QUANTUM MECHANICS I

PHYS 516

Problem Set # 2

Distributed: January 21, 2015

Due: January 30, 2015

Harmonic Oscillator

1. Analytic Solution: Write down the Schrödinger equation for the one-dimensional harmonic oscillator. Introduce dimensionless coordinates ($x = \gamma z$) and write down the resulting dimensionless equation in canonical form (coefficient of $\frac{d^2}{dz^2}$ is 1).

a. What is the value of the scaling constant γ?

b. What is the energy eigenvalue spectrum?

c. What are the analytic solutions in terms of classical functions?

d. What is the normalization constant (A & S, 22.2.14)?

e. Plot $\psi_n(x)$, $n = 0, \ldots, 5$ for $-4 \leq z \leq +4$.

2. Numerical Approximation of Second Derivative: Set $m = k = \hbar = 1$. Discretize the interval $-a \ldots + a$ (a equal to 4 or 5) into 100 equal steps with 101 equally spaced points. Approximate the second derivative by

$$\frac{d^2\psi}{dx^2}|_i \simeq \frac{\psi_{i+1} - 2\psi_i + \psi_{i-1}}{(\Delta x)^2}$$

a. Write down the Schrödinger equation as a matrix eigenvalue equation in the unknowns ψ_i, $i = 0 \ldots 100$ or $i = -50 \ldots + 50$.

b. Diagonalize this equation.

c. What are the 6 lwest eigenvalues? Compare to $n + \frac{1}{2}$ from prob. **1b**.

d. Plot the eigenvectors corresponding to the 6 lowest eigenvalues.

3. Variational Approach - Gaussian: Set $m = k = \hbar = 1$. Approximate the wavefunction $\psi(x)$ by

$$\psi(x) = \sum_i c_i \phi_i(x) \qquad \phi_i(x) = e^{-(x-x_i)^2/2\sigma^2}$$

where x_i are the 101 lattice sites used in Problem 2 above and c_i are unknown coefficients. Choose $\sigma = \Delta x$. Plug this ansatz into the Schrödinger variational principle.

a. Compute $E \int \psi^2 dx$. You can do these integrals analytically or by lookup or by Maple. You should notice that if the lattice sites are too far away from each other the integrals can be neglected: $\int \phi_i \phi_j dx \simeq 0$ for $|i - j| \geq$ small number. The result will be bilinear in the unknown coefficients c_*.

b. Compute $\int \psi^2 V(x) dx$, with $V(x) = \frac{1}{2}x^2$. You can do these integrals analytically or by lookup or by Maple. Don't bother to do the integrals that are negligible (see part **a.**.

c. Compute $\int (\nabla \psi)^2 dx$. You can do these integrals analytically or by lookup or by Maple. Don't bother to do the integrals that are negligible (see parts **a.**,**b.**.

d. Collect the three matrices (101×101) constructed in parts **a. - c.** into a single matrix generalized eigenvalue problem. Diagonalize and list the lowest 6 eigenvalues.

e. Plot the eigenvectors with the two lowest eigenvalues.