4th year "Theoretical lab"
Wave packet propagation using the split-operator method

Your task is to write a Matlab program that calculates the time evolution of a one-dimensional quantum state (wave function) according to the Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}\psi(x,t) = H\psi(x,t) = \left[\frac{\hbar k^2}{2m} + V(x)\right]\psi(x,t) = \left[-\frac{\hbar}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right]\psi(x,t), \quad (1)$$

where $\psi(x,t)$ is the wave function and $V(x)$ is a position-dependent potential. The method to use is the split operator method. The wave packet is evolved a small step dt forward in time using

$$\begin{aligned}\psi(x,t+dt) &= \exp(-iHdt/\hbar)\psi(x,t) = \exp\left[-i\frac{\hbar^2k^2}{2m}\frac{dt}{\hbar} - iV(x)\frac{dt}{\hbar}\right]\psi(x,t) \\ &\approx \exp\left[-i\frac{\hbar^2k^2}{2m}\frac{dt}{\hbar}\right]\exp\left[-iV(x)\frac{dt}{\hbar}\right]\psi(x,t). \quad (2)\end{aligned}$$

The error made when approximating $\exp(A+B)$ with $\exp(A)\exp(B)$, when A and B are operators, is of the order $[A,B]$. Here $[A,B] = AB - BA$ is the commutator of A and B. At each step dt, the error is therefore of the order $dt^2/(2m)\left[\frac{\partial^2}{\partial x^2}, V(x)\right]$, since $\hbar k = p = -i\hbar\partial/\partial x$. This is small if dt is sufficiently small.

The time evolution operator acting on $\psi(x,t)$ in (2) is efficiently calculated using the Fast Fourier Transform. The action of the exponential factor with $V(x)$ in can easily be calculated with the wave function in x-space, and the action of the exponential involving k can be easily calculated when the wave function has been transformed to the k-space. After this, one transforms the wave function back to x-space, ready to make the next time step:

$$\psi(x,t+dt) = F^{-1}\left\{\exp\left(-i\frac{\hbar^2k^2}{2m}\frac{dt}{\hbar}\right)F\left[\exp\left(-iV(x)\frac{dt}{\hbar}\right)\psi(x,t)\right]\right\}. \quad (3)$$

This can also be scaled to dimensionless $\tilde{x} = x/r$, $\tilde{t} = t/\tau$, $\widetilde{m} = m/\mu$ and $\widetilde{dt} = dt/\tau$ (using the chain rule for derivatives and where r, $\tau$and μ are parameters determining the "unit" of length, time and mass) so that time evolution step is

$$\psi(\tilde{x},\tilde{t}+\widetilde{dt}) = F^{-1}\left\{\exp\left(-ik^2\widetilde{dt}\right)F\left[\exp\left(-iV(\tilde{x})\widetilde{dt}\right)\psi(\tilde{x},\tilde{t})\right]\right\}. \quad (4)$$

It is a valuable exercise to calculate how this rescaling works.
If your Matlab program is written in terms of"real" values for $\hbar$, mass m etc., this scaling can effectively be done by setting $\hbar = 1$ and $2m = 1$.

Some initial questions to answer with the help of your program

If you finish these really quickly, there is lot of nice things to investigate with a working program. For example, different potential heights and shapes, such as a double barrier or a harmonic oscillator potential, or different initial wave packet shapes and velocites.

Question 1

Define a potential barrier $V(x)$ as

$$V(x) = 5\exp(-10x^2),$$

and an initial state

$$\psi(x, t = 0) = N\exp[-0.1(x + 5)^2]\exp(ik_{init}x),$$

with $k_{init} = 2.5$.

a) What do $V(x)$ and the initial probability distribution $|\psi(x, t)|^2$ look like? In particular, where is the initial wave packet located with respect to the potential barrier? Plot or sketch the functions either with or without the help of Matlab. N is a normalisation factor and its value is not important at this stage.

b) Evolve the wave packet in time using your program. What happens? Plot the wave packet as a function of time and explain. A good length of the total region in x-space is $x \in [-15, 15]$. Suitable values are also $dt = 0.001$ and $dx = 30/256$ (256 grid points in x-space). Running the simulation from $t = 0$ to a maximum time of $t = 2.5$ will be suitable, but you will also need to check what is happening in between in some way or another. If your program calculates a matrix, let's call it M, containing values of $|\psi(x)|^2$ for different times, then a nice plotting command to use is pcolor(M), shading interp.
If your program has parameters $\hbar$ and m in it, please use $\hbar = 1$ and $m = 0.5$, so that the algorithm becomes as in (4) on the previous page. The value of N still does not matter too much at this stage.

c) Modify your program so that it also calculates T and R, the transmission and reflection coefficients of the barrier. For this purpose, T and R can be defined as

$$T = \int_0^\infty |\psi(x)|^2 dx, \quad R = \int_{-\infty}^0 |\psi(x)|^2 dx \tag{5}$$

at the end of the calculation. For this to work, the normalisation N of the wave packet has to be correct, so that $\int_{-\infty}^{\infty} |\psi(x)|^2 dx = 1$, otherwise $T+R = 1$ won't hold. What are the numerical values for T and R for the given initial state, potential and parameters given above?

Question 2

Why does multiplying a wave function $\psi(x,t)$ with a factor of $\exp(ik_{init}x)$, where k_{init} is a constant, give it a momentum kick? In other words, the mean k of the wave function will be shifted with k_{init}. Why?
Hint: the Fourier transform of a wave function, defined as

$$\psi(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx \; \psi(x) e^{-ikx}$$

tells us what k values are most likely in the wave function. You can either give an analytical argument, or support your answer with Matlab calculations.

Question 3

You are about to submit the results of your groundbreaking numerical simulations for publication in a prestigious journal. How can you be sure that your results are correct? In other words, how do you make sure that the small error made at each time step in the calculation, and the errors made because you have also discretised x-space, do not add up so that the final result is not what it really should have been? There are at least two good answers to this question!

Question 4

Why are there fringes in the reflected part of the wave packet in question 1, when the wave packet is close to the barrier, but no fringes in the transmitted part?