PS # 5

Quantum Mechanics I — Due: 12^{th} Nov 2012

1. Consider the Hydrogen atom. Let us apply an electric field along the z direction. This leads to a Hamiltonian:

$$H = H_0 - e|E|z$$

where

$$H_0 = \frac{p^2}{2m} - \frac{e}{r} \quad \text{(Hydrogen atom)}.$$

a) Evaluate the first order energy shift to the ground state $|n=1, l=0, m=0\rangle$. Note that this state is non-degenerate.

b) In order to calculate higher order shifts (for example second order), we need to evaluate:

$$\Delta_\alpha^{(2)} = \sum_{\alpha' \neq \alpha}' \frac{|z_{\alpha\alpha'}|^2}{E_\alpha^{(0)} - E_{\alpha'}^{(0)}}$$

where α : is a collective index for $|n, l, m\rangle$. and

$$z_{\alpha\alpha} = \langle n'l'm'|z|nlm\rangle$$

Evaluate :

$$z_{\alpha 0} = \langle n'l'm'|z|100\rangle$$

(where $|100\rangle$: ground state)

for :

$2s$: $|n'=2, l=0, m=0\rangle$

$2p$: $|n'=2, l=1, m=1\rangle$, $|n'=2, l=1, m=0\rangle$, $|n'=2, l=1, m=-1\rangle$

You are given the eigenfunctions of the unperturbed Hamiltonian in (table 1). What are the only non-zero matrix elements and why?

TABLE 1

1s:

$$|1\,0\,0\rangle = \varphi_{100}(r,\theta,\varphi) = \frac{1}{\sqrt{\pi a_0^3}}\, e^{-r/a_0}$$

2s:

$$|2,0\,0\rangle = \varphi_{200}(r,\theta,\varphi) = \frac{1}{\sqrt{8\pi a_0^3}}\left(1 - \frac{r}{a_0}\right) e^{-r/2a_0}$$

2p:

$$|2\,1\,1\rangle = \varphi_{211}(r,\theta,\varphi) = -\frac{1}{8\sqrt{\pi a_0^3}}\,\frac{r}{a_0}\, e^{-r/2a_0} \sin\theta\, e^{i\varphi}$$

$$|2\,1\,0\rangle = \varphi_{200}(r,\theta,\varphi) = \frac{1}{4\sqrt{2\pi a_0^3}}\,\frac{r}{a_0}\, e^{-r/2a_0} \cos\theta$$

$$|2\,1\,-1\rangle = \varphi_{21-1}(r,\theta,\varphi) = \frac{1}{8\sqrt{\pi a_0^3}}\,\frac{r}{a_0}\, e^{-r/2a_0} \sin\theta\, e^{-i\varphi}$$

2. Consider a particle in a 2D potential:

$$V_0 = \begin{cases} 0 & \text{for } 0 \le x \le L, \quad 0 \le y \le L \\ \infty & \text{otherwise.} \end{cases}$$

Write the energy eigenfunctions for the ground and first excited states. List out degeneracies.
Add a time-independent perturbation:

$$V_1 = \begin{cases} \lambda x y & \text{for: } 0 \le x \le L, \quad 0 \le y \le L \\ 0 & \text{otherwise.} \end{cases}$$

Obtain the zeroth-order energy eigenfunctions and the first order energy eigenfunctions for the ground and the first excited states.

3. Estimate the ground state energy of a one dimensional simple Harmonic Oscillator using

$$\langle x | \tilde{0} \rangle = e^{-\beta |x|}$$

as a trial function where β is to be varied.
(Useful result:
$$\int_0^\infty e^{-\alpha x} x^n \, dx = \frac{n!}{\alpha^{n+1}} \Bigg).$$