

# Assignment 11

## OPTI 570 Quantum Mechanics

### University of Arizona

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Total time: 15 hours

## Problem I

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

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

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

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

The perturber enegy of the ground state is:

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

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

$$E_{12}^0 = E_{21}^0 = \frac{5\hbar^2 \pi^2}{2ma^2}.$$

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:

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

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

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

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:

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

## 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:

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

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 explicitly 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

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

For the degenerate subspace,

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

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 the 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:

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

The 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:

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

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

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

b) The perturbation depends only on  $r$ , so it is purely radial in position representation. 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

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

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:

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

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

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

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

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

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

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

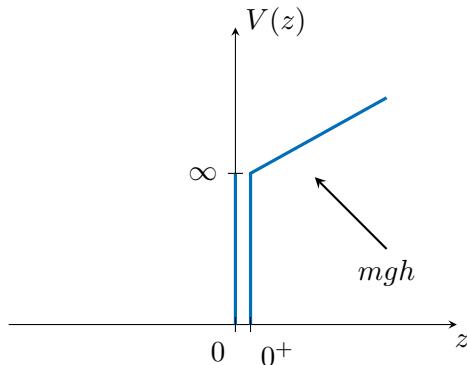
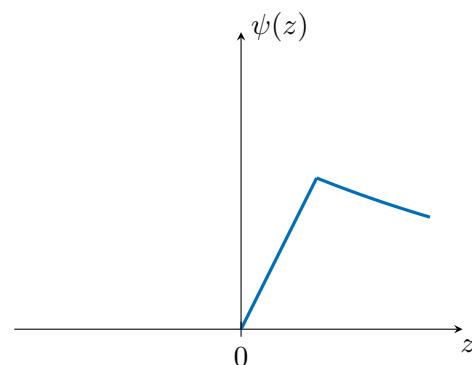
a) The potential must be infinity at  $z \leq 0$ , and at  $0^+$  it should be zero because the other tram is being evaluated:  $mg(0) = 0$ . Then, it increases linearly. For the wavefunction, we know that  $\psi(z) = 0$ ,  $z \leq 0$  and it tends to zero as  $z \rightarrow \infty$ . The sketch of the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

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:

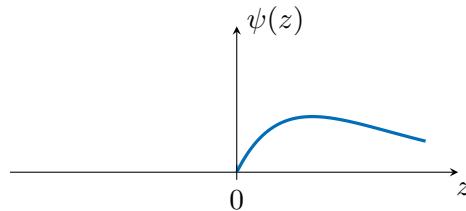
$$\begin{aligned} \int_0^\infty |\psi(z)|^2 dz &= 1 \\ \frac{A^2}{b^2} \int_0^\infty z^2 e^{-2z/b} dz &= \\ \frac{A^2 b^3}{b^2} \frac{4}{4} &= 1 \\ A = \sqrt{\frac{4}{b}} &= \frac{2}{\sqrt{b}}. \end{aligned}$$

(a) Potential  $V(z)$ (b) Wavefunction  $\psi(z)$ 

So the wavefunction is:

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

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



d) The expectation value of  $z$  is:

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

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:

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

Therefore,

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

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

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

g) The numerical value is:

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

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

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

i)

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

j) For a 100 kg mass, we have

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

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

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