Question 1

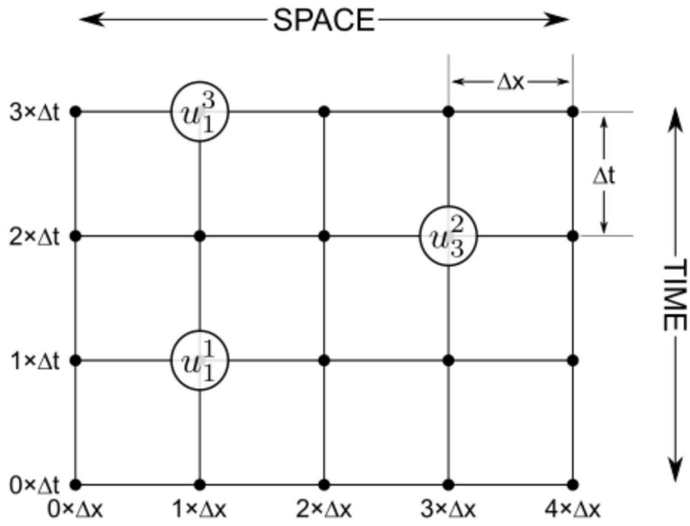

Figure 1: Visualisation of the FTCS scheme.

Using the notation $u_j^n = u(t_n, x_j)$ for $x_j = x_0 + j\Delta x$, $j = 0, 1, 2..., J$ and $t_n = t_0 + n\Delta t$, $n = 0, 1, 2, ...N$ to approximate the PDE $\frac{\partial u}{\partial t} = -D\frac{\partial u}{\partial x}$. Starting with the approximations:

$$\left.\frac{\partial u}{\partial t}\right|_{j,n} \approx \frac{u_j^{n+1} - u_j^n}{\Delta t}$$

$$\left.\frac{\partial u}{\partial x}\right|_{j,n} \approx \frac{u_{j+1}^n - u_{j-1}^n}{2\Delta x}$$

we rearrange our PDE, $i\frac{\partial \psi}{\partial t} = -\frac{\partial^2 \psi}{\partial x^2} + V\psi$ to the form $\frac{\partial \psi}{\partial t} = i\frac{\partial^2 \psi}{\partial x^2} - iV\psi$

We can now construct a discrete version of our PDE using the above listed approximations. So our equation becomes

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

By rearranging the equation so that all ψ^{n+1} are on one side of the equation and all ψ^n are on the other side, and expanding the brackets, this becomes.

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

and now bringing out common factors

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

Now to use the Crank-Nicolson Scheme we add this to

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

After adding, and once again grouping the ψ^{n+1} terms on one side and the ψ^n terms to the other, we get:

$$2\psi_j^{n+1} + i\Delta t\psi_j^{n+1} - \frac{i\Delta t}{(\Delta x)^2}\big(\psi_{j+1}^{n+1} - 2\psi_j^{n+1} + \psi_{j-1}^{n+1}\big) = \frac{i\Delta t}{(\Delta x)^2}\big(\psi_{j-1}^{n} + \psi_{n+1}^{n}\big) + \big(2 - i\Delta tV - \frac{2i\Delta t}{(\Delta x)^2}\big)\psi_j^n$$

Which simplifies to:

$$\big(2 + i\Delta tV(x_j) + \frac{2i\Delta t}{(\Delta x)^2}\big)\psi_j^{n+1} - \frac{i\Delta t}{(\Delta x)^2}\big(\psi_{j-1}^{n+1} + \psi_{j+1}^{n+1}\big) =$$
$$\big(2 - i\Delta tV(x_j) - \frac{2i\Delta t}{(\Delta x)^2}\big)\psi_j^{n} + \frac{i\Delta t}{(\Delta x)^2}\big(\psi_{j-1}^{n} + \psi_{j+1}^{n}\big)$$

Where I have also use the discrete positions to the external potential, $V(x)$.

This can be converted to a system of linear equations:

$$\begin{bmatrix} (2 + i\Delta tV(x_j) + \frac{2i\Delta t}{(\Delta x)^2}) & -\frac{i\Delta t}{(\Delta x)^2} & 0 & \cdots & 0 \\ [0.5em] -\frac{i\Delta t}{(\Delta x)^2} & (2 + i\Delta tV(x_j) + \frac{2i\Delta t}{(\Delta x)^2}) & -\frac{i\Delta t}{(\Delta x)^2} & \cdots & 0 \\ 0 & -\frac{i\Delta t}{(\Delta x)^2} & \ddots & \vdots & \vdots \\ \vdots & \vdots & \cdots & \ddots & -\frac{i\Delta t}{(\Delta x)^2} \\ 0 & 0 & -\frac{i\Delta t}{(\Delta x)^2} & (2 + i\Delta tV(x_j) + \frac{2i\Delta t}{(\Delta x)^2}) & \end{bmatrix}$$

$$\begin{bmatrix} \psi_1^{n+1} \\ \psi_2^{n+1} \\ \vdots \\ \psi_{J-2}^{n+1} \\ \psi_{J-1}^{n+1} \end{bmatrix} = \begin{bmatrix} (2 - i\Delta tV(x_1) - \frac{2i\Delta t}{(\Delta x)^2})\psi_1^n + \frac{i\Delta t}{(\Delta t)^2}(\psi_0^n + \psi_2^n) + \frac{i\Delta t}{(\Delta x)^2}\psi_0^{n+1} \\ (2 - i\Delta tV(x_2) - \frac{2i\Delta t}{(\Delta x)^2})\psi_2^n + \frac{i\Delta t}{(\Delta t)^2}(\psi_1^n + \psi_3^n) \\ \vdots \\ (2 - i\Delta tV(x_{J-2}) - \frac{2i\Delta t}{(\Delta x)^2})\psi_{J-2}^n + \frac{i\Delta t}{(\Delta t)^2}(\psi_{J-3}^n + \psi_{J-4}^n) \\ (2 - i\Delta tV(x_{J-1}) - \frac{2i\Delta t}{(\Delta x)^2})\psi_{J-1}^n + \frac{i\Delta t}{(\Delta t)^2}(\psi_{J-2}^n + \psi_J^n) + \frac{i\Delta t}{(\Delta x)^2}\psi_J^{n+1} \end{bmatrix}$$

There the final part of the first and last row are zero so cancel off leaving the RHS ψ_j^{n+1} completely dependant on the LHS ψ_j^n for eveny time step.

Because this is of the form $\mathbf{A}\underline{x} = \underline{b}$ we can solve the equivalent statement $\underline{x} = \mathbf{A}^{-1}\underline{b}$.

We use the function *complex_tridiag.c* to solve this.