interval Δt is much smaller than 1, we have to choose Δx and Δt such that

$$\Delta t \ll \frac{\hbar}{\frac{\hbar^2}{2m}\frac{1}{(\Delta x)^2} + V_{max}}. \tag{12}$$

Problems

Problem 1

Calculate initial values for $\Psi_I(x,t)$ and $\Psi_R(x,t+\frac{\Delta t}{2})$ using Eq. (8). Normalise the wave function such that

$$\int_0^L |\Psi(x,t)|^2 \, \mathrm{d}x = 1. \tag{13}$$

Make a plot of the real and imaginary parts of Ψ, selecting suitable values for Δx, x_s and σ_x to make your figure look similar to Figure 1. Make sure Δx is small enough that each oscillation of the wave function is resolved by enough points to look fairly smooth. Furthermore, make a plot of the probability density for finding the particle represented by the wave packet, given by $|\Psi(x,t)|^2$.

Problem 2

Start out a wave packet at $x_s = 5$, and propagate it a distance $\frac{L}{2} = 10$, i.e., until it reaches $x = 15$. This will take a time $T = \frac{L}{2v_g}$, where v_g, given by

$$v_g = \left.\frac{\partial\omega}{\partial k}\right|_{k_0}, \tag{14}$$

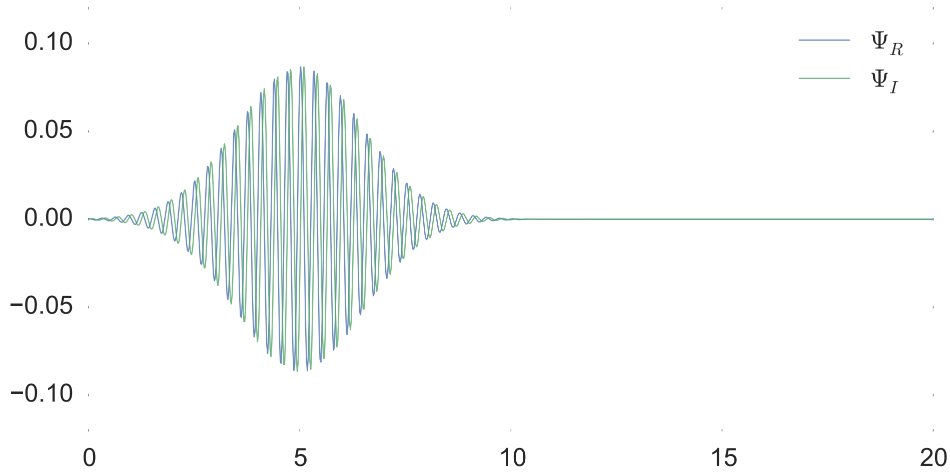

Figure 1: Real and imaginary parts of normalised wave function, as given by Eq. (8).

is the group velocity at the wave number k_0. Repeat this procedure for different values of σ_x, for example $\sigma_x = 0.5$, $\sigma_x = 1.0$ and $\sigma_x = 2.0$. Describe what happens, and produce a figure that shows the initial probability density $|\Psi(x,t)|^2$ centered on $x_s = 5$, and the same for the propagated wave centered on $x = 15$, for two different σ_x, for example $\sigma_x = 1.5$ and $\sigma_x = 0.5$.

To successfully carry out this computation, you will need to choose Δt as described in the section on numerical stability. Begin by choosing a very small number, for example 100 times smaller than the limit. Propagate the wave function a few timesteps, and plot the results. See if you can increase Δt somewhat, as that will make the computations go faster. Describe what happens if you increase Δt too much. For the rest of the problems, choose a value for Δt which is somewhat smaller than the largest value you found to work.

Note that the computations required for this problem should take no more than a few seconds of computer time.

Problem 3

Introduce a barrier of width $l = L/50$ and height $V_0 = \frac{E}{2}$ in the middle of the domain by setting $V(x)$ to

$$V(x) = \begin{cases} \frac{1}{2}E & \text{if} \quad \frac{L}{2} - \frac{l}{2} < x < \frac{L}{2} + \frac{l}{2} \\ 0 & \text{otherwise} \end{cases} \tag{15}$$

Propagate a wave packet across the barrier. You can use the same T that you found in Problem 2. Produce a plot which shows that the wave function has been partially transmitted, partially reflected. Calculate the probability of reflection

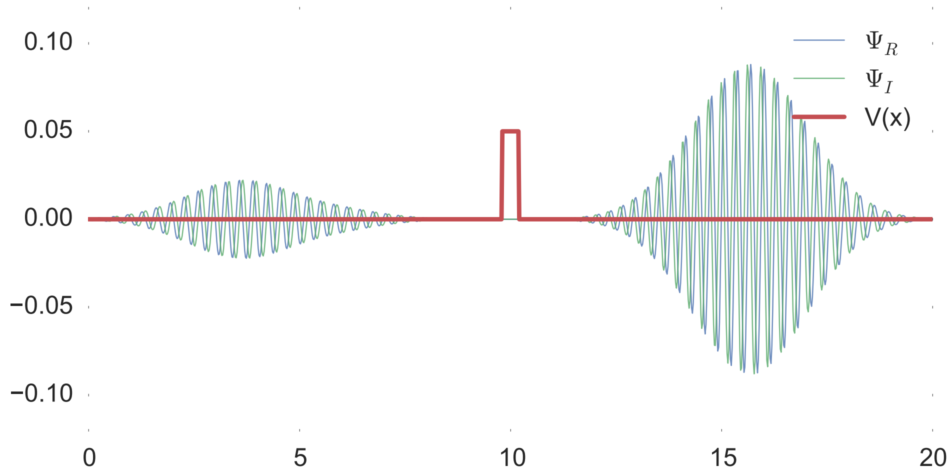

Figure 2: Wave packet has been partially transmitted, partially reflected, and has completely cleared the barrier. Note that the wave function and the potential are not measured in the same units, and the potential is included simply for visualisation, with the height of the barrier scaled to fit the graph.

and transmission by calculating

$$\int_0^{L/2} |\Psi(x,t)|^2 \mathrm{d}x \quad \text{and} \quad \int_{L/2}^{L} |\Psi(x,t)|^2 \mathrm{d}x. \tag{16}$$

You should confirm that T is large enough that the wave packet has completely cleared the barrier, i.e, your plot should look similar to Figure 2.

Problem 4

Using the same procedure as in Problem 3, calculate the probabilities of transmission an reflection for 50 different barrier heights V_0 from $0E$ to $\frac{3}{2}E$. Make a graph showing the probabilities of reflection and transmission as a function of E/V_0.

Problem 5

Using a barrier height of $\frac{9}{10}E$, calculate the probabilities of transmission and reflection for 50 different barrier widths from 0 to $L/20$. Make a graph showing the probabilities of reflection and transmission as a function of barrier width. Note that you will have to use $N_x = 1000$ or larger to be able to resolve all the different barrier thicknesses.

Bonus problem

Implement periodic boundary conditions, i.e., $\Psi(x = 0, t) = \Psi(x = L, t)$, and produce a figure with three subplots, showing three snapshots of the wave packet as it propagates to the right past $x = L$, reappearing at $x = 0$.

Bonus problem

Investigate scattering of a wave packet by an arbitrarily shaped potential. You could for example use the triangular potential described in the section about Field emission (Section 7.3.g) in Lecture notes 7.2, and vary the slope of the potential outside the metal.

THE END