Crank Nicolson method

Rosa Flaquer Galmés

Derivation of the Crank Nicolson method for the Gross-Pitaievskii equation which reads as:

$$i\frac{\partial\Psi(\tilde{z},\tilde{t})}{\partial\tilde{t}} = -\frac{1}{2}\frac{\partial^2\Psi(\tilde{z},\tilde{t})}{\partial\tilde{z}^2} + \frac{g}{|g|}\frac{n}{n_j}\Psi(\tilde{z},\tilde{t}) + V_{ext}(\tilde{z})\Psi(\tilde{z},\tilde{t}) \tag{1}$$

Here we include the external potential because altough we will set it equal to 0 when computing the time evolution of solitons it will be useful to make some tests of the method with an harmonic potential and g=0.

$$\begin{aligned}
\frac{\partial\Psi(\tilde{z},\tilde{t})}{\partial\tilde{t}} =& \frac{\Psi(\tilde{z},\tilde{t}+\frac{\Delta\tilde{t}}{2}) - \Psi(\tilde{z},\tilde{t})}{\frac{\Delta\tilde{t}}{2}} = i\frac{\partial^2\Psi(\tilde{z},\tilde{t})}{\partial\tilde{z}^2} \qquad \Rightarrow \\
\Psi(\tilde{z},\tilde{t}+\frac{\Delta\tilde{t}}{2}) =& \big[1 + i\frac{\Delta\tilde{t}}{2}\big(\frac{1}{2}\frac{\partial^2}{\partial\tilde{z}^2} + \frac{g}{|g|}\frac{|\Psi(\tilde{z},\tilde{t})|^2}{n_j} + V_{ext}(\tilde{z})\big)\big]\Psi(\tilde{z},\tilde{t}) \\
\Psi(\tilde{z},\tilde{t}+\frac{\Delta\tilde{t}}{2}) =& \big[1 - i\frac{\Delta\tilde{t}}{2}\big(\frac{1}{2}\frac{\partial^2}{\partial\tilde{z}^2} + \frac{g}{|g|}\frac{|\Psi(\tilde{z},\tilde{t}+\Delta\tilde{t})|^2}{n_j} + V_{ext}(\tilde{z})\big)\big]\Psi(\tilde{z},\tilde{t}+\Delta\tilde{t})
\end{aligned} \tag{2}$$

from where we find:

$$\begin{aligned}
&\big[1 + i\frac{\Delta\tilde{t}}{2}\big(\frac{\partial^2}{\frac{1}{2}\partial\tilde{z}^2} + \frac{g}{|g|}\frac{|\Psi(\tilde{z},\tilde{t})|^2}{n_j} + V_{ext}(\tilde{z}\big)\big]\Psi(\tilde{z},\tilde{t}) = \\
&\qquad \big[1 - i\frac{\Delta\tilde{t}}{2}\big(\frac{1}{2}\frac{\partial^2}{\partial\tilde{z}^2} + \frac{g}{|g|}\frac{|\Psi(\tilde{z},\tilde{t}+\Delta\tilde{t})|^2}{n_j} + V_{ext}(\tilde{z}\big)\big]\Psi(\tilde{z},\tilde{t}+\Delta\tilde{t})
\end{aligned} \tag{3}$$

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 $\Psi(\tilde{z},\tilde{t}+\Delta\tilde{t}) = \Psi_i^{t+1}$

$$\begin{aligned}
&\Psi_i^t + i\frac{\Delta\tilde{t}}{2}\left[\frac{1}{2}\frac{\Psi_{i+1}^t - 2\Psi_i^t + \Psi_{i-1}^t}{(\Delta\tilde{z})^2} - \frac{g}{|g|}\frac{|\Psi_i^t|^2}{n_j}\Psi_i^t - V_i|\Psi_i^t\right] = \\
&\qquad \Psi_i^{t+1} i\frac{\Delta\tilde{t}}{2}\left[-\frac{1}{2}\frac{\Psi_{i+1}^{t+1} - 2\Psi_i^{t+1} + \Psi_{i-1}^{t+1}}{(\Delta\tilde{z})^2} + \frac{g}{|g|}\frac{|\Psi_i^{t+1}|^2}{n_j}\Psi_i^{t+1} - V_i\Psi_i^{t+1}\right]
\end{aligned} \tag{4}$$

Defining $r \equiv i\frac{\Delta\tilde{t}}{4(\Delta\tilde{z})^2}$ it takes the form of

$$\begin{aligned}
&\left(1 + 2r + \frac{2g\Delta\tilde{z}^2|\Psi_i^{t+1}|^2}{|g|n_j} + 2r\Delta\tilde{z}^2V_i\right)\Psi_i^{t+1} - r\Psi_{i+1}^{t+1} - r\Psi_{i-1}^{t+1} = \\
&\qquad \left(1 - 2r - \frac{2g\Delta\tilde{z}^2|\Psi_i^t|^2}{|g|n_j} - 2r\Delta\tilde{z}^2V_i\right)\Psi_i^t + r\Psi_{i+1}^t + r\Psi_{i-1}^t
\end{aligned} \tag{5}$$

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 $\left(1+2r+\frac{2g\Delta\tilde{z}^2|\Psi_i^{t+1}|^2}{|g|n_j}+2r\Delta\tilde{z}^2 V_i\right)$ 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 $1-2r-\frac{2g\Delta\tilde{z}^2|\Psi_i^t|^2}{|g|n_j}-2r\Delta\tilde{z}^2 V_i$ in its main diagonal and r on the upper and lower diagonals, all the other elements are 0. We notice that the main diagonal of A depends on the vale of $\Psi_i^{t+1}|^2$ wich is precisely what we are trying to compute. To solve this problem we will approximate it to $\Psi_i^t|^2$.

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:

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

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

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

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:

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

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