Homework 5

PHZ 3151

Due Friday, March 27

1. Consider the Schrodinger equation we investigated in homework 4,

$$i\hbar\frac{\partial\psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2}$$

with boundary conditions $\psi(x=0,t) = \psi(x=L,t) = 0$. As you recall, in homework 4 we computed the time-dependence by integrating using the Crank-Nicholson scheme. In this problem, we will take a slightly different approach.

First, consider that the wave function $\psi(x,t)$ given by

$$\psi(x,t) = \sum_{n=1}^{\infty} c_n sin\left(\frac{n\pi x}{L}\right) e^{-i\omega_n t}$$

which means that we can find $\psi(x,t)$ at *any time* t once we know the c_n at, for example, $t=0$.

Take the initial wave function to be, as before, a Gaussian wave packet.

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

Determine the expansion coefficients c_n numerically. Recall that the c_n are given by

$$c_n = \frac{2}{L}\int_0^L sin\left(\frac{n\pi x}{L}\right)\psi(x,t=0)dx$$

This integral must be replaced by a summation to be done numerically. This is discussed in lecture and appendix C. Notice that the c_n are *complex* because the initial state $\psi(x,t=0)$ is complex.

Write the code to determine $\psi(x,t)$ in this way. Pick two times, for example $t=50$ and $t=100$, to compare with the code written in homework 4. Choose the same parameters as before ($L=200$,$\hbar=m=1$, etc.) to make an exact comparison.

2. In this problem, we will consider the concept of writing a differential operator in the form of a matrix. Consider the eigenvalue equation,

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right]\psi(x) = E\psi(x)$$

Defined over the interval $0 < x < L$. The $V(x)$ is given by,

$$V(x) = -\frac{3}{2} \exp\left[-\left(x - \frac{L}{2}\right)^2\right]$$

To solve this problem, we will use a set of basis functions $\phi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right)$. Then, we expand the eigenstates $\psi(x)$ as,

$$\psi(x) = \sum_{n=1}^{\infty} c_n \phi_n(x)$$

Use the fact that,

$$\int_0^L \phi_m(x)\phi_n(x)dx = \delta_{m,n}$$

and show that the eigenvalue equation can be written as

$$Hc = Ec$$

where c is a column vector of the coefficients c_n and H is a square matrix with elements of H given by

$$H_{mn} = \epsilon_n \delta_{mn} + V_{mn}$$

for $n, m = 1, 2, 3, 4, ...$ The elements V_{mn}, which can be found analytically and stored, are given by the expression

$$V_{mn} = \int_0^L \phi_m^*(x)V(x)\phi_n(x)dx.$$

If we take $L = 10$, it also turns out that $V(x)$ is practically zero at $x = 0$ and $x = L$, so when you perform an analytic computation of the integral, you may replace the limits by $\pm\infty$.

Solve the eigenvalue problem above for the coefficients c_n corresponding to the lowest five eigenvalues. Plot the wave function $\psi(x)$ for each of these lowest five eigenvalues, and compare to the case where $V(x) = 0$ for $0 < x < L$. You have to determine how many basis states $\phi_n(x)$ to include in your description. Try $N = 20$ so that H is a 20×20 matrix. Then, try $N = 40$, and see if the eigenvalues are perceptibly different.

Turn in the computed eigenvalues E and plotted wave functions $\psi(x)$ for the lowest five states.