QUANTUM MECHANICS I

PHYS 516

Problem Set # 3a: Beginning Numerics

Distributed: Feb 17, 2010

Due: Mar. 1, 2010

1. Simplest Analytic Problem: A particle of mass m is dropped into a potential $V(x)$ with $V = \infty$ for $x < 0$ and $x > 11$ $V = 0$ for $0 \leq x \leq 11$. Compute the eigenfunctions and their eigenvalues. Plot the lowest three eigenfucntions.

2. Oozing into Numerical Calculations: Approximate the wavefunction describing the particle in Problem # 5 above by its values at $x = 0, 1, 1, ..., 11$. Approximate the second derivative by

$$\frac{d^2\psi(i)}{dx^2} \simeq \frac{\psi(i+1) - 2\psi(i) + \psi(i-1)}{\Delta^2}$$

where Δ is the distance between adjacent points (i.e., $\Delta = 1$ in this case). Diagonalize the resulting 10×10 "kinetic energy" matrix, sort the eigenvalues from smallest to largest, and compare with the analytically determined eigenvalues computed in Problem #5. How far "up" the energy scale would you trust the numerical results? Plot the lowest three eigenfunctions. Compare with the analytic results. Are you satisfied? Why/why not?