PHYSICS 3800. Assignment 4.

1. (10 pts.) Solve the 1-D Poisson equation on $x \in [0, 1]$,

$$\frac{\partial^2 u}{\partial x^2} = f(x),$$

where $f(x) = \exp\{-1000(x - 0.5)^4\}$, with boundary conditions $u(0) = 0$ and $u(1) = 5$. This corresponds to something like a parallel plate capacitor with one plate at 0 V and the other at 5 V and a planar charge density of $\rho(x) = -\epsilon_0 f(x)$ between them. As done in class, using the central difference scheme for the second derivative transforms the PDE (really an ODE here) into a tridiagonal matrix vector equation. Use a LAPACK routine for a real general matrix to solve the problem. Time how long the program runs as you decrease Δx. Now use the appropriate LAPACK routine (SGTSV) for tridiagonal a matrix in the problem and time the code. To time the code one can use the unix utility `time`, e.g., `time ./a.out`. (Run three times to get a sense of the average time.) Plot the solution $u(x)$ as well as the electric field $[E_x = -u'(x)]$.

2. (10 pts.) Solve the 1-D time-indpendent Schödinger equation on $x \in [0, 1]$,

$$-\frac{\partial^2 \psi}{\partial x^2} + V(x)\psi = E\psi,$$

where we have chosen units so that $\hbar = 1$ and $m = 1/2$, and the potential in these units is given by $V(x) = 10^5(x - 0.5)^2$. Take the boundary conditions to be $\psi(0) = 0$ and $\psi(1) = 0$. As shown in class, upon discretization, this transforms into a tridiagonal matrix eigenvalue problem. Here the eigenvalues are real and are related to the discrete energies of a quantum harmonic oscillator. Recall that for a harmonic potential $v(x) = \frac{1}{2}m\omega^2 x^2$, the energies are $e_n = (n - \frac{1}{2})\hbar\omega$, with $n = 1, 2, \ldots$. Use the most appropriate LAPACK routine for finding eigenvalues and eigenvectors. Plot the first few eigenvectors (wavefunctions). Also plot the numerical value of e_n vs n, along with the analytical result for an unbounded quantum harmonic oscillator, for different discretization spacings Δx.

Note that once the wavelength of the solution approaches with discretization length, the solution should become inaccurate. Also, as the energy associated with the wavefunction increases, the wavefunction will extend spatially towards our artificial boundaries, and the solution will tend to that of a particle in a box. Both these factors mean that our solution will deviate from that of the harmonic oscillator for larger n.

3. (10 pts.) Using the method shown in class, solve the 1-D time-dependent Schrödinger equation on $x \in [0, 1]$,

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

where again we have chosen units so that $\hbar = 1$ and $m = 1/2$, and the potential is given by $V(x) = 10^5(x - 0.5)^2$. Take the boundary conditions to be $\psi(0) = 0$ and $\psi(1) = 0$. As shown in class, upon discretization, advancing in time is accomplished by successively solving a complex tridiagonal matrix vector equation. Use the most appropriate LAPACK routine for this task. At each time step, you will obtain the wave function. Use this to calculate the expectation value of the particle's position

$$\bar{x}(t) = \int_0^1 x|\psi(x, t)|^2 dx$$

using the trapezoid rule. How does $\bar{x}(t)$ compare with a classical harmonic oscillator (plot the classical trajectory over top)?