Department of Physics
IIT-Madras

PCD_STiAP_Self_Assesment_4
30 marks

1. What are the relativistic corrections due to the perturbation added to the Schrödinger energy levels of the one electron atomic system. Express the terms in detail and explain the dependency of each term with orbital quantum number. – 6 marks

The energy correction terms are:

i. Relativistic kinetic energy term:

$$\Delta E_{\substack{\text{Rel.}\\ \text{K.E.}}} = -E_n \; (Z\alpha)^2 \; \frac{1}{n^2}\left[\frac{3}{4} - \frac{n}{\left(\ell + \frac{1}{2}\right)}\right]$$

; Kinetic energy term is included for all $l$ value

ii. Spin-orbit interactions:

$$\langle H_{\text{spin-orbit}} \rangle = -E_n \; (Z\alpha)^2 \; \frac{\left\{ j(j+1) - \ell(\ell+1) - \frac{3}{4} \right\}}{2n\ell\left(\ell + \frac{1}{2}\right)(\ell+1)}$$

; This term is included for $l \neq 0$; since for s subshell the value is the same.

iii. Darwin term:

$$\langle h'''_{\text{Darwin}} \rangle = \frac{\pi\hbar^2 Z e^2}{2m^2c^2} \langle \psi_{n,\ell=0,m=0} | \delta^3(\vec{r}) | \psi_{n,\ell=0,m=0} \rangle = \frac{\pi\hbar^2 Z e^2}{2m^2c^2} |\psi_{n,\ell=0,m=0}(r=0)|^2 = -\frac{E_n}{n} \; (Z\alpha)^2$$

; This term is included for $l = 0$ subshell alone.

---

2. The good quantum numbers to solve the relativistic fine structure Hamiltonian of Hydrogen atom are $n, l, m_l, m_s$. – 1+2+1 marks

   a. Is the above statement true? If not what are the good quantum numbers?
   The above statement is false. The good quantum numbers for this problem are $n, l, j, m_j$.

   b. Why these are chosen as good quantum number for this problem?
   In this problem, where spin-orbit interaction is included, the angular momentum is no longer $L \bullet S$ as it does not commute with $L_Z$ or $S_Z$. The angular momentum is now the addition of L and S which is represented as $j = L + S$, where

$L \bullet S = \frac{1}{2}\left(J^2 - L^2 - S^2\right)$. With this quantum numbers the operator $L \bullet S$ is diagonal and commutes with all the other operators.

c. Give the eigen values of these quantum numbers.
The eigen values are $E_n, l(l+1)\hbar^2, j(j+1)\hbar^2$ and $m_j\hbar$

---

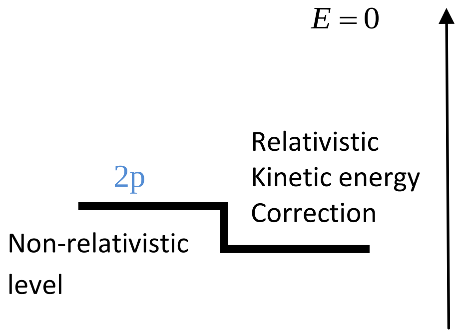
3. For a non-relativistic 2p state, apply the corrections mentioned in question no 1 individually and state the corrected energy level. Sketch roughly the energy level diagram for each correction – 6 marks (2+3+1)

2p state: $n = 2, l = 1$

i. Relativistic Kinetic energy term:

$$\Delta E_{\substack{Rel.\\K.E.}} = -E_n \; (Z\alpha)^2 \; \frac{1}{n^2}\left[\frac{3}{4} - \frac{n}{\left(\ell + \frac{1}{2}\right)}\right]$$

$$= -E_2\left(\frac{Z\alpha}{n}\right)^2\left(-\frac{7}{12}\right)$$




The intrinsically negative energy becomes more negative by a factor of 7/12

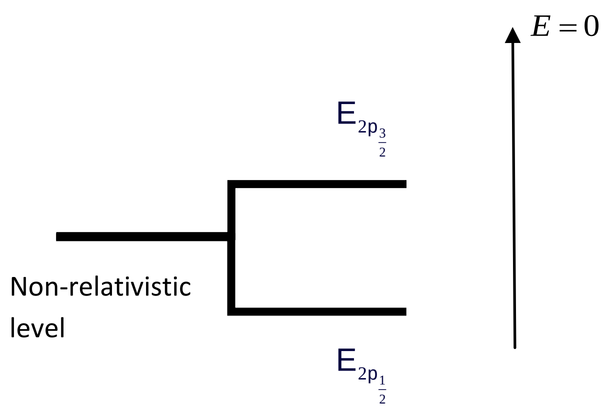
ii. Spin-orbit correction term

$$\left\langle H_{spin-orbit}\right\rangle = -E_n \; (Z\alpha)^2 \; \frac{\left\{j(j+1) - \ell(\ell+1) - \frac{3}{4}\right\}}{2n\ell\left(\ell + \frac{1}{2}\right)(\ell+1)}$$

For $l = 1; j = 1 + \frac{1}{2} = \frac{3}{2}$ or $j = 1 - \frac{1}{2} = \frac{1}{2}$; The numerator will become 1 for j=3/2 and (-2) for j=1/2

$E_{2p_{\frac{3}{2}}} = E_{2p} - E_{2p}\frac{(Z\alpha)^2}{12}$; $E_{2p}$ is intrinsically negative, so we are adding the $E_{2p_{3/2}}$ level which makes the correction less negative than the actual energy level.

$E_{p_{\frac{1}{2}}} = E_{2p} + E_{2p}\frac{(Z\alpha)^2}{6}$ $E_{2p}$ is intrinsically negative, so we are subtracting the $E_{2p_{1/2}}$ level which makes the correction more negative than the actual energy level.




iii. Darwin correction: This correction is applied only for $l=0$ states.

---

4. Fill in the blanks accordingly: _______ + ________ $\longrightarrow$ $A^{**}$ $\longrightarrow$ $e+A^{+*}$ - 2 marks
    a. In photoionization process - $h\nu + A$
    b. In electron-ion scattering process - $e+A^{+}$

---

5. Given the radial equation $R''+\frac{2}{r}R'-\frac{l(l+1)}{r^2}R+\frac{2\mu}{\hbar^2}\left[E-V(r)\right]R=0$; where $R_{\varepsilon l}(r)=\frac{y_{\varepsilon l(r)}}{r}$

   Find out the solution for this differential equation in $y_{\varepsilon l(r)}$ for $s$ wave in zero potential.

   – 5 marks

$$R''+\frac{2}{r}R'-\frac{l(l+1)}{r^2}R+\frac{2\mu}{\hbar^2}\left[E-V(r)\right]R=0 \qquad R_{\varepsilon l}(r)=\frac{y_{\varepsilon l(r)}}{r}$$

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dr^2}+\left\{V(r)+\frac{1}{2m}\frac{l(l+1)}{r^2}\right\}-E\right]y_{\varepsilon l}(r)=0$$

For zero potential: V(r) = 0

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dr^2}+\left\{\frac{1}{2m}\frac{l(l+1)}{r^2}\right\}-E\right]y_{\varepsilon l}(r)=0$$

For s state: $l=0$

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dr^2}-E\right]y_{\varepsilon,l=0}(r)=0$$

$$\frac{(\hbar k)^2}{2m}=\frac{p^2}{2m}=E$$

$$k=\frac{p}{\hbar}=\frac{\sqrt{2mE}}{\hbar}$$

$$\left[\frac{d^2}{dr^2}+k^2\right]y_{\varepsilon,l=0}(r)=0$$

$$\Rightarrow y_{\varepsilon,l=0}(r) = rR_{\varepsilon,l=0}(r) = Ne^{\pm ikr}$$

$$\Rightarrow R_{\varepsilon,l=0}(r) = N\frac{e^{\pm ikr}}{r} \rightarrow N\frac{\sin(kr)}{r};$$

$\frac{\cos(kr)}{r}$ blows up as r $\longrightarrow$ 0 and N is normalization constant.

---

6. Given the solution for the plane wave equation along z direction $e^{i\vec{k}\bullet\vec{r}} = \sum_{l=0}^{\infty} a_l P_l(\cos\theta) j_l(\rho)$ in terms of spherical Bessel functions: Show that the value of $a_l = i^l(2l+1)$ with $\rho = kr$ and $\mu = \cos\theta$ and $\int_{-1}^{+1} e^{i\rho\mu} P_l(\mu)\, d\mu = a_l\left[\frac{2}{2l+1}\right] j_l(\rho)$ - 4 marks

Taking LHS of given equation $\int_{-1}^{+1} e^{i\rho\mu} P_l(\mu)\, d\mu = \int_{-1}^{+1} P_l(\mu) e^{i\rho\mu} d\mu$; Integrating by parts

$$= \left[P_l(\mu)\frac{e^{i\rho\mu}}{i\rho}\right]_{-1}^{+1} - \int_{-1}^{+1} P_l^{'}(\mu)\frac{e^{i\rho\mu}}{i\rho}\, d\mu$$

We know that
$$P_l(\mu = 1) = 1$$
$$P_l(\mu = -1) = (-1)^l P_l(\mu = 1) = (-1)^l$$

$\int_{-1}^{+1} e^{i\rho\mu} P_l(\mu)\, d\mu = \frac{e^{i\rho} - (-1)^l e^{-i\rho}}{i\rho} - \frac{1}{i\rho}\int_{-1}^{+1} P_l^{'}(\mu) e^{i\rho\mu} d\mu$; The second term can be ignored as the further integration will give $1/\rho^2$ which is negligible when compared to $1/\rho$ .

Now we have: $\frac{e^{i\rho} - (-1)^l e^{-i\rho}}{i\rho} = a_l\left[\frac{2}{2l+1}\right] j_l(\rho)$ --------------------- (1)

Taking LHS $e^{il\pi} = \left(e^{i\pi}\right)^l = (-1)^l$ Sub in eq (1)

$$\frac{e^{i\rho} - e^{il\pi} e^{-i\rho}}{i\rho} = a_l\left[\frac{2}{2l+1}\right] j_l(\rho)$$

$$\left[\frac{e^{i\rho} - e^{i\frac{l\pi}{2}} e^{i\frac{l\pi}{2}} e^{-i\rho}}{i\rho}\right] = a_l\left[\frac{2}{2l+1}\right] j_l(\rho)$$

$$e^{i\frac{l\pi}{2}}\left[\frac{e^{i\rho} e^{-i\frac{l\pi}{2}} - e^{i\frac{l\pi}{2}} e^{-i\rho}}{i\rho}\right] = a_l\left[\frac{2}{2l+1}\right] j_l(\rho) \text{ --------------------------- (2)}$$

$$e^{il\pi} = \left(e^{i\pi}\right)^l = (-1)^l = \left(i^2\right)^l = i^{2l}$$

$$e^{i\frac{l\pi}{2}} = i^l$$

Sub this in eq (2)

$$a_l\left[\frac{2}{2l+1}\right] j_l(\rho) = i^l\left[\frac{e^{i\left(\rho-\frac{l\pi}{2}\right)} - e^{-i\left(\rho-\frac{l\pi}{2}\right)}}{i\rho}\right] = i^l\left[\frac{2i\sin\left(\rho-\frac{l\pi}{2}\right)}{i\rho}\right]$$

$$Now, \quad j_l(\rho) \underset{\rho\to\infty}{=} \frac{\sin\left(\rho-\frac{l\pi}{2}\right)}{\rho} \Rightarrow a_l = i^l\left(2l+1\right)$$

---

7.

a. What is that symmetry which connect the solutions of scattering theory with photoionization process : Time reversal symmetry

b. The above mentioned symmetry is a discrete symmetry like parity and charge conjugation.

c. State true or false:

$[\vec{r},\Theta]_- = 0$ : True

$[\vec{p},\Theta]_- = 0$ : False

- 2 mark

---