Spin Dependent Selection Rules for Photonic Transitions in Hydrogen-Like Atoms

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Abstract

Spin dependent selection rules for photonic transitions in hydrogen-like atoms is derived by using the solution of Dirac equation for hydrogen-like atoms. It is shown that photonic transitions occur when \( \Delta j = 0, \pm 1, \pm 2 \) while \( \Delta m_j = 0, \pm 1, \pm 2 \). By applying the spin dependent selection rules, we can explain the observed \( (6s \rightarrow 7s) \) transition in Cesium (Cs) atom.

Keywords: Dirac Hydrogen Atom, Hydrogen-Like (Hydrogenic) Atoms, Photonic Transitions, Selection Rules, Fermi-Golden Rule, Transition Rate

1. Introduction

Applications of hydrogen-like atoms in technology are more than the hydrogen atom itself. Accurate determination of the excited-state properties of atomic and molecular systems, such as fine and hyperfine coupling constants, oscillator strengths play important roles for testing the high-precision atomic theory and quantum mechanics. The aim of the present study is to find spin dependent selection rules for photonic transitions in hydrogen-like atoms. We first derive the spin dependent eigenstates of the hydrogen-like atoms then find a more accurate correspondence between these eigenstates. So far in literature the states have been denoted by the quantum numbers \( (n, l, j) \) [1] but not by the quantum numbers \( (n, l, m_j) \). In this way, we distinguish the states in the Zeeman sense including the quantum number, \( m_j \). By using the Fermi-Golden rule, we calculate the non-zero matrix elements and then develop the spin dependent selection rules for the photonic transitions in the hydrogen-like atoms. We show that photonic transitions occur when \( \Delta j = 0, \pm 1, \pm 2 \) and \( \Delta m_j = 0, \pm 1, \pm 2 \). By applying the spin dependent selection rules, we can explain the observed \( (6s \rightarrow 7s) \) transition in Cesium (Cs) atom. The outline of the present study is as follows. In Section 2 we give a short summary of the Dirac hydrogen atom and then extend it to the hydrogen-like atoms. In Section 3 we develop the spin dependent transition rates for Dirac hydrogen-like atoms. In Section 4 we give the explanation of the \( (6s \rightarrow 7s) \) transition of Cs in terms of the spin dependent selection rules. In Section 5 we give the conclusions.

2. The Dirac Hydrogen Atom

To find the eigenvalue of the Dirac hydrogen-like atom, we will begin with the Dirac Hamiltonian of the hydrogen atom [2-4]:

\[
H_D = \alpha \cdot p c + \beta m c^2 + V(r)
\]  

(1)

where \( V(r) = -e^2 / r \) is the Coulomb potential, \( m \) is the mass of an electron, \( c \) is the velocity of light, \( \alpha \) and \( \beta \) are the standard Dirac matrices in the Dirac representation:

\[
\alpha = \begin{pmatrix} 0 & \sigma \\ \sigma & 0 \end{pmatrix} \quad \beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}
\]  

(2)

Here the 1’s and 0’s stand for 2 × 2 unit and zero matrices respectively and the \( \sigma \) is the standard vector composed of the three Pauli matrices \( \sigma = (\sigma_x, \sigma_y, \sigma_z) \). Since the Hamiltonian is invariant under rotations, we look for simultaneous eigenfunctions of \( H_D \), \( |J|^2 \), and \( J_z \), where

\[
S = \frac{1}{2} \sum \hbar \left( \begin{array}{cc} \sigma & 0 \\ 0 & \sigma \end{array} \right)
\]  

(3a)

and
\[ J_z = L_z + S_z \text{ or } m_j = m + m_s \tag{3b} \]

We remark that the spin operator is diagonal in terms of \( 2 \times 2 \) Pauli spin matrices; therefore the angular part should be precisely that of the Pauli two-component theory. Defining

\[ \chi_+ = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \text{ and } \chi_- = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \]

the spin dependent wave functions can be written as [5]:

\[
\begin{align*}
|n, l, m, \uparrow\rangle_{\text{hydrogen}} &= \Psi_{n, j=1/2, m_j} = \\
&\sqrt{\frac{l+\frac{1}{2}m_j+\frac{1}{2}}{2l+1}}R_{nl}(r)Y_{l\frac{1}{2}m_j}^{\frac{1}{2}}\chi_+ + \sqrt{\frac{l-\frac{1}{2}m_j+\frac{1}{2}}{2l+1}}R_{nl}(r)Y_{l\frac{1}{2}m_j}^{-\frac{1}{2}}\chi_- \tag{4a} \\
&= G_lY_{l\frac{1}{2}m_j}^{\frac{1}{2}}\chi_+ + G_lY_{l\frac{1}{2}m_j}^{-\frac{1}{2}}\chi_- \\
|n, l, m, \downarrow\rangle_{\text{hydrogen}} &= \Psi_{n, j=-1/2, m_j} = \\
&\sqrt{\frac{l+\frac{1}{2}m_j+\frac{1}{2}}{2l+1}}R_{nl}(r)Y_{l\frac{1}{2}m_j}^{-\frac{1}{2}}\chi_+ + \sqrt{\frac{l-\frac{1}{2}m_j+\frac{1}{2}}{2l+1}}R_{nl}(r)Y_{l\frac{1}{2}m_j}^{\frac{1}{2}}\chi_- \tag{4b} \\
&= -G_lY_{l\frac{1}{2}m_j}^{\frac{1}{2}}\chi_+ + G_lY_{l\frac{1}{2}m_j}^{-\frac{1}{2}}\chi_- 
\end{align*}
\]

where \( R_{nl}(r) \) is the radial wave function, \( Y_{lj}^{m_j} \) are the spherical harmonics. Further in Equation (4a), \( l \) can be replaced by \( (j - \frac{1}{2}) \) (spin-up case); and in Equation (4b), \( l \) can be replaced by \( (j + \frac{1}{2}) \) (spin-down case). In a hydrogen-like atom the potential \( V(r) = -e^2/r \) is replaced by \( V(r) = -Ze^2/r \), where \( Z \) is the atomic number. The spin dependent eigenfunctions for hydrogen-like atoms are written as:

\[
\begin{align*}
|n, l, m, \uparrow\rangle_{\text{H-like}} &= \Psi_{n, j=1/2, m_j} = \\
&\sqrt{\frac{l+\frac{1}{2}m_j+\frac{1}{2}}{2l+1}}R_{nl}(r)Y_{l\frac{1}{2}m_j}^{\frac{1}{2}}\chi_+ + \sqrt{\frac{l-\frac{1}{2}m_j+\frac{1}{2}}{2l+1}}R_{nl}(r)Y_{l\frac{1}{2}m_j}^{-\frac{1}{2}}\chi_- \tag{5a} \\
|n, l, m, \downarrow\rangle_{\text{H-like}} &= \Psi_{n, j=-1/2, m_j} = \\
&\sqrt{\frac{l+\frac{1}{2}m_j+\frac{1}{2}}{2l+1}}R_{nl}(r)Y_{l\frac{1}{2}m_j}^{-\frac{1}{2}}\chi_+ + \sqrt{\frac{l-\frac{1}{2}m_j+\frac{1}{2}}{2l+1}}R_{nl}(r)Y_{l\frac{1}{2}m_j}^{\frac{1}{2}}\chi_- \tag{5b}
\end{align*}
\]

where

\[
R_{nl}(r)_{\text{H-like}} = \sqrt{\frac{2Z}{na_o}} \left( \frac{n-l-1}{n(n+1)!} \right)^{2/na_o} e^{-2r/na_o}
\]

\[
X \left[ \frac{2Z}{na_o} \right] I_{n-l+1}^{2l+1} \left( \frac{2Z}{na_o} \right)
\]

Here \( I_{n-l+1}^{2l+1} \) are the Laguerre polynomials and \( a_o = \hbar^2/mc^2 \) is the Bohr radius.

3. Developing Spin Dependent Transition Rates for Photonic Transitions in Dirac Hydrogen-Like Atoms

To develop the spin dependent selection rules for hydrogen-like atoms, we need to consider energy shifts coming from the electric field \( E \) and the magnetic field \( B \) separately. When the atom is subject to an external electric and magnetic field, it will have interactions through the Hamiltonians: \( H'(E) = -\vec{d} \cdot \vec{E} \) and \( \dot{H}'(B) = -\vec{\mu} \cdot \vec{B} \).

However, the electric and the magnetic field of a photon are not independent fields and they are related to each other with the same vector potential \( \vec{A}(x, y, z) \) which obeys the Coulomb gauge condition \( \nabla \cdot \vec{A} = 0 \).

In this case the electric and the magnetic field vectors are given by:

\[
\vec{E}(x, y, z) = -ik\vec{A}(x, y, z) \tag{6a}
\]

and

\[
\vec{B}(x, y, z) = \vec{\nabla} \times \vec{A}(x, y, z) \tag{6b}
\]

where \( \vec{k} \) is the wave vector of the photon.

In general the effect of the vector potential \( \vec{A}(x, y, z) \) on electron is considered through the canonical momentum that produces an interaction potential \( H'(A) \) which has the linear and the quadratic terms [6]:

\[
H'(\vec{A}) = -\frac{e}{mc} (\vec{A} \cdot \vec{p}) + \frac{e^2}{2mc^2} A^2 \tag{7}
\]

where \( \vec{p} \) is the linear momentum of the electron.

We will see that to develop the selection rules for photonic transitions, the Hamiltonian \( H'(E) = -\vec{d} \cdot \vec{E} \) will be adequate and the Hamiltonian \( \dot{H}'(B) = -\vec{\mu} \cdot \vec{B} \) will not produce anything new.

Let us first start with the effect of the electric field. In Dirac notations, if at \( t = 0 \) the electron is at an initial state

\[ |i> = |n, l, m, \uparrow\rangle_{\text{H-like}} \]

given by Equation (5a) and Equation (5b), then at \( t > 0 \), because of the interaction with \( H' \), there will be a non-zero transition rate to some other states

\[ |f> = |n', l', m', \downarrow\rangle_{\text{H-like}} \]

which will be called the final states. According to the
Golden rule, the transition probability will be proportional to the square of the matrix element of $H'$ between the initial and the final states: $\langle f | H' | i \rangle^2$. To calculate the matrix element $\langle f | H' | i \rangle = \langle f | \overrightarrow{d} \cdot \mathbf{E} | i \rangle$, we follow a similar way as followed by Saglam et al. [5]. Namely we will consider two different cases: 
a) The polarization of the electric field is in x-y plane (along the x- or the y-axis) b) The polarization of the electric field is in z-direction. Since the dipole moment vector $\overrightarrow{d}$ is equal to $(-e\mathbf{r})$, for the case a), we calculate the matrix elements of the quantities $x \pm iy = r \sin \theta \exp(\pm i\phi)$ and for the case b) we calculate the matrix elements of the quantity: $rcos \theta$. For the case a) we can write:

$$\langle f | H' | i \rangle = \left\{ n', l', m'_l \uparrow \downarrow \left| r \sin \theta \exp(\pm i\phi) \right| n, l, m, \uparrow \downarrow \right\}_{H'-like}$$

$$= \left\{ n', l', m'_l \uparrow \left| r \sin \theta \exp(\pm i\phi) \right| n, l, m, \uparrow \right\}_{H'-like}$$

$$+ \left\{ n', l', m'_l \downarrow \left| r \sin \theta \exp(\pm i\phi) \right| n, l, m, \downarrow \right\}_{H'-like}$$

$$+ \left\{ n', l, m'_l \uparrow \left| r \sin \theta \exp(\pm i\phi) \right| n, l, m, \uparrow \right\}_{H'-like}$$

$$+ \left\{ n', l, m'_l \downarrow \left| r \sin \theta \exp(\pm i\phi) \right| n, l, m, \downarrow \right\}_{H'-like}.$$ (8)

Substitution of Equation (5a) in $I_1$ we obtain:

$$I_1 = F'_1 F'_2 \left( \begin{array}{cc} \phantom{-} & \phantom{-} \\ \phantom{-} & \phantom{-} \\ \end{array} \right) ^* \left[ \begin{array}{cc} AY^{m_1/2} & BY^{m_1/2} \\ \end{array} \right] \left[ \begin{array}{cc} AY^{m_1/2} & BY^{m_1/2} \\ \end{array} \right] d\Omega$$

$$+ \left[ AY^{m_1/2} + BY^{m_1/2} \right] \left[ \begin{array}{cc} AY^{m_1/2} & BY^{m_1/2} \\ \end{array} \right] d\Omega$$

$$+ F'_2 F'_2 \left( \begin{array}{cc} \phantom{-} & \phantom{-} \\ \phantom{-} & \phantom{-} \\ \end{array} \right) ^* \left[ \begin{array}{cc} CY^{m_1/2} & DY^{m_1/2} \\ \end{array} \right] \left[ \begin{array}{cc} CY^{m_1/2} & DY^{m_1/2} \\ \end{array} \right] d\Omega$$

$$+ \left[ CY^{m_1/2} + DY^{m_1/2} \right] \left[ \begin{array}{cc} CY^{m_1/2} & DY^{m_1/2} \\ \end{array} \right] d\Omega.$$ (9)

which will be non-zero for:

$$\Delta j = 1; \; \Delta m_j = 0, -2$$ \hspace{1cm} (10a)

$$\Delta j = -1; \; \Delta m_j = \pm 1$$ \hspace{1cm} (10b)

To evaluate the integral (9) we have used the relation:

$$\sin \theta \cdot Y_l^m = \sqrt{\frac{(l+1-m)(l+2-m)}{(2l+1)(2l+3)}} Y_{l+1}^{m-1}$$

$$+ \sqrt{\frac{(l+m)(l+1+m)}{(2l+1)(2l+1)}} Y_{l+1}^{m-1} e^{i\phi}.$$ \hspace{1cm} (11)

Next substituting Equation (5b) in $I_2$ we obtain:

$$I_2 = F'_1 F'_1 \left( \begin{array}{cc} \phantom{-} & \phantom{-} \\ \phantom{-} & \phantom{-} \\ \end{array} \right) ^* \left[ \begin{array}{cc} AY^{m_1/2} + BY^{m_1/2} \\ \end{array} \right] \left[ \begin{array}{cc} AY^{m_1/2} + BY^{m_1/2} \\ \end{array} \right] d\Omega$$

$$+ \left[ AY^{m_1/2} + BY^{m_1/2} \right] \left[ \begin{array}{cc} AY^{m_1/2} + BY^{m_1/2} \\ \end{array} \right] d\Omega$$

$$+ F'_1 F'_2 \left( \begin{array}{cc} \phantom{-} & \phantom{-} \\ \phantom{-} & \phantom{-} \\ \end{array} \right) ^* \left[ \begin{array}{cc} CY^{m_1/2} + DY^{m_1/2} \\ \end{array} \right] \left[ \begin{array}{cc} CY^{m_1/2} + DY^{m_1/2} \\ \end{array} \right] d\Omega$$

$$+ \left[ CY^{m_1/2} + DY^{m_1/2} \right] \left[ \begin{array}{cc} CY^{m_1/2} + DY^{m_1/2} \\ \end{array} \right] d\Omega.$$ \hspace{1cm} (12)

which will be non-zero for:

$$\Delta j = 1; \; \Delta m_j = 0, -2$$ \hspace{1cm} (13a)

$$\Delta j = -1; \; \Delta m_j = \pm 1$$ \hspace{1cm} (13b)

where we have used Equation (11) again.

Similarly substitution of Equations (5a) and (5b) in $I_3$ we obtain:

$$I_3 = F'_1 F'_2 \left( \begin{array}{cc} \phantom{-} & \phantom{-} \\ \phantom{-} & \phantom{-} \\ \end{array} \right) ^* \left[ \begin{array}{cc} AY^{m_1/2} + BY^{m_1/2} \\ \end{array} \right] \left[ \begin{array}{cc} AY^{m_1/2} + BY^{m_1/2} \\ \end{array} \right] d\Omega$$

$$+ \left[ AY^{m_1/2} + BY^{m_1/2} \right] \left[ \begin{array}{cc} AY^{m_1/2} + BY^{m_1/2} \\ \end{array} \right] d\Omega$$

$$+ F'_2 F'_1 \left( \begin{array}{cc} \phantom{-} & \phantom{-} \\ \phantom{-} & \phantom{-} \\ \end{array} \right) ^* \left[ \begin{array}{cc} CY^{m_1/2} + DY^{m_1/2} \\ \end{array} \right] \left[ \begin{array}{cc} CY^{m_1/2} + DY^{m_1/2} \\ \end{array} \right] d\Omega$$

$$+ \left[ CY^{m_1/2} + DY^{m_1/2} \right] \left[ \begin{array}{cc} CY^{m_1/2} + DY^{m_1/2} \\ \end{array} \right] d\Omega.$$ \hspace{1cm} (14)

which will be non-zero for:

$$\Delta j = 2; \; \Delta m_j = 0, -2$$ \hspace{1cm} (15a)

$$\Delta j = 0; \; \Delta m_j = \mp 1$$ \hspace{1cm} (15b)

Similarly substitution of Equations (5a) and (5b) in $I_4$ we obtain:

$$I_4 = -F'_1 F'_1 \left( \begin{array}{cc} \phantom{-} & \phantom{-} \\ \phantom{-} & \phantom{-} \\ \end{array} \right) ^* \left[ \begin{array}{cc} AY^{m_1/2} + BY^{m_1/2} \\ \end{array} \right] \left[ \begin{array}{cc} AY^{m_1/2} + BY^{m_1/2} \\ \end{array} \right] d\Omega$$

$$+ \left[ AY^{m_1/2} + BY^{m_1/2} \right] \left[ \begin{array}{cc} AY^{m_1/2} + BY^{m_1/2} \\ \end{array} \right] d\Omega$$

$$+ F'_2 F'_1 \left( \begin{array}{cc} \phantom{-} & \phantom{-} \\ \phantom{-} & \phantom{-} \\ \end{array} \right) ^* \left[ \begin{array}{cc} CY^{m_1/2} + DY^{m_1/2} \\ \end{array} \right] \left[ \begin{array}{cc} CY^{m_1/2} + DY^{m_1/2} \\ \end{array} \right] d\Omega$$

$$+ \left[ CY^{m_1/2} + DY^{m_1/2} \right] \left[ \begin{array}{cc} CY^{m_1/2} + DY^{m_1/2} \\ \end{array} \right] d\Omega.$$ \hspace{1cm} (16)

which will be non-zero for:

$$\Delta j = 0; \; \Delta m_j = 0, -2$$ \hspace{1cm} (17a)

$$\Delta j = 0; \; \Delta m_j = \pm 1$$ \hspace{1cm} (17b)
where we used the relations:

\[
\cos \theta \cdot Y_l^m = \frac{(l + 1 + m)(l + 1 - m)}{(2l + 1)(2l + 3)} Y_{l+1}^m + \frac{(l + m)(l - m)}{(2l + 1)(2l - 1)} Y_{l-1}^m
\]

Similarly substitution of Equation (5b) in \( I_2' \) we obtain:

\[
I_2' = F_1' F_2' \int \left( y_{j_2}^{-1} \right) \left( AY_{j_2}^{m_2} \right. \left. + BY_{j_2}^{m_2} \right) d\Omega
\]

which will be non-zero for

\[
\Delta j = \pm 1; \Delta m_j = 0
\]

Substitution of Equations (5a) and (5b) in \( I_3' \) we obtain:

\[
I_3' = -F_1' F_2' \int \left( y_{j_3}^{-1} \right) \left( AY_{j_3}^{m_3} \right. \left. + BY_{j_3}^{m_3} \right) d\Omega
\]

which will be non-zero for

\[
\Delta j = 0; \Delta m_j = 0
\]

According to the conventional selection rules (\( \Delta l = \pm 1 \) and \( \Delta s = 0 \)) which are derived from the Schrödinger equation in the same way as in Section 3, a transition such as \( 6s \rightarrow 7s \) is not allowed (because this is a transition \( l = 0 \rightarrow l = 0 \) in which \( \Delta l = 0 \), so it does not meet the condition \( \Delta l = \pm 1 \)). But \( 6s \rightarrow 7s \) transition in Cs atom has been already observed \([7-9]\). However, the present spin dependent selection rules allow the transition: \( 6s \uparrow \rightarrow 7s \uparrow \) in Cs atom. Because here we have \( \Delta j = 0 \) and \( \Delta m_j = 0 \) which are allowed by the
present spin dependent selection rules given in Equation (28). To prove the above transition in detail, let us assume that the outer electron of the Cs atom is initially at the state \( |6s \uparrow \rangle = |6,0,0,1/2 \rangle \) \(_{\text{H-like}}\). From Equation (5a) we write:

\[
|i\rangle = |6,0,0,1/2 \rangle >_{\text{H-like}} = R_{6,0}(r)_{\text{H-like}} Y_0^0 \chi_s = A Y_0^0 \chi_s. \tag{29}
\]

where A is the normalization constant. When it is excited to the \( |7s \rangle\) state, the possible final states are:

\[
|7s \uparrow\rangle \quad \text{and} \quad |7s \downarrow\rangle \quad \text{\(_{\text{H-like}}\).}
\]

From Equations (5a) and (5b) these states are:

\[
|f\rangle = |7,0,0,1/2 >_{\text{H-like}} = R_{7,0}(r)_{\text{H-like}} Y_0^0 \chi_s = B Y_0^0 \chi_s, \tag{30a}
\]

\[
|f\rangle = |7,0,0,-1/2 >_{\text{H-like}} = - R_{7,0}(r)_{\text{H-like}} Y_0^1 \chi_s = C Y_0^1 \chi_s \tag{30b}
\]

where \( B \) and \( C \) are the normalization constants. Substituting the wave functions from Equation (29) and Equations (30a)-(30b) in Equations (8) and (18) we find:

\[
\langle 7,0,0,1/2 | - \vec{d} \cdot \vec{E} | 6,0,0,1/2 \rangle \approx \int_{0}^{\pi} \sin \theta' \mathrm{d} \theta' \neq 0 \tag{31}
\]

\[
\langle 7,0,0,-1/2 | - \vec{d} \cdot \vec{E} | 6,0,0,1/2 \rangle = 0 \tag{32}
\]

Therefore the non-zero matrix element in Equation (31) gives us a non-transition between the states \( |6s \uparrow \rangle\) and \( |7s \uparrow\rangle\) which is also allowed by the present spin dependent selection rules given in Equation (28) (\( \Delta j = 0 \) and \( \Delta m_j = 0 \)).

5. Conclusions

We have derived the spin dependent selection rules for photonic transitions in hydrogen-like atoms by using the solution of Dirac equation for hydrogen-like atoms. It is shown that photonic transitions occur when \( \Delta j = 0, \pm 1, \pm 2 \) \( \text{while} \ \Delta m_j = 0, \pm 1, \pm 2 \). By applying the present spin dependent selection rules we can explain the observed \((6s \rightarrow 7s)\) transition in Cesium (Cs) atom [7,8]. Because in the \((6s \rightarrow 7s)\) transition in Cesium (Cs) atom we have \( \Delta j = 0 \) \( \text{while} \ \Delta m_j = 0 \) which is an allowed transition according to the present selection rules given in Equation (28). The present result is believed to be helpful for a deeper understanding of the photonic transitions and the spectrum of Cs atom [1]. A detailed study will be presented in the future.

6. References


