Department of Physics
IIT-Madras

PCD_STiAP_Self_Assesment_2
70 marks

Q1. [a] The radial part of the Schrodinger differential equation for the Hydrogen atom is written below with an unknown 'C':

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dR(r)}{dr}\right)+C_\ell(r)+\frac{2m}{\hbar^2}\left[E-V(r)\right]R(r)=0.$$

Find C and express your answer here: $C_\ell(r)=-\frac{l(l+1)}{r^2}R(r)$, Centrifugal term

→2 marks

Q1. [b] The radial part of the Schrodinger differential equation for the Hydrogen atom, **inclusive** of the 'centrifugal' term $C_\ell(r)$ has eigenvalues E which can be written as one the two expressions given below.

Place a tick mark ✓ in the box corresponding to the correct expression below:

$E=E_n \rightarrow$ independent of ℓ [√]

$E=E_{n,\ell} \rightarrow$ depending on ℓ [ ]

→2 marks

Q1. [c] (i) The Casimir operator for the SO(3) symmetry group of the Hydrogen atom is_______J^2________________ and its eigenvalues is $\hbar j(j+1)$

(ii) One of the two Casimir operators for the SO(4) symmetry group of the Hydrogen atom is: $c_1=I^2+K^2$ and its eigenvalues are: $\hbar^2 i(i+1)$; $\hbar^2 k(k+1)$

(iii) The *other* Casimir operator for the SO(4) symmetry group of the Hydrogen atom is: $c_2=I^2-K^2$ and its eigenvalues are: $\hbar^2 i(i+1)$; $\hbar^2 k(k+1)$

→6 marks

Q2. [a] When the angular momentum is half-integer, place a tick mark ✓ in the box corresponding to the correct expression below, $U_R(\theta)$ being the rotation operator corresponding to rotation through the angle θ:

$U_R(\theta+2\pi)=-U_R(\theta)$ [√]

or

$U_R(\theta+2\pi)=+U_R(\theta)$ [ ]

<u>Write your 'proof' in the space below</u>:

For half integer angular part $\vec{J}=\frac{1}{2}\hbar\vec{\sigma}$

$$U_R\left(\theta\hat{\theta}\right) = \mathrm{e}^{-i\frac{\theta}{2}\hat{\theta}\cdot\vec{\sigma}}$$

$$U_R\left(\theta = 2\pi, \hat{\theta} = \hat{e}_z\right) = \mathrm{e}^{-i\frac{2\pi}{2}\hat{e}_z\cdot\vec{\sigma}} = \mathrm{e}^{-i\pi\sigma_z}$$

$$= \cos\left(\pi\sigma_z\right) - i\sin\left(\pi\sigma_z\right)$$

$$= \cos\left(\pi\begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix}\right) - i\sin\left(\pi\begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix}\right)$$

$$= \begin{bmatrix}\cos\pi & 0\\ 0 & \cos(-\pi)\end{bmatrix}$$

$$= \begin{bmatrix}-1 & \\ & -1\end{bmatrix} = -1\begin{bmatrix}1 & \\ & 1\end{bmatrix}$$

$U(\theta + 2\pi) = -U(\theta)$ →5 marks

Q2. [b] (i) The 'orbital angular momentum selection rule' for electric dipole transition is:

$$\Delta l = 0, \pm 1$$

(ii) The 'spin angular momentum selection rule' for electric dipole transition is:

$$\Delta s = 0$$

(iii) The 'total angular momentum selection rule' for electric dipole transition is:

$$\Delta j = 0, \pm 1$$

(iv) The Wigner-Eckart theorem is:

$$\left\langle j'm'\middle|T_q^{(k)}\middle| jm\right\rangle = \frac{\left\langle j'\left\|T_q^{(k)}\right\| j\right\rangle}{\sqrt{2j'+1}}\left(j'm'\middle|mq\right)$$ →5 marks

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Q3(a). Obtain the matrix representation for the operator $J_- = J_x - iJ_y$ in the common eigenbasis of J^2, J_z for the case of spin-half angular momentum and <u>write the required matrix representation in the space below</u>: j=1/2; m=1/2,-1/2 ; 2 dimensional basis $\left\{\left|\frac{1}{2},\frac{1}{2}\right\rangle, \left|\frac{1}{2},-\frac{1}{2}\right\rangle\right\}$

$$\mathbb{J}_- = \begin{bmatrix}\left\langle\frac{1}{2},\frac{1}{2}\middle|J_-\middle|\frac{1}{2},\frac{1}{2}\right\rangle & \left\langle\frac{1}{2},\frac{1}{2}\middle|J_-\middle|\frac{1}{2},-\frac{1}{2}\right\rangle\\ \left\langle\frac{1}{2},-\frac{1}{2}\middle|J_-\middle|\frac{1}{2},\frac{1}{2}\right\rangle & \left\langle\frac{1}{2},-\frac{1}{2}\middle|J_-\middle|\frac{1}{2},-\frac{1}{2}\right\rangle\end{bmatrix}$$ ----------- (1)

$$\mathbb{J}_- = \begin{bmatrix} 0 & 0 \\ \left\langle \frac{1}{2},-\frac{1}{2} \middle| J_- \middle| \frac{1}{2},\frac{1}{2} \right\rangle & 0 \end{bmatrix} \text{----------- (2)}$$

$$\langle j, m-1 | J_- | jm \rangle = +\hbar\sqrt{j(j+1) - m(m-1)}$$

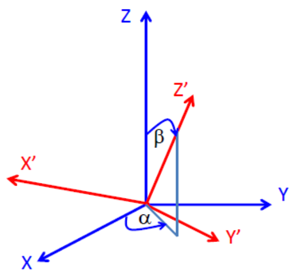
From eq (2)

$$\left\langle \frac{1}{2},-\frac{1}{2} \middle| J_- \middle| \frac{1}{2},\frac{1}{2} \right\rangle = +\hbar\sqrt{\frac{1}{2}\left(\frac{1}{2}+1\right) - \frac{1}{2}\left(\frac{1}{2}-1\right)} = +\hbar\sqrt{\frac{3}{4}+\frac{1}{4}} = \hbar$$

$$\mathbb{J}_- = \hbar \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix}$$

→4 marks

Q3(b). It is given that $Y_{\ell m}(\theta\varphi) = \sum_{m'=-\ell}^{\ell} D_{mm'}^{(\ell)*}(R) Y_{\ell m'}(\theta'\varphi')$ → we have expanded the spherical harmonic function using the Wigner D functions. Find $Y_{\ell m}(\theta\varphi)$ corresponding to a point on the Z' axis. Give your answer in the space below:



$$Y_{\ell m}(\theta\varphi) = \sum_{m'=-\ell}^{\ell} D_{mm'}^{(\ell)*}(R) Y_{\ell m'}(\theta'\varphi')$$

For a point on Z' axis $\theta = \beta; \varphi = \alpha; \theta' = 0$

$$Y_{\ell m}(\beta\alpha) = \sum_{m'=-\ell}^{\ell} D_{mm'}^{(\ell)*}(R) Y_{lm'}(0\varphi') \text{ ----------- (1)}$$

For every value of l and m'; $$Y_{lm'}(0\varphi') = \sqrt{\frac{2l+1}{4\pi}}\delta_{m'0} \text{ ---------------- (2)}$$

$$Y_{\ell m}(\beta\alpha) = D_{m0}^{(\ell)*}(R)\sqrt{\frac{2l+1}{4\pi}} \text{ -------------- (3)}$$

We know that, $$Y_{\ell m}(\theta'\varphi') = \sum_{m'=-\ell}^{\ell} D_{m'm}^{(\ell)}(R) Y_{\ell m'}(\theta\varphi)$$

for $m = 0$: $$Y_{\ell 0}(\theta'\varphi') = \sum_{m'=-\ell}^{\ell} D_{m'0}^{(\ell)}(R) Y_{\ell m'}(\theta\varphi)$$ from eq (3)

$$Y_{\ell 0}(\theta'\varphi') = \sum_{m'=-\ell}^{\ell} \sqrt{\frac{4\pi}{2l+1}} Y^*_{lm'}(\beta,\alpha) Y_{\ell m'}(\theta\varphi)$$

Using m instead of m' and substituting Legendre polynomial

$$\sqrt{\frac{2\ell+1}{4\pi}} P_\ell(\cos\theta') = \sum_{m=-\ell}^{\ell} \sqrt{\frac{4\pi}{2\ell+1}} Y^*_{\ell m}(\beta,\alpha) Y_{\ell m}(\theta\varphi)$$

$$P_\ell(\cos\theta') = \frac{4\pi}{2\ell+1} \sum_{m=-\ell}^{\ell} Y^*_{\ell m}(\beta,\alpha) Y_{\ell m}(\theta\varphi)$$

→4 marks

Q3(c). Is the transition (j=0) → (j=0) allowed as per the dipole selection rules? Explain your answer in the space below:

The transition (j=0) → (j=0) cannot take place under any selection rules. Since this transitions do not possess a net orbital angular momentum.

From triangular law of inequality, we have $|j-j'| \le 1 \le |j+j'|$ For (j=0) → (j'=0)

$j+j'=0$; This is not greater or equal to unity.

Therefore, the selection rule is violated.

→2 marks

Q4. A point mass particle whose rest-mass is m and energy E moves at a constant velocity v (with respect to an inertial frame S) in a 'zero-potential' region. Given: $\gamma = 1/\sqrt{1-(v^2/c^2)}$.

Place a tick mark ✓ in the 'appropriate True/False boxes' below:

(a) According to classical non-relativistic mechanics, $E = \gamma mc^2$ ☐ True ☑ False

Give a brief reason justifying your answer in the little space below & if false, rectify the statement:

$$E = \gamma mc^2 = \left(1 - \frac{v^2}{c^2}\right)^{-1/2} mc^2$$

$$= \left(1 + \frac{1}{2}\frac{v^2}{c^2} + \frac{1}{4}\frac{v^2}{c^2} + \ldots\ldots\ldots\right) mc^2$$

In Classical non-relativistic mechanic, $v << c$

$$\therefore E = \left(1 + \frac{1}{2}\frac{v^2}{c^2}\right) mc^2 \qquad \Rightarrow E = mc^2 + \frac{1}{2}mv^2$$

(b) According to classical relativistic mechanics, the 4-velocity is given by $\gamma \frac{d\vec{r}}{dt}$ ☐ True ☑ False

Give a brief reason justifying your answer in the little space below & if false, rectify the statement:

The four velocity is given by $\eta^\mu (\mu = 0,1,2,3)$, where

$$\eta^0 = \gamma c; \eta^1 = \gamma \frac{dx^1}{dt}; \eta^2 = \gamma \frac{dx^2}{dt}; \eta^3 = \gamma \frac{dx^3}{dt}$$

$$\eta^\mu = \gamma c, \gamma \frac{d\vec{r}}{dt}$$

(c) According to relativistic mechanics, the 'momentum' is given by $\vec{p} = \gamma \vec{v}$ ☐True ☑False

Give a brief reason justifying your answer in the little space below & if false, rectify the statement:

Proper momentum; $p^\mu (\mu = 0,1,2,3)$

$$p^0 = m\gamma c;\ p^1 = m\gamma \frac{dx^1}{dt};\ p^2 = m\gamma \frac{dx^2}{dt};\ p^3 = m\gamma \frac{dx^3}{dt}$$

$$p^\mu = m\gamma c, m\gamma \vec{v}$$

(d) According to quantum relativistic mechanics, the leading term in the relativistic correction to the kinetic energy goes as $\frac{v^2}{c^2}$. ☑True ☐False

Give a brief reason justifying your answer in the little space below & if false, rectify the statement:

$$K.E = E - mc^2$$

$$= mc^2 \left(1 - \frac{v^2}{c^2}\right)^{-1/2} - mc^2$$

$$= mc^2 \left(1 + \frac{1}{2}\frac{v^2}{c^2} + \frac{1}{4}\frac{v^2}{c^2} + ...\right) - mc^2$$

$$= mc^2 \left(\frac{1}{2}\frac{v^2}{c^2} + \frac{1}{4}\frac{v^2}{c^2} + ...\right)$$

(e) The spin-orbit interaction for an electron in $n = 10$ excited state is just as strong as that for the electron in the ground state $n = 1$ for the H atom. ☐True ☑False

Give a brief reason justifying your answer in the little space below & if false, rectify the statement:

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

$$\Rightarrow \langle H_{spin-orbit} \rangle \alpha \frac{1}{n^2}$$

→10 marks

Q5. The first Foldy-Woutheysen transformation of the Dirac Hamiltonian

$$H = \beta mc^2 + c\vec{\alpha}\cdot(\vec{p} - e\vec{A}) + e\phi$$

$$= \beta mc^2 + \quad \theta + \quad \varepsilon \quad \{\text{where } \theta = c\vec{\alpha}\cdot(\vec{p} - e\vec{A}) \text{ and } \varepsilon = e\phi\}$$

for an electron in an EM field is effected through the operator $S_1 = \frac{-i\beta\theta}{2mc^2}$.

Find the coefficients X,B and C in the following expression:

$$\boxed{i[S,H]_- = X\theta + B\beta\theta^2 + C[\theta,\varepsilon]_-}$$

NOTE: You may use additional space at the end of this book, or a supplement (<u>which also must be submitted</u>), but <u>the final answer MUST be given below in the space provided</u>:

$$i[S,H]_- = i\left[\frac{-i\beta\theta}{2mc^2}, \beta mc^2 + \theta + \varepsilon\right]_-$$

$$= \left[\frac{\beta\theta}{2mc^2}, \beta mc^2\right]_- + \left[\frac{\beta\theta}{2mc^2}, \theta\right]_- - \left[\frac{\beta\theta}{2mc^2}, \varepsilon\right]_-$$

$$= \frac{1}{2}\left(\beta\theta\beta - \beta^2\theta\right) + \frac{1}{2mc^2}\left(\beta\theta^2 - \theta\beta\theta\right) + \frac{1}{2mc^2}\left(\beta\theta\varepsilon - \varepsilon\beta\theta\right)$$

$$\beta\theta = -\theta\beta$$
$$\beta\varepsilon = \varepsilon\beta$$

$$= \frac{1}{2}\left(-\beta\beta\theta - \beta^2\theta\right) + \frac{1}{2mc^2}\left(\beta\theta^2 + \beta\theta\theta\right) + \frac{1}{2mc^2}\left(\beta\theta\varepsilon - \beta\varepsilon\theta\right)$$

$$i[S,H]_- = -\theta + \frac{\beta\theta^2}{mc^2} + \frac{1}{2mc^2}\beta[\theta,\varepsilon]_-$$

$$X = -1; B = \frac{1}{mc^2}; C = \frac{\beta}{2mc^2}$$

→10 marks

Q6(a). Consider 2-electron wavefunction $\psi(q_1,q_2) = \phi(\vec{r}_1,\vec{r}_2)\chi(\zeta_1,\zeta_2)$ made up as an antisymmetrized product of 1-electron spin-orbitals $\phi_{n_i,l_i,m_{l_i}}(\vec{r}_j)\,\chi_{m_{s_i}}(\zeta_j)$. Now, if the two-electron state has for its spin-part the function given by $\chi(\zeta_2,\zeta_1) = +\chi(\zeta_1,\zeta_2)$, write its spatial-part $\phi(\vec{r}_1,\vec{r}_2)$ <u>in the blank space below</u>:

$$\phi(\vec{r}_1,\vec{r}_2) = -\phi(\vec{r}_1,\vec{r}_2)$$

→2 marks

Q6(b). Find the basis of spatial functions in which the coulomb interaction $1/r_{12}$ has a diagonal representation and <u>write your answer in the blank space below</u>:

The required two-dimensional basis is:

$\{\varphi_1(\vec{r}_1)\varphi_2(\vec{r}_2), \varphi_1(\vec{r}_2)\varphi_2(\vec{r}_1)\}$ In this basis the coulomb interaction is not diagonal; so operate

$T_{2\times 2} = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & -1 \\ 1 & 1 \end{bmatrix}$ on the basis to diagonalize.

$$= T_{2\times 2}\begin{bmatrix} \varphi_1(\vec{r}_1)\varphi_2(\vec{r}_2) \\ \varphi_1(\vec{r}_2)\varphi_2(\vec{r}_1) \end{bmatrix}$$

$$= \frac{1}{\sqrt{2}}\begin{bmatrix} \varphi_1(\vec{r}_1)\varphi_2(\vec{r}_2) - \varphi_1(\vec{r}_2)\varphi_2(\vec{r}_1) \\ \varphi_1(\vec{r}_1)\varphi_2(\vec{r}_2) + \varphi_1(\vec{r}_2)\varphi_2(\vec{r}_1) \end{bmatrix} = \begin{bmatrix} \phi^{Triplet} \\ \phi^{Single} \end{bmatrix}$$

→2 marks

Q6(c). Write in the space below the mathematical equality that expresses the Koopmans theorem and explain each term that goes into the equation.

$$E\left(\psi^{(N)}\right) - E\left(\psi^{(N-1)}\right)_{(n_k=0)} = \varepsilon_k = -\lambda_{kk}$$

1st term: Energy equation for N electron system
2nd term: Energy term for N-1 electron system, i.e after removal of one electron from kth orbital under frozen orbital approximation
The difference gives the energy of the kth orbital of the system. λ being the Lagrange variational multiplier; n_k occupation no: of kth electron.

→3 marks

Q6(d). Explain, in the space below, what is meant by the 'frozen orbital approximation'.

Variations in the single particle orbitals are made one at a time, which is to say that the other N-1 orbitals are considered 'frozen' during the consideration of variation in each orbital.

→3 marks

Q7 Fill in the blanks below:

(i) Given that the total electron scattering wavefunction is:

$$\psi_{Tot} \xrightarrow[r\to\infty]{} \frac{1}{2ikr}\sum_l c_l(2l+1)\left[P_l(\cos\theta)e^{i(kr+\delta_l)} - P_l(-\cos\theta)e^{-i(kr+\delta_l)}\right].$$

As per the 'outgoing' wave boundary conditions, $c_l = e^{i\delta_l(k)}$.

(ii) As per the 'ingoing' wave boundary conditions, $c_l = e^{-i\delta_l(k)}$.

(iii) The physical dimensions of the quantity

$$\left(\frac{qA_0(\omega)}{mc}\right)^2 \left|\left\langle f \,|\, e^{i\vec{k}\bullet\vec{r}}\hat{\varepsilon}\bullet\vec{\nabla} \,|\, i\right\rangle\right|^2 \times 2\pi\delta(\tilde{\omega})$$

are: T^{-1} (transition probability per unit time)

(iv) In the presence of an electric field, the lifetime of the 2s state of the hydrogen atom would **(place a tick mark ✓ in the appropriate box below)**:

decrease [$\surd$], *or* *remain same* [ ], *or* *increase* [ ], as compared to the atom being just by itself in vacuum.

Reason (state in the space below):

In the presence of the applied electric field, the metastable 2s state develops some character of the unstable 2p state. This results in a slight shortening of the lifetime of the 2s state via a radiative (2s, 2p) mixed state to 1s transition.

→3+2=5 marks for Q7.

Q8. Express the coupled angular momentum with $j=\frac{1}{2}, m=-\frac{1}{2}$ as a linear combination of direct product vectors resulting from the coupling of two angular momenta $j_1=1,\ j_2=\frac{1}{2}$. Use the CGC tables given below and write your answer in the space provided below that:

TABLE 1³. $(j_1\ \tfrac{1}{2}\ m_1\ m_2 | j_1\ \tfrac{1}{2}\ j\ m)$

$j=$	$m_2=\frac{1}{2}$	$m_2=-\frac{1}{2}$
$j_1+\frac{1}{2}$	$\sqrt{\dfrac{j_1+m+\frac{1}{2}}{2j_1+1}}$	$\sqrt{\dfrac{j_1-m+\frac{1}{2}}{2j_1+1}}$
$j_1-\frac{1}{2}$	$-\sqrt{\dfrac{j_1-m+\frac{1}{2}}{2j_1+1}}$	$\sqrt{\dfrac{j_1+m+\frac{1}{2}}{2j_1+1}}$

Write your answer in this box:

Given $j=1/2; m=-1/2$

For $m=-1/2$ the values m_1 and m_2 can take are -1,1/2 and 0,-1/2

The direct product equation is given by

$\left|\frac{1}{2}-\frac{1}{2}\right\rangle = C_1\left|-1\frac{1}{2}\right\rangle + C_2\left|0-\frac{1}{2}\right\rangle$ From the table C_1 and C_2 can be found.

C_1: Given $j_1 = 1$ and $j=1/2$; $m_2 = ½$ and $m = -1/2$

$$C_1 = -\sqrt{\frac{j_1 - m + \frac{1}{2}}{2j_1 + 1}} = -\sqrt{\frac{1 - \left(-\frac{1}{2}\right) + \frac{1}{2}}{2(1) + 1}} = -\sqrt{\frac{2}{3}}$$

C_2: Given $j_1 = 1$ and $j=1/2$; $m_2 = -1/2$ and $m = -1/2$

$$C_2 = \sqrt{\frac{j_1 + m + \frac{1}{2}}{2j_1 + 1}} = -\sqrt{\frac{1 + \left(-\frac{1}{2}\right) + \frac{1}{2}}{2(1) + 1}} = \sqrt{\frac{1}{3}}$$

$$\left|\frac{1}{2} - \frac{1}{2}\right\rangle = -\sqrt{\frac{2}{3}}\left|-1\frac{1}{2}\right\rangle + \sqrt{\frac{1}{3}}\left|0 - \frac{1}{2}\right\rangle$$

$$\left|\left(1, \ \frac{1}{2}\right) \ \frac{1}{2}, \ -\frac{1}{2}\right\rangle = -\sqrt{\frac{2}{3}}\left|-1\frac{1}{2}\right\rangle + \sqrt{\frac{1}{3}}\left|0 - \frac{1}{2}\right\rangle$$

→5 marks.