Computational Physics
Spring 2014, Shoemaker
UPDATED Homework 3 (Due date April 18 end of day)

Email homework as an attachment to (`deirdre@gatech.edu` and `kjani3@gatech.edu`). Include a `README` file that lists the files included with a short description (e.g. programs, plots, etc).

Write a program that solves the one-dimensional, time-dependent Schroedinger equation without a potential barrier (free particle) using the iterative Crank-Nicolson method. The computational domain is $-L/2 \leq x \leq L/2$ with $L = 100$. Use 200 points in your computational domain. The initial profile of the wave function is

$$\Psi(x, t = 0) = A\, e^{i\,k\,x}\, \exp\left(-\frac{(x - x_o)^2}{2\,\sigma^2}\right) \tag{1}$$

with $x_0 = 0$, $k = 0.25$ and $\sigma = L/10$. Use periodic boundary conditions.

Your program must at every 200 steps output a snapshot of the profile of $|\Psi|^2$ versus x. Also, the program must write to the command window the value of the integral

$$N = \int_{-L/2}^{L/2} |\Psi|^2\, dx \tag{2}$$

after each 200 step, a sanity check that your evolution preserves the unitary condition. Be sure that you start the evolution with a wave function that satisfies this condition. Note, N might not be equal to one but it should be maintained during the evolution.

Your homework must include a discussion on the stability of the method and convergence tests.