Homework 4

PHZ 3151

Due Friday, March 6, 2009

1. Consider a function $y(t)$ that is periodic in time t with periodicity $2T$. Hence, $y(t+2MT) = y(t)$ where M is any integer.

a) Which of the following three series is an appropriate Fourier representation of $y(t)$? (choose one)

$$y(t) = \frac{a_0}{2} + \sum_{n=1}^{\infty} a_n \cos\left(2n\pi t/T\right) + \sum_{n=1}^{\infty} b_n \sin\left(2n\pi t/T\right)$$

$$y(t) = \frac{a_0}{2} + \sum_{n=1}^{\infty} a_n \cos\left(n\pi t/T\right) + \sum_{n=1}^{\infty} b_n \sin\left(n\pi t/T\right)$$

$$y(t) = \sum_{n=1}^{\infty} a_n \sin\left(n\pi t/T\right)$$

b) Using the appropriate series chosen in part a), determine the appropriate expansion coefficients a_n and (possibly) b_n for $y(t)$ defined by,

$$y(t) = T - t$$

on the interval from $-T < t < T$. Sketch the periodic function $y(t)$ for a few periods.

2. Assume we have sampled some signal $y(t)$ at discrete times $t_m = m\Delta t$. The sampling interval is regular, so we can assume m is an integer. In total, we collect M data points, so that the total time we sample is $T = M\Delta t$.

Write an expression for the discrete Fourier transform (following appendix C). What is the maximum frequency we can determine? Explain what what would happen if the actual signal $y(t)$ contains frequency components greater than this function?

3. Consider the diffusion equation for the scalar field $u(x,t)$, written in the form

$$\frac{1}{\alpha^2}\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2}$$

Use separation of variables to write this partial differential equation as two first-order differential equations,

$$\frac{dT}{dt} = -\alpha^2 k^2 T$$
$$\frac{d^2X}{dx^2} = -k^2 X$$

Obtain the solutions in the case of the boundary conditions $X(0) = X(L) = 0$. Show then that the solution to the diffusion equation can be written in the form,

$$u(x,t) = \sum_{n=1}^{\infty} a_n \sin\left(\frac{n\pi x}{L}\right) e^{-\alpha^2 k^2 t}$$

4. In this computer project, you will simulate a particle of mass m in a box with $V(x) = 0$ for $0 < x < L$, and $V(x) = \infty$ everywhere else. The wave function $\psi(x,t)$ is governed in this case, for $0 < x < L$ by the time-dependent Schrodinger equation,

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

with boundary conditions $\psi(x=0,t) = \psi(x=L,t) = 0$. In this case, the analytical solutions can be written in the form obtained in class,

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

where $\omega_n = \frac{h\pi n^2}{4mL^2}$ $(\hbar = \frac{h}{2\pi})$. Notice the similarity to the analytical solutions we wrote down for waves on a string with fixed endpoints. As we have seen, the coefficients a_n, in this case complex, are determined by the initial conditions.

We will write a code to integrate the time-dependent Schrodinger equation. We will implement the Crank-Nicholson method as described in class. The initial conditions will be given by the Gaussian wave packet,

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

Take the total length to be $L = 200$ and choose an appropriate spatial step Δx and hence j_{max}. Use units with $\hbar = m = 1$. Pick an appropriate (i.e. stable) time step Δt. Note that $j = -1, 0, 1, 2, ..., j_{max}$ and $n = 0, 1, ..., t_{max}/\tau$. The boundary conditions are such that $\psi^n_{j=-1} = 0$ and $\psi^n_{j=j_{max}} = 0$. Thus, show that the problem reduces to solving j_{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 $E_0 = k_0^2/2$ 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 Δx and time step Δt. Also, what is an acceptable total simulation time τ 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 $|\psi(x,t)|^2$.