# Assignment 11

## OPTI 570 Quantum Mechanics

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## Problem I

a) Using the information from Complement $G_{II}$, the wave function is:

$$\psi_{n_x,n_y}(x,y) = \frac{2}{a}\sin\frac{n_x\pi x}{a}\sin\frac{n_y\pi y}{a}, \quad \text{with} \quad E^0_{n_x,n_y} = \frac{\hbar^2\pi^2}{2ma^2}(n_x^2+n_y^2).$$

The first-order correction in the eigenvalue of the ground state $\psi_{1,1}$ depends on the mean value of $W$:

$$E^{(1)}_{1,1} = \langle\psi_{1,1}|W|\psi_{1,1}\rangle = \omega_0\int_0^{a/2}\int_0^{a/2}|\psi(x,y)|^2\,dxdy = \frac{4\omega_0}{a^2}\int_0^{a/2}\sin^2\frac{\pi x}{a}\,dx\int_0^{a/2}\sin^2\frac{\pi y}{a}\,dy$$

$$E^{(1)}_{1,1} = \frac{4\omega_0}{a^2}\frac{a}{4}\frac{a}{4} = \frac{\omega_0}{4}.$$

The integration is divided in two simple ones.

The perturbed enegy of the ground state is then:

$$E_{11} \approx E^{(0)}_{11} + E^{(1)}_{1,1} = \frac{\hbar^2\pi^2}{ma^2} + \frac{\omega_0}{4}.$$

b) In this case, we have a two-degenerate eigenvalue with states $|1,2\rangle$ and $|2,1\rangle$. The eigenvalue is:

$$E^{(0)}_{12} = E^{(0)}_{21} = \frac{5\hbar^2\pi^2}{2ma^2}.$$

The mean values are:

$$\langle 12|W|12\rangle = \langle 21|W|21\rangle = \frac{4\omega_0}{a^2}\int_0^{a/2}\sin^2\frac{\pi x}{a}\,dx\int_0^{a/2}\sin^2\frac{2\pi y}{a}\,dy = \frac{\omega_0}{4}.$$

The off-diagonal elements are:

$$\langle 12|W|21\rangle = \langle 21|W|12\rangle = \frac{4\omega_0}{a}^2\left(\int_0^{a/2}\sin\frac{\pi x}{a}\sin\frac{2\pi x}{a}\,dx\right)^2 = \frac{16\omega_0}{9\pi^2}.$$

In the $\{|12\rangle, |21\rangle\}$ basis, $W$ is represented as:

$$W = \omega_0 \begin{bmatrix} \frac{1}{4} & \frac{16}{9\pi^2} \\ \frac{16}{9\pi^2} & \frac{1}{4} \end{bmatrix}.$$

We obtain the perturbation term by looking the eigenvalues and eigenstates of this matrix which lives in the eigensubspace $\mathscr{E}_\pm$. The eigenvalues are:

$$E_\pm^{(1)} = \omega_0 \left( \frac{1}{4} \pm \frac{16}{9\pi^2} \right).$$

So the two split energies are:

$$E_\pm \approx \frac{5\hbar^2\pi^2}{2ma^2} + \omega_0 \left( \frac{1}{4} \pm \frac{16}{9\pi^2} \right).$$

The corresponding zero-order eigenstates are:

$$\psi_\pm(x, y) = \frac{1}{\sqrt{2}}[\psi_{12}(x, y) \pm \psi_{21}(x, y)].$$

# Problem II

a) Because $H_0$ is purely written in terms of $J_z$, it is diagonal in the $\{|1\rangle, |0\rangle, |-1\rangle\}$ basis:

$$J_z|m\rangle = m\hbar|m\rangle, \quad m = 1, 0, -1.$$

Therefore,

$$H_0|m\rangle = (aJ_z + \frac{b}{\hbar}J_z^2)|m\rangle = (am\hbar + \frac{b}{\hbar}m^2\hbar^2)|m\rangle = \hbar(am + bm^2)|m\rangle.$$

The energy eigenvalues are:

$$\begin{aligned} m = 1 &\Longrightarrow E_{+1} = \hbar(a + b) \\ m = 0 &\Longrightarrow E_0 = 0 \\ m = -1 &\Longrightarrow E_{-1} = \hbar(b - a). \end{aligned}$$

Degeneracy occurs when at least two energies are equal. This can happen when $a = b$, which implies that $E_{-1} = E_0$ and therefore, the ratio is:

$$\frac{b}{a} = 1.$$

The states $|0\rangle$ and $|-1\rangle$ are degenerate with energy $E = 0$.

b) The spin-1 operator are:

$$J_x = \frac{\hbar}{\sqrt{2}} \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}, \quad J_y = \frac{\hbar}{\sqrt{2}} \begin{bmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{bmatrix}, \quad J_z = \hbar \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix}.$$

Putting these in the $J_u$ operator and the replacing in $W = \omega_0 J_u$ yields:

$$W = \hbar\omega_0 \begin{bmatrix} \cos\theta & \frac{\sin\theta}{\sqrt{2}e^{-i\varphi}} & 0 \\ \frac{\sin\theta}{\sqrt{2}}e^{i\varphi} & 0 & \frac{\sin\theta}{\sqrt{2}}e^{-i\varphi} \\ 0 & \frac{\sin\theta}{\sqrt{2}}e^{i\varphi} & -\cos\theta \end{bmatrix}$$

c) If $a = b$, then there is a degeneracy with $|0\rangle$ and $|-1\rangle$. Also, oriented to Ox axis means that $\theta = \pi/2$ and $\varphi = 0$, so $J_u = J_x$. For $j = 1$, we have the following unperturbed Hamiltonian:

$$H_0 = aJ_z + \frac{a}{\hbar}J_z^2 = a\hbar \begin{bmatrix} 2 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}.$$

We see explictly that $|0\rangle$ and $|-1\rangle$ share the same eigenvalue 0. We have colored the two subspaces we have. The perturbation is:

$$W = \omega_0 J_x = \hbar\omega_0 \frac{1}{\sqrt{2}} \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}.$$

For the nondegenerate state $|1\rangle$ we have

$$E_1^{(1)} = \langle 1|W|1\rangle = \hbar\omega_0 \frac{1}{\sqrt{2}} 0 = 0 \Longrightarrow E_1 \approx 2a\hbar.$$

For the degenerate subpace,

$$W = \hbar\omega_0 \frac{1}{\sqrt{2}} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \Longrightarrow \lambda_\pm = \pm\frac{\hbar\omega_0}{\sqrt{2}}.$$

The corresponding eigenstates are:

$$|\psi_\pm\rangle = \frac{1}{\sqrt{2}}(|0\rangle \pm |-1\rangle).$$

The energies to first order are:

$$E_+ \approx 0 + \frac{\hbar\omega_0}{\sqrt{2}}, \quad \text{and} \quad E_- \approx 0 - \frac{\hbar\omega_0}{\sqrt{2}}.$$

These two eigenvalues are linked with the zero-order eigenstates found from $W$.

d) Now th eigenvalues of $H_0$ becomes:

$$H_1^0 = \hbar(a+b) = 3a\hbar, \quad E_0^0 = 0, \quad E_{-1}^0 = \hbar(b-a) = a\hbar.$$

The matrix $J_u$ for this case is:

$$J_u = \hbar \begin{bmatrix} \cos\theta & \frac{\sin\theta}{\sqrt{2}}e^{-i\varphi} & 0 \\ \frac{\sin\theta}{\sqrt{2}}e^{i\varphi} & 0 & \frac{\sin\theta}{\sqrt{2}}e^{-i\varphi} \\ 0 & \frac{\sin\theta}{\sqrt{2}}e^{i\varphi} & -\cos\theta \end{bmatrix}$$

Te only non-zero elements that connects $|0\rangle$ with the other states are:

$$\langle 1|W|0\rangle = \omega_0\hbar\frac{\sin\theta}{\sqrt{2}}e^{-i\varphi}, \quad \langle -1|W|0\rangle = \omega_0\hbar\frac{\sin\theta}{\sqrt{2}}e^{i\varphi}.$$

The ground state is represented as:

$$|\psi_0\rangle \approx |0\rangle + \sum_{n\neq 0}\frac{\langle n|W|0\rangle}{E_0^0 - E_n^0}|n\rangle = |0\rangle + \frac{\langle 1|W|0\rangle}{E_0^0 - E_1^0} + \frac{\langle -1|W|0\rangle}{E_0^0 - E_{-1}^0} = |0\rangle - \frac{\omega_0\sin\theta}{3\sqrt{2}a}e^{-i\varphi}|1\rangle - \frac{\omega_0\sin\theta}{\sqrt{2}a}e^{i\varphi}|-1\rangle.$$

It needs to be normalized by its norm:

$$|\psi_0'\rangle = \frac{|\psi_0\rangle}{\sqrt{1 + \frac{5}{9}\frac{\omega_0^2\sin^2\theta}{a^2}}}.$$

# Problem III

a) For an s state, the angular part is $Y_{00}$ and it integrates to one, so we just need the radial integration:

$$\langle n00|W|n00\rangle = 2E_1 a_0 \int_0^b r^2 |R_{n0}(t)|^2 (\frac{1}{r} - \frac{1}{b})\ dr.$$

For $n = 1$ and $n = 2$, we have:

$$\langle 100|W|100\rangle \approx 2E_1 a_0 \frac{4}{a_0^3} \int_0^b r^2 (\frac{1}{r} - \frac{1}{b})\ dr = \frac{8E_1}{a_0^2} \int_0^b (r - \frac{r^2}{b})\ dr = \frac{4}{3} E_1 \left(\frac{b}{a_0}\right)^2$$
$$\langle 200|W|200\rangle \approx 2E_1 a_0 \frac{1}{8a_0^3} \int_0^b r^2 (2 - \frac{r}{a_0})^2 (\frac{1}{r} - \frac{1}{b})\ dr = \frac{1}{6} E_1 \left(\frac{b}{a_0}\right)^2.$$

b) The perturbation depends only on $r$, so it is purely radial in posittion representatino. The matrix elements is:

$$\langle 100|W|21m\rangle = \int_0^\infty dr\ r^2 R_{10}(r) W(r) R_{21}(t) \int d\Omega Y_{00}^*(\theta, \phi) Y_{1m}(\theta, \phi).$$

But in the angular part, we have $l = 0$ and $l = 1$, which are orthogonal each other and therefore its integral is zero. So in both cases we have a zero value.

c) The five states with $n = 1, 2$ are:

$$\{|100\rangle, |200\rangle, |21-1\rangle, |210\rangle, |211\rangle\}.$$

We have the elements we can use to construct the matrix $W$, which is then

$$W = \begin{bmatrix} \frac{4}{3}E_1(\frac{b}{a_0})^2 & \beta E_1(\frac{b}{a_0})^2 & 0 & 0 & 0 \\ \beta E_1(\frac{b}{a_0})^2 & \frac{1}{6}E_1(\frac{b}{a_0})^2 & 0 & 0 & 0 \\ 0 & 0 & \varepsilon & 0 & 0 \\ 0 & 0 & 0 & \varepsilon & 0 \\ 0 & 0 & 0 & 0 & \varepsilon \end{bmatrix}$$

d) The energies in the Hydrogen is $E_n^0 = -E_1/n^2$. For the five states we have:

$$E_{100}^{(0)} = -E_1, \quad E_{200}^{(0)} = E_{21m}^{(0)} = -E_1/4.$$

The $n = 1$ and $n = 2$ levels are not degenerate with each other, so we can use non-degenerate perturbation theory. To first order, the energy shift of each nondegenerate state is just the diagonal matrix element of $W$. So:

$$E_{100} \approx -E_1 + \frac{4}{3} E_1 (\frac{b}{a_0})^2$$
$$E_{200} \approx -\frac{E_1}{4} + \frac{E_1}{6} (\frac{b}{a_0})^2$$
$$E_{21m} \approx -\frac{E_1}{4}$$

Second order involves the off-diagonal which are not considered.

e) From d), the shift on $n = 2$ is the $2s$ shift:

$$\Delta E_{2s} = \frac{E_1}{6}(\frac{b}{a_0})^2.$$

For the $2p$ level is $-E_1/4$. The energy difference between $2s$ and $2p$ from the finite proton size is

$$\Delta E_{\text{finite proton}} = \frac{1}{6}E_1(\frac{b}{a_0})^2 = \frac{E_1}{6}10^{-10} \longrightarrow \Delta f_{\text{finite proton}} = \frac{\Delta E}{\hbar} = \frac{E_1}{6\hbar}10^{-10} = 5.5 \cdot 10^4 \ Hz.$$

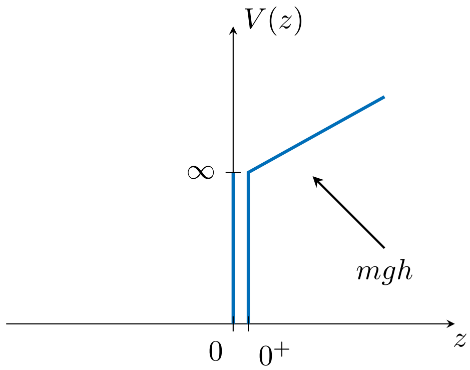
The Lamb shift is $\Delta f_{\text{Lamb}} = 10^9 \ Hz$, so the ratio is:

$$\frac{\Delta f_{\text{finite proton}}}{\Delta f_{\text{Lamb}}} = \frac{5.5 \cdot 10^4}{10^9} = 5.5 \cdot 10^{-5}.$$

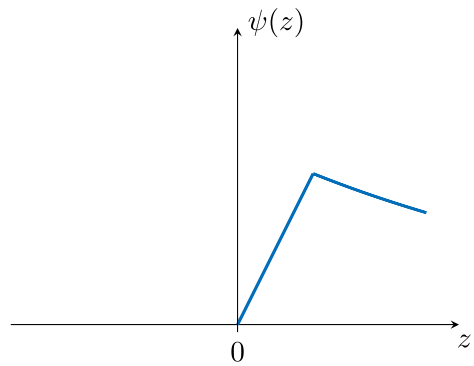
Therefore, for accurately determining the hydrogen energy levels, the Lamb shift is far more significant than the finite extent of the proton.

## Problem IV

a) The potential must be infinity at $z \leq 0$, and at $0^+$ it should be zero because the other tram is being evaluated: $mg(0) = 0$. Then, it increases linearly. For the wavefuction, we know that $\psi(z) = 0, \ z \leq 0$ and it tends to zer oas $z \to \infty$. The sketch of the potential and the ground state are shown below.




(a) Potential $V(z)$




(b) Wavefunction $\psi(z)$

b) The Hamiltonian is:

$$H = -\frac{\hbar^2}{2m}\partial_z^2 + V(z), \quad V(z) = \begin{cases} \infty, & z \leq 0 \\ mgz, & z > 0 \end{cases}.$$

c) The coefficients are found by the normalization condition:

$$\int_0^\infty |\psi(z)|^2 \, dz = 1$$

$$\frac{A^2}{b^2}\int_0^\infty z^2 e^{-2z/b} \, dz =$$

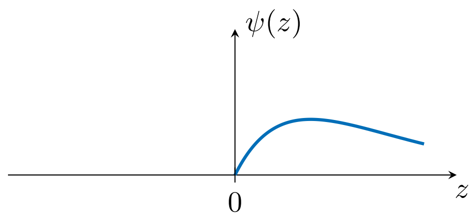
$$\frac{A^2}{b^2}\frac{b^3}{4} = 1$$

$$A = \sqrt{\frac{4}{b}} = \frac{2}{\sqrt{b}}.$$

The integral was computed with calculator. The wavefunction is therefore:

$$\psi(z) = \frac{2}{\sqrt{b}}\frac{z}{b}e^{-z/b}.$$

The sketch is below. It is similar to my guess but softer.




d) The expectation value of $z$ is:

$$\int_0^\infty z|\psi(z)|^2\,dz = \frac{4}{b^3}\int_0^\infty z^3 e^{-2z/b}\,dz = \frac{4}{b^3}\frac{3}{8}b^4 = \frac{3}{2}b.$$

This integral was computed with calculator.

e) We do the analogous process for the expectation value of $H$. The potential energy is easy to compute:

$$\langle V\rangle = \langle mgz\rangle = mg\langle z\rangle = \frac{3}{2}mgb.$$

While, for the kinetic energy, we use direct integration:

$$\begin{aligned}
\langle T\rangle &= \int_0^\infty \psi^*(z)\left[-\frac{\hbar^2}{2m}\partial_z^2\right]\psi(z)\,dz \\
&= -\frac{\hbar^2}{2m}\int_0^\infty \psi^*(z)[\partial_z^2\psi(z)]\,dz \\
&= -\frac{\hbar^2}{2m}\int_0^\infty [\frac{2}{b^{3/2}}ze^{-z/b}][-\frac{2}{b^{1/2}}\frac{1}{b^2}e^{-z/b}(2-z/b)]\,dz \\
&= \frac{\hbar^2}{2m}\frac{4}{b^4}\int_0^\infty z(2-z/b)e^{-2z/b}\,dz \\
&= \frac{\hbar^2}{2m}\frac{4}{b^4}\left[2\int_0^\infty ze^{-2z/b}\,dz - \frac{1}{b}\int_0^\infty z^2e^{-z/b}\,dz\right] \\
&= \frac{\hbar^2}{2m}\frac{4}{b^4}\frac{b^2}{4} \\
\langle T\rangle &= \frac{\hbar^2}{2mb^2}.
\end{aligned}$$

Therefore, because of linearity we have

$$\langle H\rangle = \langle T\rangle + \langle V\rangle = \frac{\hbar^2}{2mb^2} + \frac{3}{2}mgb.$$

f) Minimize $\langle H\rangle$ is the same that select the $b_o$ such that $[\partial_b\langle H\rangle]\big|_{b=b_o} = 0$.

$$\partial_b\langle H\rangle = -\frac{\hbar^2}{mb^3} + \frac{3}{2}mg = 0 \longrightarrow b_0 = \left(\frac{2\hbar^2}{3m^2g}\right)^{1/3} = \left(\frac{h^2}{6\pi^2m^2g}\right)^{1/3}.$$

g) The numberical value is:

$$b_0 = \left[ \frac{(6.626 \times 10^{-34})^2}{6\pi^2 (1.5 \times 10^{-25})^2 (9.8)} \right]^{1/3} \approx 3.2 \times 10^{-7}\ m.$$

h) Putting $b_0$ in $\langle H \rangle$:

$$\langle H \rangle = \frac{(1.055 \times 10^{-34})^2}{2(1.5 \times 10^{-25})(9.8)} + \frac{3}{2}(1.5 \times 10^{-25}(9.8)(3.2 \times^{-7})) \approx 1.1 \times 10^{-30}\ J.$$

i)

$$\frac{\langle H \rangle}{k_B} = \frac{1.1 \times 10^{-30}}{1.4 \times 10^{-23}} = 0.8 \times 10^{-7}\ K.$$

j) For a 100 $kg$ mass, we have

$$b = \left( \frac{4.4 \times 10^{-67}}{5.8 \times 10^{6}} \right)^{1/3} \approx 1.9 \times 10^{-25}\ m.$$

The associated $\langle H \rangle / k_b$ is:

$$\frac{\langle H \rangle}{k_b} = \frac{3 \times 10^{-22}}{1.4 \times 10^{-23}} \approx 21\ K.$$