PHYS3071 Assignment 5

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1 Part A

To numerically solve the ordinary Schrodinger equation (with no mean field potential term), we initiated the system with an initial state

$$\vec{u}_0 = \psi(x,0) = Ne^{-x^2}; \qquad N = \left(\int_{-\infty}^{\infty} e^{-2x^2}\, dx\right)^{-1/2} \tag{1}$$

which is a Gaussian function centered at 0. The solution to the next time step could then be calculated with a central difference/Crank-Nicholson method, with

$$\vec{u}_{j+1} = \left(\mathbb{I} - \frac{\Delta t}{2}M\right)^{-1}\vec{v}_j; \qquad \vec{v}_j = \left(\mathbb{I} + \frac{\Delta t}{2}M\right)\vec{u}_j \tag{2}$$

where

$$M = \begin{pmatrix} 2a + b(V_i + g|\psi_{i,j}|^2) & 0 & 0 & \cdots & 0 \\ -a & 2a + b(V_i + g|\psi_{i,j}|^2) & -a & \cdots & 0 \\ 0 & -a & 2a + b(V_i + g|\psi_{i,j}|^2) & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & -a \\ 0 & 0 & \cdots & 0 & 2a + b(V_i + g|\psi_{i,j}|^2) \end{pmatrix} \tag{3}$$

and

$$a = \frac{i\hbar\Delta t}{2m\Delta x^2}; \qquad b = \frac{i\Delta t}{\hbar}; \qquad V = \frac{2\hbar^2 x^2}{m} \tag{4}$$

The parameters here are complex valued, and so the probability value at any point in the grid is given by $|\psi_{i,j}|^2 = \psi_{i,j}\psi^*_{i,j}$. The left side term in equation (2) could easily be solved with with a tridiagonal matrix solver, adapted from PHYS3071 Assignment 2 to handle complex valued input vectors.
In our initial case, we set $g = 0$ to simulate no interactions within the Bose-Einstein Condensate, and the time-series probability distribution is shown in Figure 1. We performed the simulation with 100 space steps ($\Delta x = 8/100$) and 1000 time steps ($\Delta t = (\pi/2)/1000$), with $\hbar = 1$ and $m = 1/2$ for ease of calculation. The magnitude of these parameter steps were chosen so that we could satisfy the condition $\Delta t/\Delta x^2 < \frac{1}{2}$, and with our step sizes we obtain $\Delta t/\Delta x^2 \simeq 0.244$ as required to converge to an appropriate solution.

We see in our solution that the probability distribution is unchanging in time (both in position and variance) and so this must be an eigenfunction of the system.

2 Part B

In order to test how the system behaved when starting with some initial momentum (as opposed to the stationary initial state in part A), we set the initial state of the system to

$$\psi(x,0) = e^{-x^2}e^{ipx/\hbar} \Longrightarrow \psi(x,0) = e^{-x^2}\left[\cos\left(\frac{px}{\hbar}\right) + i\sin\left(\frac{px}{\hbar}\right)\right] \tag{5}$$

for some momentum $p = 2\hbar$ in our simulation. In the above, the imaginary component corresponds to the momentum in probability space.
Unfortunately, there was an error in the C++ code used to simulate this system and we saw no change in the system over time (i.e. the output was identical to that in Figure 1, but with a lower maximum probability value due to the presence of an extra, imaginary component in the state vector).

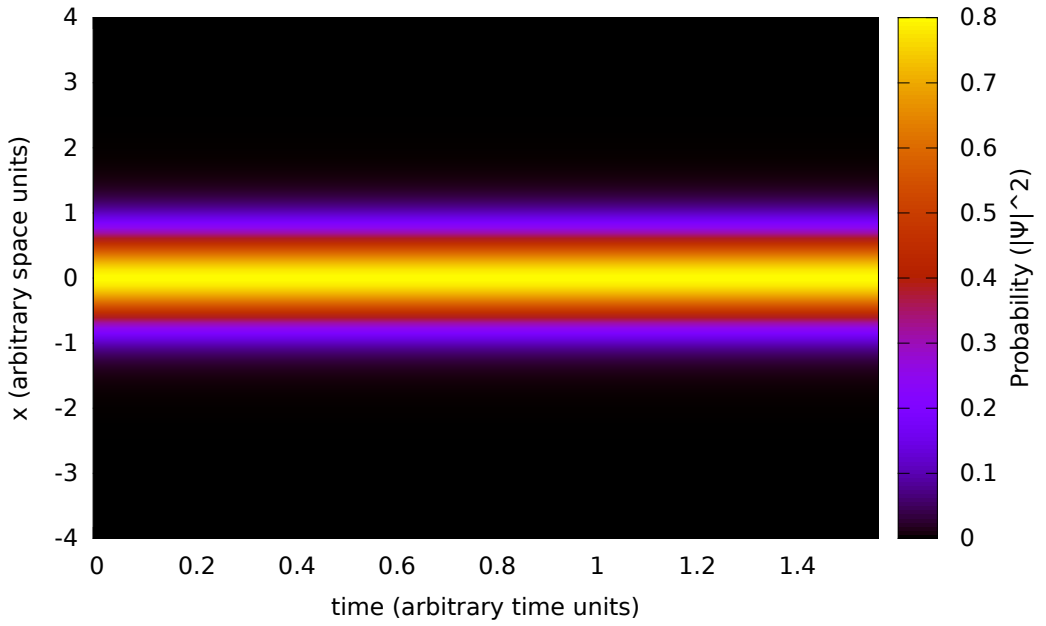

Figure 1: Solution to the ordinary Schrodinger equation with no mean field potential term, and a stationary Gaussian initial state function. The simulation was performed on a grid of $x \in [-4, 4]$ and over a time duration of $t \in [0, \pi/2]$, with 100 linear steps in the domain and 1000 linear steps in time.

3 Part C

Now, to simulate interactions within the BEC, we set $g = 30$ in a separate simulation with the initial stationary Gaussian (given by equation (1)). As in Part B, the code was unable to generate a dynamic solution and we unfortunately see data identical to that in Figure 1.