Crank Nicolson method

Rosa Flaquer Galmés

To start the resoluiton of the problem we compute the time evolution for $g = 0$ and $V_{ext} = 0$ then the equation reads as:

$$i\frac{\partial\Psi(\tilde{z},\tilde{t})}{\partial\tilde{t}} = -\frac{\partial^2\Psi(\tilde{z},\tilde{t})}{\partial\tilde{z}^2} \tag{1}$$

We will use the Crank Nicolson method which we will derive for this particular case. We start writing the time partial derivative as:

$$\begin{aligned}
\frac{\partial\Psi(\tilde{z},\tilde{t})}{\partial\tilde{t}} =& \frac{\Psi(\tilde{z},\tilde{t}+\frac{\Delta\tilde{t}}{2}) - \Psi(\tilde{z},\tilde{t})}{\frac{\Delta\tilde{t}}{2}} = i\frac{\partial^2\Psi(\tilde{z},\tilde{t})}{\partial\tilde{z}^2} \quad \Rightarrow \\
\Psi(\tilde{z},\tilde{t}+\frac{\Delta\tilde{t}}{2}) =& (1 + i\frac{\Delta\tilde{t}}{2}\frac{\partial^2}{\partial\tilde{z}^2})\Psi(\tilde{z},\tilde{t}) \\
\Psi(\tilde{z},\tilde{t}+\frac{\Delta\tilde{t}}{2}) =& (1 - i\frac{\Delta\tilde{t}}{2}\frac{\partial^2}{\partial\tilde{z}^2})\Psi(\tilde{z},\tilde{t}+\Delta\tilde{t})
\end{aligned} \tag{2}$$

from where we find:

$$(1 + i\frac{\Delta\tilde{t}}{2}\frac{\partial^2}{\partial\tilde{z}^2})\Psi(\tilde{z},\tilde{t}) = (1 - i\frac{\Delta\tilde{t}}{2}\frac{\partial^2}{\partial\tilde{z}^2})\Psi(\tilde{z},\tilde{t}+\Delta\tilde{t}) \tag{3}$$

We then use a three point formula for the spatial derivative and change the notation to $\Psi(\tilde{z},\tilde{t}) \equiv \Psi_i^t$ so that $\Psi(\tilde{z}+\Delta\tilde{z},\tilde{t}) = \Psi_{i+1}^t$ and $\Psi(\tilde{z},\tilde{t}+\Delta\tilde{t}) = \Psi_i^{t+1}$

$$\Psi_i^t + i\frac{\delta\tilde{t}}{(\Delta\tilde{z})^2}[\Psi_{i+1}^t - 2\Psi_i^t + \Psi_{i-1}^t] = \Psi_i^{t+1} - i\frac{\delta\tilde{t}}{(\Delta\tilde{z})^2}[\Psi_{i+1}^{t+1} - 2\Psi_i^{t+1} + \Psi_{i-1}^{t+1}] \tag{4}$$

Defining $r \equiv i\frac{\delta\tilde{t}}{(\Delta\tilde{z})^2}$ it takes the form of

$$2(1+r)\Psi_i^{t+1} - r\Psi_{i+1}^{t+1} - r\Psi_{i-1}^{t+1} = 2(1-r)\Psi_i^t + r\Psi_{i+1}^t + r\Psi_{i-1}^t \tag{5}$$

Which turns to be a matrix equation if we define a vector u^t that contains all Ψ_i^t values at a given time

$$Au^{t+1} = Bu^t \tag{6}$$

A is a tridiagonal matrix with $2(1+r)$ in its main diagonal and $-r$ on the upper and lower diagonals, all the other elements are 0. B is also a tridiagonal matrix with $2(1-r)$ in its main diagonal and r on the upper and lower diagonals, all the other elements are 0.

There are various ways to check if the method is working properly: conservation of the norm and conservation of the energy. The easiest is the first one. First of all we ensure that our $\Psi(\tilde{z},\tilde{t})$ is well normalizet to 1 using any integration method, for instance Simpson:

$$1 = \|N\|^2\int_a^b \Psi^*(\tilde{z},\tilde{t})\Psi(\tilde{z},\tilde{t})d\tilde{z} \approx \|N\|^2\frac{d\tilde{z}}{3}\sum_{k=0}^{M/2-1}(u_{2k}^t + 4u_{2k+1}^t + u_{2k+2}^t) \tag{7}$$

Where M is the number of points where the function is avaluated. Once we have the wave-function propperly normalized we can check at every step of the Crank-Nicolson method if it is conserved by computing the norm of u^{t+1} and storing the maximum difference between the norm at $\tilde{t} = 0$ and the evolved function.

To compute the expextation value of the energy:

$$\langle E \rangle = \int_{-\infty}^{\infty} \Psi^*(\tilde{z}, \tilde{t}) \hat{H} \Psi(\tilde{z}, \tilde{t}) d\tilde{z} = \int_{-\infty}^{\infty} \Psi^*(\tilde{z}, \tilde{t}) \big(-\frac{\partial^2}{\partial \tilde{z}^2}\big) \Psi(\tilde{z}, \tilde{t}) d\tilde{z} = \int_{-\infty}^{\infty} \Psi^*(\tilde{z}, \tilde{t}) \big(i \frac{\partial \Psi(\tilde{z}, \tilde{t})}{\partial \tilde{t}}\big) d\tilde{z} \quad (8)$$

It is useful to write $(\hat{H})$ like this (using equation 1) because we can then write $\frac{\partial \Psi(\tilde{z}, \tilde{t})}{\partial \tilde{t}}$ as:

$$\frac{\partial \Psi(\tilde{z}, \tilde{t})}{\partial \tilde{t}} \approx \frac{\Psi(\tilde{z}, \tilde{t} + \delta \tilde{t}) - \Psi(\tilde{z}, \tilde{t})}{\delta \tilde{t}} \quad (9)$$

and both of this terms are known in every iteration of the Crank Nicolson method so we only have to focus on computing the integral. Using the u_1^t notation:

$$\langle E \rangle = \int_{-\infty}^{\infty} (u_i^t)^* \frac{i}{\delta \tilde{t}} (u_i^{t+1} - u_i^t) d\tilde{z} \quad (10)$$

This integral can be solved using, for example, the Simpson's method again.

1 Firts test, gaussian

To start testing the method we compute the time evolution for a gaussian function centered at zero and with $\sigma = 1$. We expect it to evolve as it is not an eigenfunction of $H = -\frac{\partial^2}{\partial \tilde{z}^2}$.

We compute the method for a spacing of $\Delta\tilde{z} = 0.01$ with $\tilde{z} \in [-3, 3]$ and a time interval $\delta\tilde{t} = 0.001$.

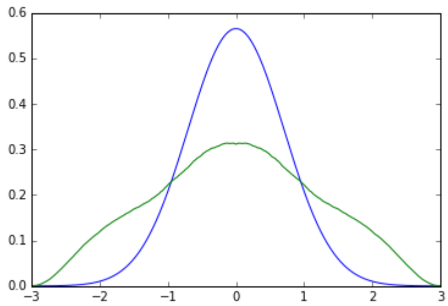

Figure 1: $|\Psi|^2$ *at time* $\tilde{t} = 0$ *in blue and at time* $\tilde{t} = 5$ *in green*

The maximum diference between the norm at $\tilde{t} = 0$ and the norm of the evolving function was: $1.16233793701x10^{-7}$

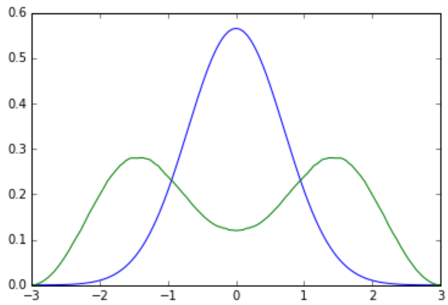

Figure 2: $|\Psi|^2$ *at time* $\tilde{t} = 0$ *in blue and at time* $\tilde{t} = 10$ *in green*

The maximum diference between the norm at $\tilde{t} = 0$ and the norm of the evolving function was: $1.16241938852x10^{-7}$

2 Second test, bright soliton

2.1 null velocity

We compute the method for a spacing of $\Delta\tilde{z} = 0.01$ with $\tilde{z} \in [-10, 10]$ and a time interval $\delta\tilde{t} = 0.001$ for a bright soliton solution with null velocity and $n_0 = 1$

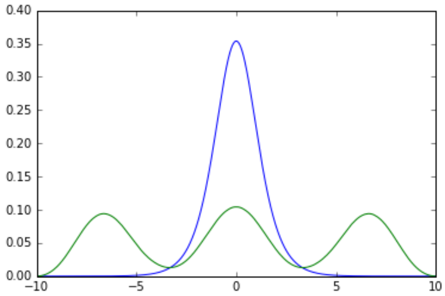

Figure 3: $|\Psi|^2$ *at time* $\tilde{t} = 0$ *in blue and at time* $\tilde{t} = 10$ *in green*

The maximum diference between the norm at $\tilde{t} = 0$ and the norm of the evolving function was: $1.4.59786764218x10^{-9}$

2.2 0.5 velocity

We compute with $\tilde{v} = 0.5$ and two diferent time intervals: $\delta\tilde{t} = 0.001$ and $\delta\tilde{t} = 0.01$

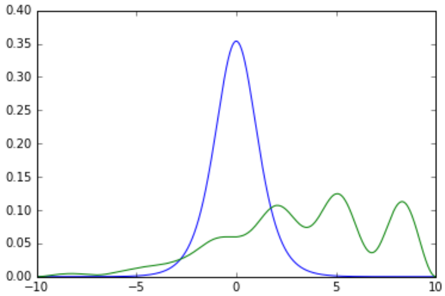

Figure 4: $|\Psi|^2$ *at time* $\tilde{t} = 0$ *in blue and at time* $\tilde{t} = 5$ *in green with* $\delta\tilde{t} = 0.01$

The maximum diference between the norm at $\tilde{t} = 0$ and the norm of the evolving function was: $3.06995195931x10^{-9}$

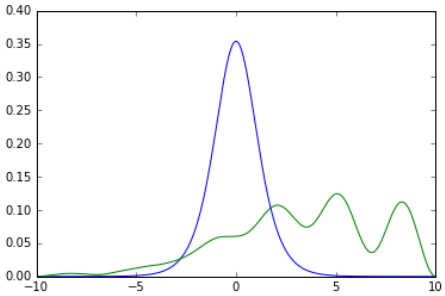

Figure 5: $|\Psi|^2$ *at time* $\tilde{t} = 0$ *in blue and at time* $\tilde{t} = 10$ *in green with* $\delta\tilde{t} = 0.001$

The maximum diference between the norm at $\tilde{t} = 0$ and the norm of the evolving function was: $3.45472594976x10^{-9}$
Here we have also computed the time that the program's been runing to obtain the result. For $\delta\tilde{t} = 0.01$ it was only $19.82s$ whereas the running time for $\delta\tilde{t} = 0.001$ it was $87.26s$ and yet there is no significant improvement on the result.

3 Third test, grey soliton

We run the code for the grey solution for a spacing of $\Delta\tilde{z} = 0.01$ with $\tilde{z} \in [-10, 10]$ and a time interval $\delta\tilde{t} = 0.01$ and the results found are:

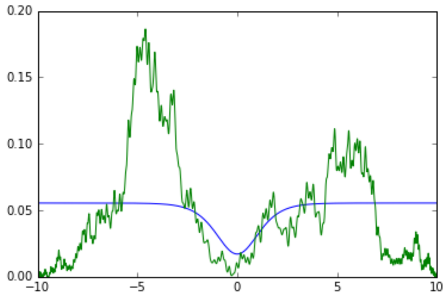

Figure 6: $|\Psi|^2$ *at time* $\tilde{t} = 0$ *in blue and at time* $\tilde{t} = 5$ *in green with* $\tilde{v} = 0.5$

The maximum diference between the norm at $\tilde{t} = 0$ and the norm of the evolving function was: $9.4415014253x10^{-5}$

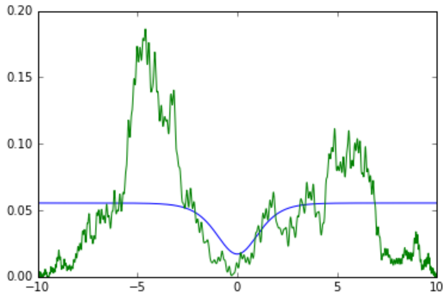

Figure 7: $|\Psi|^2$ *at time* $\tilde{t} = 0$ *in blue and at time* $\tilde{t} = 5$ *in green with* $\tilde{v} = 0$

The maximum diference between the norm at $\tilde{t} = 0$ and the norm of the evolving function was: $9.70332161562x10^{-5}$