Computer project 2

PHZ 5156

Results due Thursday, September 30

Please submit your code and plots wherever requested. Results can be handed in either as a hardcopy, or as an electronic document (e.g. tex, latex, MS word, or even a .pdf) sent via email.

1. A wave function in one dimension evolves according to the Schrodinger equation as,

\[ i\hbar \frac{\partial \psi (x, t)}{\partial t} = \left[ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \right] \psi (x, t) \]

Show that if \( V(x) = 0 \) for a \( t = 0 \) wave packet given by

\[ \psi (x, t = 0) = \frac{1}{\sigma_0 \pi^{\frac{1}{4}}} e^{ik_0 x} e^{-(x-x_0)^2/2\sigma_0^2} \]

that the analytic expression for the time evolution is given by

\[ \psi (x, t) = \frac{1}{(\sigma_0 \sigma)^{\frac{1}{4}}} e^{ik_0(x-st/2)} e^{-(x-x_0-st)^2/2\sigma_0 \sigma} \]

with \( s = \hbar k_0 / m \) and \( \sigma = \sigma_0 + \frac{i \hbar t}{m \sigma_0} \). Simply prove that the solution works at \( t = 0 \) and then satisfies the time-dependent Schrodinger equation. This result can be found analytically also using Green functions.

2. Implement the Crank-Nicholson scheme to calculate the quantum-mechanical time evolution of a one-dimensional Gaussian wave packet with hard wall boundaries, so that the wave function vanishes at \( x = 0 \) and \( x = l \). For the evolution, use the definitions,

\[ x_j = (j + 1)h \]
\[ t_n = n \Delta t \]
\[ \psi_j^n = \psi(x_j, t_n) \]

Take the total length to be \( L = 200 \) and choose an appropriate spatial step \( h \) and hence \( j_{\text{max}} \). Use units with \( \hbar = m = 1 \). Pick an appropriate (i.e. stable) time step \( \Delta t \). Note that \( j = -1, 0, 1, 2, ..., j_{\text{max}} \) and \( n = 0, 1, ..., t_{\text{max}} / \tau \). The boundary conditions are such that \( \psi_{j = -1}^n = 0 \) and \( \psi_{j = j_{\text{max}}}^n = 0 \). Thus, show that the problem reduces to solving \( j_{\text{max}} \) linear equations. The resulting matrix equation is actually
tridiagonal. Solving this problem is not too computationally difficult, and we will work on a subroutine tridiag.f to solve it. Note that because the matrix equation has so many zero values, that we should avoid storing all of the elements in the matrix to save memory. After considering how to implement the scheme, code it in and view the evolution. Use a Gaussian wave packet as the initial $t = 0$ state, using $x_0 = L/6$, $\sigma_0 = 3$, and energy $E_0 = 4$ (with $E_0 = k^2/2$ in units of $\hbar = m = 1$. Occasionally output the wave function. Plot the time evolution at a few points and compare directly to the exact analytical result. Consider the appropriate spatial step $h$ and time step $\Delta t$. Also, what is an acceptable total simulation time $\tau$ so that you can see some waves bounce off of the boundaries. Verify in your code that probability density is conserved. Finally, in your write up, include pictures of a few snapshots compared to the analytical results. Include enough to really show the time evolution. It might be useful to plot the real and imaginary parts of the wave function. Also, it might be useful to plot $|\psi(x,t)|^2$. 