Modern Comp Coursework Part 2

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The problem

Use the finite difference method to calculate values for the TDSE. (Using Python.)
I have the time dependent Schrodinger equation

$$i\frac{\partial\psi_j^n}{\partial t} = -\frac{1}{2}\frac{\partial^2\psi_j^n}{\partial x^2} + \frac{1}{2}x^2\psi_j^n \qquad (eq. 1.1)$$

This can be written in the form

$$i\frac{\partial\psi_j^n}{\partial t} = \hat{H}\psi_j^n \qquad (eq. 1.2)$$

with

$$\hat{H} = -\frac{1}{2}\frac{\partial^2}{\partial x^2} + \frac{1}{2}x^2 \qquad (eq. 1.3)$$

Part A

Step 1 (Normalising the wavefunction.)

I will first derive the finite difference equation(s) to be used in my Python programme that allow for the calculation of the next set of values in a time step. I first set the notation I will use such that it is consistent throughout this document.

I have been given the boundary condition for $\psi(x, t = 0)$.

$$\psi(x, t = 0) = Ne^{-(x-1)^2} \qquad (eq. 2.0)$$

I can calculate N from the normalisation of ψ. This is achieved by integrating the square of

$$\int_{-\infty}^{\infty} |\psi|^2 dx = 1$$

$$N^2 \int_{-\infty}^{\infty} \left|e^{-(x-1)^2}\right|^2 dx = 1$$

$$\therefore N = \sqrt{\frac{1}{\int_{-\infty}^{\infty}\left|e^{-(x-1)^2}\right|^2}} \qquad (eq. 3.0)$$

The programme automatically calculates the normalised function for $\psi(x, t = 0)$. A different wavefunction to the one stated in eq. 2.0 can be used at any time by altering the programme at the function named nopsi_sq.

Step 2 (Finding the finite difference equations to be used in the programme.)

I have $\psi(x, t)$ which I will write as ψ_j^n such that j and n represent the x and t components respectively. If I am to talk about the next step in t (that is to say $t + dt$) it would take the form ψ_j^{n+1} and similarly for $x + dx$, ψ_{j+1}^n. (dt and dx are the time and x step intervals respectively.)

I know from lectures that the general form of discretisation of the first and second differential equations are;

$$\frac{\partial u(x,t)}{\partial t} = \frac{u(x,t+1) - u(x,t)}{\Delta t}$$

and

$$\frac{\partial^2 u(x,t)}{\partial x^2} = \frac{u(x+1,t) - 2u(x,t) + u(x-1,t)}{\Delta x^2}$$

I can infer then that the components of the TDSE equation, $\frac{\partial \psi_j^n}{\partial t}$ and $\frac{\partial^2 \psi_j^n}{\partial x^2}$, can be written as follows;

$$\frac{\partial \psi_j^n}{\partial t} = \frac{\psi_j^{n+1} - \psi_j^n}{\Delta t} \qquad (eq. 4.1)$$

and

$$\frac{\partial^2 \psi_j^n}{\partial x^2} = \frac{\psi_{j+1}^n - 2\psi_j^n + \psi_{j-1}^n}{\Delta x^2} \qquad (eq. 4.2)$$

Putting $eq. 4.1$ and $eq. 4.2$ into $eq. 1.0$ we get the discretised version of the TDSE as

$$i\frac{\psi_j^{n+1} - \psi_j^n}{\Delta t} = -\frac{1}{2}\frac{\psi_{j+1}^n - 2\psi_j^n + \psi_{j-1}^n}{\Delta x^2} + \frac{1}{2}x^2\psi_j^n \qquad (eq. 5.0)$$

We have the tools now to find ψ_j^{n+1} as we have calculated in **step 1** the value of $\psi_j^{n=0}$. It will just take some working to allow this to be usable in Python.

$eq. 5$ can be written in Hermitian form as

$$i\left(\frac{\psi^{n+1} - \psi^n}{\Delta t}\right) = \hat{H}\psi^n \qquad (eq. 6.0)$$

Evaluating $eq. 6.0$ with the right-hand side (RHS) being the previous time step, ψ^n, we come to an unusable solution. The same is true for evaluating $eq. 6.0$ with the RHS being the next time step, ψ^{n+1} (Robertson, 2011). A way to approach this will be to take the average time step on the RHS. This gives rise to the equation

$$i\left(\frac{\psi_j^{n+1} * \psi_j^n}{\Delta t}\right) = \frac{1}{2}\left(\hat{H}\psi_j^{n+1} + \hat{H}\psi_j^n\right) \qquad (eq. 6.1)$$

This leads to the equation for solving for the next time step

$$\psi_j^{n+1} = \left(\frac{1}{1 + \frac{i\Delta t}{2}\hat{H}}\right)\left(1 - \frac{i\Delta t}{2}\hat{H}\right)\psi_j^n \qquad (eq. 6.2)$$

Rearranging this and substituting in $eq. 1.2$ and $eq. 1.3$ we arrive at

$$\psi_{j+1}^{n+1} + \psi_{j-1}^{n+1} + A_j\psi_j^{n+1} = B_j \qquad (eq. 6.3)$$

with the values of A_j and B_j evaluated as

$$A_j = -2 + \frac{4i\Delta x^2}{\Delta t} - (\Delta x^2 \cdot x^2) \qquad (eq. 6.4)$$

$$B_j = -\psi_{j+1}^n - \psi_{j-1}^n + \psi_j^n\left(2 + \frac{4i\Delta x^2}{\Delta t} + (\Delta x^2 \cdot x^2)\right) \qquad (eq. 6.5)$$

$eq. 6.3$ can be written in matrix form as is shown below;

$$\begin{pmatrix} A_1 & 1 & 0 & 0 & \cdots \\ 1 & A_2 & 1 & 0 & \cdots \\ 0 & 1 & A_3 & 1 & \cdots \\ 0 & 0 & 1 & \ddots & \cdots \\ \vdots & \vdots & \vdots & \vdots & A_j \end{pmatrix} \begin{pmatrix} \psi_1^{n+1} \\ \psi_2^{n+1} \\ \psi_3^{n+1} \\ \vdots \\ \psi_j^{n+1} \end{pmatrix} = \begin{pmatrix} B_1^n \\ B_2^n \\ B_3^n \\ \vdots \\ B_j^n \end{pmatrix} \qquad (eq. 6.7)$$

This takes the form of the B_j matrix being the current time step, the ψ_j^{n+1} matrix being the next time step and the A_j matrix being the operator. To calculate the array of wavefunction values for the next time step, ψ_j^{n+1}, one can multiply the current time step, B_j, by the reciprocal of the A_j matrix.

$$\begin{pmatrix} \psi_1^{n+1} \\ \psi_2^{n+1} \\ \psi_3^{n+1} \\ \vdots \\ \psi_j^{n+1} \end{pmatrix} = \begin{pmatrix} A_1 & 1 & 0 & 0 & \cdots \\ 1 & A_2 & 1 & 0 & \cdots \\ 0 & 1 & A_3 & 1 & \cdots \\ 0 & 0 & 1 & \ddots & \cdots \\ \vdots & \vdots & \vdots & \vdots & A_j \end{pmatrix}^{-1} \begin{pmatrix} B_1^n \\ B_2^n \\ B_3^n \\ \vdots \\ B_j^n \end{pmatrix} \qquad (eq. 6.8)$$

Using the following set of equations, we can simplify the above equation into a new matrix.

$$U_i = \frac{1}{A_i - U_{i-1}} \qquad (eq. 7.1)$$

$$R_i = (B_i - R_{i-1})U_i \qquad (eq. 7.2)$$

$$\begin{pmatrix} 1 & U_1 & 0 & 0 & \cdots \\ 0 & 1 & U_2 & 0 & \cdots \\ 0 & 0 & 1 & U_3 & \cdots \\ 0 & 0 & 0 & \ddots & \cdots \\ \vdots & \vdots & \vdots & \vdots & 1 \end{pmatrix} \begin{pmatrix} \psi_1^{n+1} \\ \psi_2^{n+1} \\ \psi_3^{n+1} \\ \vdots \\ \psi_j^{n+1} \end{pmatrix} = \begin{pmatrix} R_1 \\ R_2 \\ R_3 \\ \vdots \\ R_j \end{pmatrix} \qquad (eq. 7.3)$$

Solving $eq. 6.7$ in reverse order using our new equations we can get

$$\psi_J^{n+1} = R_J \qquad (eq. 7.4)$$

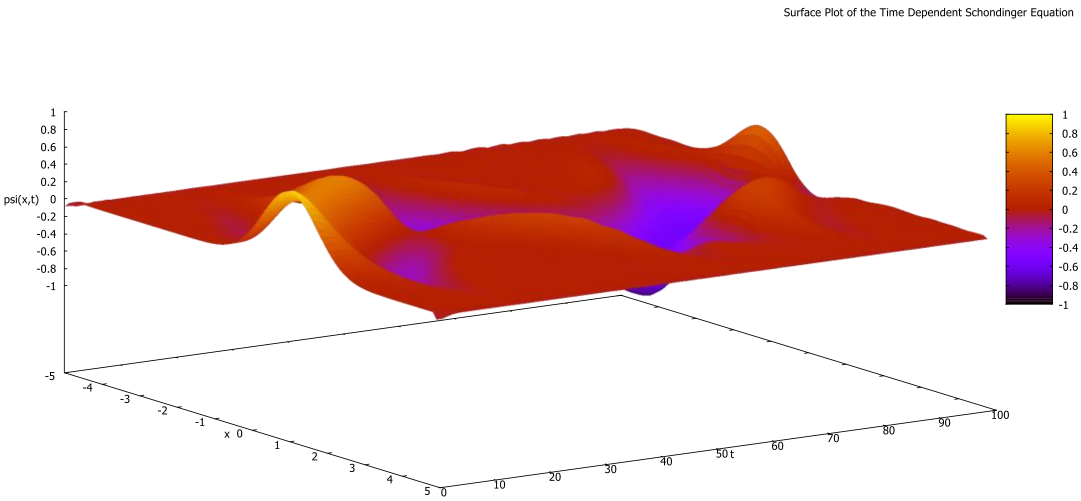
The next value backwards, $J - 1$, we get

$$\psi_{J-1}^{n+1} = R_{J-1} - U_{J-1}\psi_J^{n+1} \qquad (eq. 7.5)$$

When simplified to make the expression more general it reads

$$\psi_i^{n+1} = R_i - U_i\psi_{i+1}^{n+1} \qquad (eq. 7.6)$$

And thus, we arrive at the equation we will be utilising in the programme to calculate the wavefunction at a future time step.

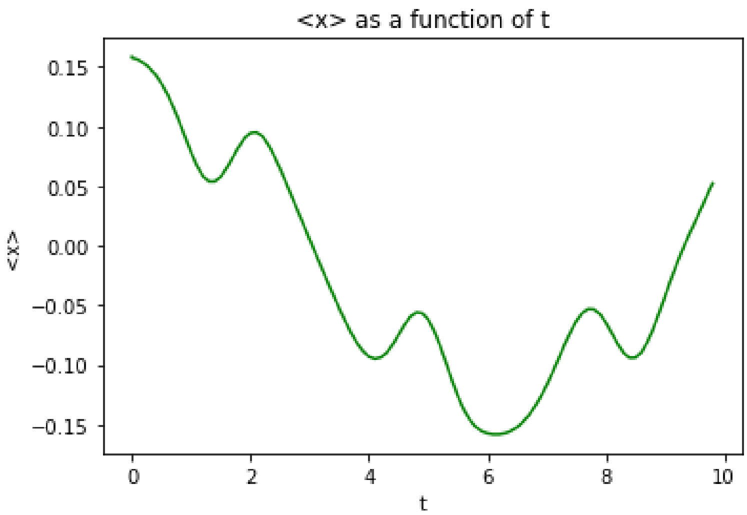


Surface plot of the TDSE. Generated using a GNUplot command with data from the Python programme.

An example of the data file and plot file have been included in the submission folder. The data file output by the Python programme needs to be altered such that there is a space between data sets at each time step. This image was generated using data produced by the Python programme. It is included just in case the marker cannot use GNUplot.

Part B

The expectation of x, $< x >$, at time t is required to be calculated and plotted. The expectation can be characterised as the average $x - value$ over a range, at time t. Therefore, instead of using the integration method as outlined in the assignment brief, I will take the average of the $x - values$ at each time step, t. I found this method to be equal to the integrating method (which takes the form of the trapezium rule in my programme). I have included the trapezium method – commented out – for comparison if desired.



Plot of the <x> as a function of t generated by the Python programme.

This is a plot of the expectation value of x at each time step, t. I have included it for completeness. It was generated by the Python programme.

Final Notes

I have submitted this document, the image files of the plots above, an example of the output data file, the GNUplot command file and the Python programme. The programme has been submitted as a python file (.py) and as a text file (.txt) so that it can be read by the marker regardless of what method of compiling, they prefer. I wrote the programme using Spyder (Python 3.8).

Works Cited

Robertson, D. G. (2011, October 10). Solving the Time-Dependent Schrodinger Equation. Westerville: Department of Physics, Otterbein University.