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

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

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

\[ \Rightarrow 2 \text{ marks} \]

Q1. [b] The radial part of the Schrödinger 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 \( \checkmark \) in the box corresponding to the correct expression below:

\[ E = E_n \rightarrow \text{independent of } \ell \ \checkmark \]
\[ E = E_{n,\ell} \rightarrow \text{depending on } \ell \ \square \]

\[ \Rightarrow 2 \text{ marks} \]

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: \( \hbar^2 i(i+1) \); \( \hbar^2 k(k+1) \)

\[ \Rightarrow 6 \text{ marks} \]

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

\[ U_\ell(\theta + 2\pi) = -U_\ell(\theta) \ \checkmark \]

or

\[ U_\ell(\theta + 2\pi) = +U_\ell(\theta) \ \square \]

Write your ‘proof’ in the space below:

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

\[ \langle j'm'|T_q^{(k)}|jm \rangle = \frac{\langle j'|T_q^{(k)}|j \rangle}{\sqrt{j'+1}} \langle j'm'|mq \rangle \] → 5 marks

Q3(a). Obtain the matrix representation for the operator \( J_z = J_x - iJ_y \) in the common eigenbasis of \( J^2, J_z \) for the case of spin-half angular momentum and write the required matrix representation in the space below:

\[
J_z = \begin{bmatrix}
\langle \frac{1}{2}, \frac{1}{2} | J | \frac{1}{2}, \frac{1}{2} \rangle & \langle \frac{1}{2}, \frac{1}{2} | J | \frac{1}{2}, -\frac{1}{2} \rangle \\
\langle \frac{1}{2}, -\frac{1}{2} | J | \frac{1}{2}, \frac{1}{2} \rangle & \langle \frac{1}{2}, -\frac{1}{2} | J | \frac{1}{2}, -\frac{1}{2} \rangle
\end{bmatrix}
\] → 5 marks

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\[ \mathcal{J}_- = \begin{bmatrix} 1 & 0 \\ -1 & 0 \\ 1 & 0 \end{bmatrix} \quad \text{(2)} \]

\[ \langle j, m - 1 | J_- | jm \rangle = +h \sqrt{j(j+1) - m(m-1)} \]

From eq (2)

\[ \langle \frac{1}{2}, -\frac{1}{2} | J_- | \frac{1}{2}, \frac{1}{2} \rangle = +h \sqrt{\left(\frac{1}{2} + 1\right) - \left(\frac{1}{2} - 1\right)} = +h \sqrt{\frac{3}{4} + \frac{1}{4}} = h \]

\[ \mathcal{J}_- = h \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix} \]

→ 4 marks

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

\[ Y_{lm}(\theta\phi) = \sum_{m'=-\ell}^{\ell} D_{mm'}^{(l\ast)}(R) Y_{lm}(\theta'\phi') \]

For a point on Z’ axis \( \theta = \beta; \varphi = \alpha; \theta' = 0 \)

\[ Y_{lm}(\beta\alpha) = \sum_{m'=-\ell}^{\ell} D_{mm'}^{(l\ast)}(R) Y_{lm}(0\phi') \quad \text{(1)} \]

For every value of \( l \) and \( m' \);

\[ Y_{lm}(0\phi') = \sqrt{\frac{2l+1}{4\pi}} \delta_{m,0} \quad \text{(2)} \]

\[ Y_{lm}(\beta\alpha) = D_{m0}^{(l\ast)}(R) \sqrt{\frac{2l+1}{4\pi}} \quad \text{(3)} \]

We know that,

\[ Y_{lm}(\theta'\phi') = \sum_{m'=-\ell}^{\ell} D_{mm'}^{(l)}(R) Y_{lm}(\theta\phi) \]

for \( m = 0 \) \( Y_{l0}(\theta'\phi') = \sum_{m=-\ell}^{\ell} D_{m0}^{(l)}(R) Y_{l0m}(\theta\phi) \) from eq (3)
\[ Y_{\ell m}(\theta, \phi) = \sum_{m=-\ell}^{\ell} \sqrt{\frac{4\pi}{2\ell + 1}} Y_{m}^{*} (\beta, \alpha) Y_{\ell m} (\theta, \phi) \]

Using \( m \) instead of \( m' \) and substituting Legendre polynomial \( P_{\ell} (\cos \theta') = \sum_{m=\ell}^{\ell} \sqrt{\frac{4\pi}{2\ell + 1}} Y_{m}^{*} (\beta, \alpha) Y_{\ell m} (\theta, \phi) \)

\[ \rightarrow 4 \text{ marks} \]

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

The transition \( (j=0) \rightarrow (j=0) \) 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 \( |j - j'| \leq 1 \leq |j + j'| \) For \( (j=0) \rightarrow (j'=0) \)

\( j + j' = 0 \); This is not greater or equal to unity.

Therefore, the selection rule is violated.

\[ \rightarrow 2 \text{ marks} \]

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 \( \checkmark \) in the ‘appropriate True/False boxes’ below:

(a) According to classical non-relativistic mechanics, \( E = \gamma mc^2 \) \( \square \) True \( \sqrt{\text{False}} \)

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

\[ E = \gamma mc^2 = \left(1 - \frac{v^2}{c^2}\right)^{-1/2} mc^2 = \left(1 + \frac{1}{2} \frac{v^2}{c^2} + \frac{1}{4} \frac{v^2}{c^2} + \ldots \right) mc^2 \]

In Classical non-relativistic mechanic, \( v << c \)

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

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

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**

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

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

\[ p^0 = mc; p^1 = mc, \gamma \frac{d\vec{r}}{dt}; p^2 = mc \frac{dx^2}{dt}; p^3 = mc \frac{dx^3}{dt} \]

\[ p^\mu = mc, \gamma v \]

(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**

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

\[ \begin{align*}
K.E &= E - mc^2 \\
&= mc^2 \left(1 - \frac{v^2}{c^2}\right)^{-1/2} - mc^2 \\
&= mc^2 \left(1 + \frac{1}{2} \frac{v^2}{c^2} + \frac{1}{4} \frac{v^2}{c^2} + \ldots \right) - mc^2 \\
&= mc^2 \left(1 + \frac{1}{4} \frac{v^2}{c^2} + \ldots \right)
\end{align*} \]

(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. **False**

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

\[ \begin{align*}
\langle H_{\text{spin-orbit}} \rangle &= -E_n \ (Z\alpha)^2 \ \frac{j(j+1) - \ell(\ell+1) - \frac{3}{4}}{2n\ell\left(\ell + \frac{1}{2}\right)(\ell+1)} \\
\Rightarrow \langle H_{\text{spin-orbit}} \rangle &= \frac{1}{n^2} \quad \rightarrow 10 \text{ marks}
\end{align*} \]
Q5. The first Foldy-Wouthuysen transformation of the Dirac Hamiltonian
\[ H = \beta mc^2 + c\alpha \cdot (\vec{p} - e\vec{A}) + e\phi \]

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

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

Find the coefficients \( X, B \) and \( C \) in the following expression:
\[ i[S,H] = X\theta + B\beta\theta^2 + C[0,\varepsilon] \]

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

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

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

\[ = \frac{1}{2} (\beta\theta - \beta^2\theta) + \frac{1}{2mc^2} (\beta\theta^2 - \theta\beta\theta) + \frac{1}{2mc^2} (\beta\theta\varepsilon - \varepsilon\beta\theta) \]

\[ \beta\theta = -\theta \quad \beta\varepsilon = \varepsilon \beta \]

\[ = \frac{1}{2} (\beta\theta - \beta^2\theta) + \frac{1}{2mc^2} (\beta\theta^2 + \beta\theta\theta) + \frac{1}{2mc^2} (\beta\theta\varepsilon - \beta\varepsilon\theta) \]

\[ i[S,H] = -\theta + \frac{\beta\theta^2}{m c^2} + \frac{1}{2mc^2} \beta[0,\varepsilon] \]

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

\( \rightarrow 10 \text{ marks} \)

Q6(a). Consider 2-electron wavefunction \( \psi(q_1, q_2) = \phi(r_1, r_2) \chi(\zeta_1, \zeta_2) \) made up as an antisymmetrized product of 1-electron spin-orbitals \( \phi_{n_i l_i m_i} (\vec{r}_i) \chi_{m_i} (\zeta_j) \). 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 \( \phi(r_1, r_2) \) in the blank space below:

\[ \phi(r_1, r_2) = -\phi(r_1, r_2) \]

\( \rightarrow 2 \text{ marks} \)

Q6(b). Find the basis of spatial functions in which the coulomb interaction \( 1/r_2 \) has a diagonal representation and write your answer in the blank space below:

The required two-dimensional basis is:
\[
\{ \varphi_1(\vec{r}_1), \varphi_2(\vec{r}_1), \varphi_3(\vec{r}_2), \varphi_2(\vec{r}_1) \}\text{ In this basis the coulomb interaction is not diagonal; so operate}
\]
\[
T_{2 \times 2} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & -1 \\ 1 & 1 \end{bmatrix}
\]
on the basis to diagonalize.

\[
=T_{2 \times 2} \begin{bmatrix} \varphi_1(\vec{r}_1), & \varphi_2(\vec{r}_2) \\ \varphi_3(\vec{r}_2), & \varphi_2(\vec{r}_1) \end{bmatrix}
\]
\[
= \frac{1}{\sqrt{2}} \begin{bmatrix} \varphi_1(\vec{r}_1) & \varphi_2(\vec{r}_2) - \varphi_1(\vec{r}_2) \varphi_2(\vec{r}_1) \\ \varphi_3(\vec{r}_2) & \varphi_2(\vec{r}_1) + \varphi_1(\vec{r}_1) \varphi_3(\vec{r}_1) \end{bmatrix} = \begin{bmatrix} \phi_{\text{Triple}} \\ \phi_{\text{Single}} \end{bmatrix}
\]

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

\[
E(\psi^{(N)}) - E(\psi^{(N-1)}) = \epsilon_k = -\lambda_{kk}
\]

1\textsuperscript{st} term: Energy equation for N electron system
2\textsuperscript{nd} 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. \( \lambda \) being the Lagrange variational multiplier; \( n_k \) occupation no: of kth electron.

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.

Q7 Fill in the blanks below:

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

\[
\psi_{\text{Tot}} \rightarrow \infty
\]

\[
= \frac{1}{2ikr} \sum c_i (2l+1) \left[ P_l(\cos \theta)e^{i(kr+\delta)} - P_l(-\cos \theta)e^{-i(kr+\delta)} \right]
\]

As per the ‘outgoing’ wave boundary conditions, \( c_i = e^{i\delta_i(k)} \).

(ii) As per the ‘ingoing’ wave boundary conditions, \( c_i = e^{-i\delta_i(k)} \).

(iii) The physical dimensions of the quantity

\[
\left( \frac{qA_0(\omega)}{mc} \right)^2 \left| \int f e^{i\vec{k} \cdot \vec{r}} \hat{E} \cdot \hat{V} |i \right|^2 \times 2\pi \delta(\omega)
\]

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 \( \sqrt{\_} \), 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.  
\[ \rightarrow 3+2=5 \text{ marks for Q7.} \]

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>
<thead>
<tr>
<th>TABLE 1a. ((j_1 \frac{1}{2} m_1 m_2 \mid j_1 \frac{1}{2} j m))</th>
</tr>
</thead>
<tbody>
<tr>
<td>( j = )</td>
</tr>
<tr>
<td>( j_1 + \frac{1}{2} )</td>
</tr>
<tr>
<td>( j_1 - \frac{1}{2} )</td>
</tr>
<tr>
<td>( m_2 = \frac{1}{2} )</td>
</tr>
<tr>
<td>( \sqrt{j_1 + m + \frac{1}{2}} )</td>
</tr>
<tr>
<td>( \sqrt{2j_1 + 1} )</td>
</tr>
<tr>
<td>( m_2 = -\frac{1}{2} )</td>
</tr>
<tr>
<td>( \sqrt{j_1 - m + \frac{1}{2}} )</td>
</tr>
<tr>
<td>( \sqrt{2j_1 + 1} )</td>
</tr>
</tbody>
</table>

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

\[
\begin{pmatrix}
\frac{1}{2} \\
\frac{1}{2}
\end{pmatrix} = C_1 \begin{pmatrix} 1 \\
\frac{1}{2}
\end{pmatrix} + C_2 \begin{pmatrix} 0 \\
\frac{1}{2}
\end{pmatrix}
\]

From the table \( C_1 \) and \( C_2 \) can be found.
C₁: Given \( j₁ = 1 \) and \( j = \frac{1}{2} \); \( m₂ = \frac{1}{2} \) and \( m = -\frac{1}{2} \)

\[
C₁ = \sqrt{\frac{j₁ - m + \frac{1}{2}}{2j₁ + 1}} = \sqrt{\frac{1 - \left(-\frac{1}{2}\right) + \frac{1}{2}}{2(1)+1}} = \sqrt{\frac{2}{3}}
\]

C₂: Given \( j₁ = 1 \) and \( j = \frac{1}{2} \); \( m₂ = -\frac{1}{2} \) and \( m = -\frac{1}{2} \)

\[
C₂ = \sqrt{\frac{j₁ + m + \frac{1}{2}}{2j₁ + 1}} = \sqrt{\frac{1 + \left(-\frac{1}{2}\right) + \frac{1}{2}}{2(1)+1}} = \sqrt{\frac{1}{3}}
\]

\[
\left| \frac{1}{2} - \frac{1}{2} \right| = -\sqrt{\frac{2}{3}} \left| -\frac{1}{2} \right| + \sqrt{\frac{1}{3}} \left| 0 - \frac{1}{2} \right|
\]

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

⇒ 5 marks.