PHYS-4007/5007
COMPUTATIONAL PHYSICS PROJECT:
The Quantum Harmonic Oscillator

1 Introduction

The equation of motion of quantum mechanics for a particle is given by the Schrödinger equation,

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + V\Psi. \tag{1}$$

Here, Ψ is the wave function of the particle, which is a function of both time, t, and position, x, moving in a potential field described by V. Solution of the Schrödinger equation typically uses the method of separating the time- from the space-dependent part of the equation. The spatial portion is the so-called *stationary* (or *time-independent*) Schrödinger equation — an eigenvalue equation which, in the coordinate representation, takes the form of a linear differential equation. The solutions of of this equation are wave functions $\psi(\boldsymbol{r})$, which assign a complex number to every point $\boldsymbol{r}$. More specifically, they describe those states of the physical system for which the probability $|\psi(\mathbf{r})|^2$ does not change with time. To obtain a numerical solution of the Schrödinger equation, one can either approximately discretize the linear differential equation and put it in matrix form, or expand $\psi(\mathbf{r})$ in terms of a complete set of wave functions $\psi_n(\mathbf{r})$ and consider only a finite number of them. In both cases, the stationary Schrödinger equation leads to an eigenvalue equation of a finite matrix.

This project is composed of three stages. Stages (1) and (2) are to be completed by the undergraduate students. Stages (1) – (3) are to be completed by graduate students and those students taking this course in the honors section (*i.e.*, PHYS-4007-088).

Stage (1): Quantum Mechanical Harmonic Oscillator in One-Dimension

You are to investigate a one-dimensional problem where a mass m moves in the quadratic potential $V(x) = m\omega^2x^2/2$. Here, x is the spatial coordinate and ω is the angular frequency of the harmonic oscillator. The Hamiltonian for such a system is

$$H = \frac{1}{2}\left(\frac{p^2}{m} + m\omega^2x^2\right) , \tag{2}$$

or in operator format,

$$\hat{H} = \frac{1}{2m}\left(\hbar^2 \frac{\partial^2}{\partial x^2} + m^2\omega^2 x^2\right) \ . \tag{3}$$

The eigenfunctions (*i.e.*, wave functions) of H_0 are

$$\psi_n(\xi) = \left(\frac{m\omega}{\pi\hbar}\right) \frac{1}{\sqrt{2^n n!}} H_n(\xi)\, e^{-\xi^2/2} \ , \quad n = 0, 1, 2, ..., \tag{4}$$

where the $H_n(\xi)$ here represents the **Hermite polynomial** set of functions (and <u>not</u> the Hamiltonian H) and ξ is related to the position coordinate via $\xi = \sqrt{(m\omega/\hbar)}\, x$. From these eigenfuctions, we can set up the following eigenvalue equation to represent the time-independent Schrödinger equation:

$$H|\psi_n\rangle = E_n|\psi_n\rangle, \tag{5}$$

(see any quantum mechanics book for a definition of the "bra-ket" notation: $|\psi_n\rangle$) where the eigenvalues (*i.e.*, energies) of H are

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega \ . \tag{6}$$

The quantum mechanics harmonic oscillator has actual analytic solutions to the Schrödinger equation (which you can find in any quantum mechanics book). You are to numerically calculate $\psi_n(x)$, and E_n for the first 20 energy states of your harmonic oscillator (once again, using both numeric methods mentioned above). Compare your numerical solution with the analytic solutions (do this with graphs) that are typically derived in most quantum mechanics books. Your code should also calculate expectation values, probabilities, and HUP for each state numerically as well. Set the code up such that the user can input any "n" up to the maximum listed.

Stage (2): Quantum Mechanical Harmonic Oscillator in Three-Dimensions

In this stage of this project, you will now carry out the above calculations, but for a 3-dimensional harmonic oscillator. Your task is to numerically solve the PDE listed in Equation (1) — the Schrödinger equation but with the Hamiltonian being given by

$$\hat{H} = \frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right) + \frac{1}{2}m\omega^2\left(x^2 + y^2 + z^2\right) \ . \tag{7}$$

Make comparisons between the numerical wave function solution for the 3-D case with respect to the 1-D case. As well, compare the energies between these 2 cases for all of the "n" calculated in Stage (1).

Stage (3): Time-Varying Quantum Mechanical Harmonic Oscillator

Add a periodic variability to the harmonic potential of the form

$$V(x,t) = \frac{1}{2} m\omega^2 x^2 \cos(\omega t) \ . \tag{8}$$

2 Computer Coding Techniques

Follow what was done in Stage (1), but also describe how the first 5 wave functions and energies change with time. Follow what is described in §XI.B in terms of using separation of variables to set up a set of ordinary differential equations (ODE) and then use either the $4th$-order Runge-Kutta or the Adams Method to solve these sets of ODEs.

Honors Section and Graduate Students will also need to design a graphics package to display the time variability of the potential and wave functions on a computer screen. Note that you will not be able to make any comparisons to analytic solutions since they don't exist!

3 Analysis

It will be up to the student to design a set of analysis questions to answer for this project. These questions should be addressed in your project's proposal that you will have to write for the second homework set. The final computer project report must be written in LaTeX! I will have a LaTeX template file called `template.tex` on the course web page.