Assignment 12 —- The Schrödinger equation

1 Purpose: Quantum tunneling

The Schrödinger equation is one of the fundamental equations of quantum mechanics and, in its time-dependent form, describes the evolution of wave functions. In quantum mechanics, wave functions $\psi(x,t)$ are complex functions whose norms $|\psi(x,t)|^2$ describe the probability of finding particles in specific locations x at specific times t.

In this assignment, your goal is to write a program that solves the Schrödinger equation with finite-differences and the Crank-Nicolson method. In particular, you should find the numerical solution to the (1-D / time-dependent) Schrödinger equation with some local potential

$$i\hbar\frac{\partial}{\partial t}\psi(x,t) = \hat{H}\psi(x,t) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x,t) + V(x)\psi(x,t) \tag{1}$$

For this assignment we are going to work in 'natural units', effectively rescaling t and x such that $\hbar = 1$ and $m = \frac{1}{2}$. This reduces the above equation to the following problem:

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

Note that the wave function $\psi(x,t)$ of a particle is a complex function, while e.g. x and t are real numbers, so you will have to pay close attention in your program which data type you use for which variable.

Problem 1

Show that the Crank-Nicolson scheme applied to equation 2 leads to the following equation:

$$\left(2 + i\Delta t V(x) + \frac{2i\Delta t}{\Delta x^2}\right)\psi_j^{n+1} - \frac{i\Delta t}{\Delta x^2}\left(\psi_{j-1}^{n+1} + \psi_{j+1}^{n+1}\right) = \left(2 - i\Delta t V(x) - \frac{2i\Delta t}{\Delta x^2}\right)\psi_j^{n} + \frac{i\Delta t}{\Delta x^2}\left(\psi_{j-1}^{n} + \psi_{j+1}^{n}\right) \tag{3}$$

In order to derive eq. 3, follow the same steps as done in the lecture, i.e. first derive the equation for the explicit FTCS scheme and then add the corresponding equation for an implicit FTCS scheme. When done bring all unknown future values (ψ^{n+1}) to the left-hand side and all known values (ψ^n) to the right hand side. Like for assignment 11, create a PDF file showing your derivation and name this file `as12-problem1-surname-studentid.pdf`. You can again either use Word/TeX to create the PDF file or write the derivation down by hand and scan what you wrote.

Problem 2 - The unperturbed case

Your first goal is to write a program that simulates a particle in a harmonic potential $V(x) = x^2$. The eigensolutions to this equation are well known and are given by

$$\psi_k(x) = \frac{1}{\sqrt{2^k k! \sqrt{\pi}}}\exp\left[-\frac{x^2}{2}\right]H_k(x) \tag{4}$$

where k denotes the oscillator energy level and $H_k(z)$ are the Hermite polynomials. The corresponding energy levels are given by $E_k = k + \frac{1}{2}$. The first few Hermite polynomials are given by

$$\begin{aligned} H_0(x) &= 1 \\ H_1(x) &= 2x \\ H_2(x) &= 4x^2 - 2 \\ H_3(x) &= 8x^3 - 12x \\ &\dots \end{aligned} \tag{5}$$

This gives you an opportunity to check if your code is working. Implement the Crank-Nicolson scheme in a program. An updated version of the `tridiag` function which can deal with complex numbers can be found on Blackboard. Choose as limits of the integration interval $x_0 = -20$ and $x_e = 20$ and integrate the evolution up to $t_{fin} = 10$. Choose 2000 grid points in the x direction and choose a timestep of $\Delta t = 0.0025$ and an output time step of $\Delta t_{out} = 0.05$. You can assume that $\psi_0^n = \psi_J^n = 0$ as boundary conditions. Choose one of the above eigensolutions as the intial condition of your program. These solutions are constant in time, so if your code works correctly the wave function should also be constant in your simulation. In order to test if the wave function is constant in your program, output at each output time the following quantities to the screen:

- column 1: The current time t_n.
- column 2: The Norm of the solution at current time via numerical integration

$$\text{Norm}(t_n) = \int_{-\infty}^{\infty} \psi^*(x,t_n)\psi(x,t_n)\,dx \approx \sum_{j=1}^{N_x} \Delta x\, |\psi(x_j,t_n)|^2$$

- column 3: the average location of the function at current time via numerical integration!

$$\langle x\rangle(t_n) = \int_{-\infty}^{\infty} \psi^*(x,t_n)x\,\psi(x,t_n)\,dx \approx \sum_{j=1}^{N_x} \Delta x\, x_j\, |\psi(x_j,t_n)|^2$$

- column 5: the square-root of the variance of the distribution at current time via numerical integration!

$$\sigma(t_n) = \sqrt{\langle x^2\rangle(t_n) - (\langle x\rangle(t_n))^2} \quad \text{where} \quad \langle x^2\rangle(t_n) \approx \sum_{j=1}^{N_x} \Delta x\, x_j^2\, |\psi(x_j,t_n)|^2$$

Note: since the Crank-Nicolson method is unitary this means that the Norm is conserved for each iteration (to machine precision). This is again an excellent validation of your code!

Problem 3: Quantum tunneling

Now, for the real problem, you need to propagate through a central barrier. Modify your program such that the potential contains a potential barrier given by $V(x) = B_0 \cdot exp(-16x^2)$ in addition to the harmonic potential. The starting condition of your program should be the ground state wave function of the previous problem but now shifted in x such that it is centered around $x = 4$ instead of $x = 0$. Your program should ask the user for the following parameters:

- The height B_0 of the potential barrier
- The two points x_0 and x_e of the grid boundary
- The number J of spatial grid points
- The time step Δt.
- The output time step Δt_{out}.
- The final time t_{fin} for the integration

At each output time, the program should print the same information as the program for problem 2 to the screen. It should also determine with which probability the particle can be found on the left ($x < 0$) side of the barrier and print it to the screen. At the end it should write x_j and $|\psi(x_j, t_{fin})|^2$ for all j into a file. Send us this program as `as12-problem3-surname-studentid.c`.

Problem 4: Simulating tunneling

Run your program with the same input as the program for problem 2. Use as barrier potential $B_0 = 50, 100, 150$ and plot the resulting $|\psi(x, t_f)|^2$ at $t = t_{fin}$ in a postscript file called `as12-problem4-surname-studentid.ps`.

Problem 5: Visualizing the tunneling effect

Send us an animation of the quantum tunneling for the ground-state wave function for $B_0 = 50$. Your movie should show how $|\psi(x)|^2$ evolves as a function of time t. To produce the animation you can use the scripts that I've provided for last week's worksheet problem together with `gnuplot`, or do it your own way! Submit your animation to the server by giving it the name `as12-problem5-surname-studentid.gif`. Make sure that it is no larger than 5MB in size.

Submission

The full set of files you will have when you are done should be:

- `as12-problem1-surname-studentid.pdf`
- `as12-problem3-surname-studentid.c`
- `as12-problem4-surname-studentid.ps`
- `as12-problem5-surname-studentid.gif`

As always, to submit your assignment, mount your directory on the submission server, create a subdirectory called `as12` under your student ID, eg. `s1234567/as12/` and copy your files into this subdirectory. You must submit your files into this subdirectory. Be sure to follow the above submission instructions, otherwise you make the marking of the assignments unnecessary complicated for us.

PHYS3071/7073 - Due Friday, 6th of June, 2014 by 11am

Grading Sheet – Assignment 12 —- Schrödinger function

A: /20% **Theory**: Was a derivation of eq. 3 submitted with the solution and is this derivation correct?

B: /30% **Function**: Does the program run and produce the correct output?

C: /10% **Usability**: Is the program easy to use? Are the input requirements and output formatting easy to understand?

D: /10% **Readability**: Is the program easy to read and comprehend? Is it well-commented? If the code is sufficiently complex, has it been broken up into manageable subroutines, each of which is well-documented?

E: /10% **Efficiency**: Does the program run efficiently? Is the coding clunky or unnecessarily complicated?

F: /10% **Presentation (Plots)**: Does the plot clearly convey the results? Does it have an appropriate title? Are the axes and the plot items clearly labeled?

G: /10% **Movie**: Was a movie produced that shows the evolution of the wave function for the specified case ?

Total Points: $\boxed{\quad\quad /100}$