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 perturber enegy of the ground state is:

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

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:

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

The eigenvalues are:

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

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:

$$\psi_+(x, y) = \frac{1}{\sqrt{2}}(\psi_{12}(x, y) + \psi_{21}(x, y))$$
$$\psi_-(x, y) = \frac{1}{\sqrt{2}}(\psi_{12}(x, y) - \psi_{21}(x, y)).$$

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:

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

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 fround 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:

$$\langle n00|W|n00\rangle = 2E_1a_0\int_0^b r^2|R_{n0}(t)|^2(\frac{1}{r}-\frac{1}{b})\,dr.$$

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

$$\langle 100|W|100\rangle \approx 2E_1a_0\frac{4}{a_0^3}\int_0^b r^2(\frac{1}{r}-\frac{1}{b})\,dr = \frac{8E_1}{a_0^2}\int_0^b(r-\frac{r^2}{b})\,dr = \frac{4}{3}E_1\left(\frac{b}{a_0}\right)^2$$
$$\langle 200|W|200\rangle \approx 2E_1a_0\frac{1}{8a_0^3}\int_0^b r^2(2-\frac{r}{a_0})^2(\frac{1}{r}-\frac{1}{b})\,dr = \frac{1}{6}E_1\left(\frac{b}{a_0}\right)^2.$$

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

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

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:

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

Second order involver 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) sgasga

b) agas

c) safasf

d) asfasf (only compute the expansion asked)

e) dsgsdg

f) sdgsdg

g) sdgsdg

h) sdgsdg

i) sdggs

j) asfasf