QUANTUM MECHANICS I

PHYS 516

Problem Set # 2

Distributed: Jan. 15, 2016

Due: January 22, 2016

1. Harmonic Oscillator 1: Plot the harmonic oscillator wavefunctions for the ground state $\psi_0(x)$ and the five lowest excited states $\psi_i(x)$, $i = 1 - 5$.

$$\psi_n(x) = \frac{1}{\sqrt{2^n n! \sqrt{\pi}}} H_n(x) e^{-x^2/2}$$

where $H_n(x)$ are the classical Hermite polynomials with standard normalization: $H_n(x) = (2x)^n +$ terms of lower degree.

2. Harmonic Oscillator 2: Solve the equation $-\frac{1}{2}\frac{d^2\psi}{dx^2} + \frac{1}{2}x^2\psi = E\psi$ (obtained by setting $m = k = \hbar = 1$ in the Schrödinger equation) numerically by discretizing along the line using a step size Δ and extending the part of the line that is discretized from $-a$ to $+a$. Play around with the parameters Δ and a until you find reasonable values. Describe your frustration as you iterate to 'reasonable values'. What values are you using? Then plot the ground state (no zero crossings) and the five lowest excited states and brag that you've done an analytically solvable problem numerically.

3. Normalization Problem: If you look at the vertical scales on the plots of Problems 1 and 2, they are different. How do you reconcile this difference. Be quantitative.

4. Plot $|\psi_{10}(x)|^2$ and compare with the plot by Dicke and Wittke in the handout.

5. Diatomic Molecules: Schrödinger derives an approximation to the spectrum of a diatomic molecule:

$$E_i \simeq \frac{l(l+1)\hbar^2}{2I_0}\left(1 - \frac{\epsilon}{1+3\epsilon}\right) + (n + \frac{1}{2})\hbar\omega_0\sqrt{1+3\epsilon} \qquad \epsilon = \frac{l(l+1)\hbar^2}{(I_0\omega_0)^2}$$

This occurs as Eq. (51) in his second paper. I have made the following modifications in his equations. (1) Interchanged $n \leftrightarrow l$, where n is now the harmonic oscillator quantum number and l is the orbital angular momentum quantum number, (2) $h \to \hbar$, $\nu_0 \to \omega_0$, (3) $\mu r_0^2 = A \to I_0$.

Carry out a Taylor series expansion of this energy expression in powers of ϵ (!! Please use Maple or other !!) and express the result in powers of $(n+\frac{1}{2})$ and $l(l+1)$:

$$E_i \simeq \sum_{p,q} D_{p,q}(n+\frac{1}{2})^p \, [l(l+1)]^q$$