Ex6212: Hydrogen atom in magnetic field, probed by electric field

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The problem:

Consider a Hydrogen atom that is placed in a constant homogeneous magnetic field $\mathcal{B}$ that points in the Z direction. An electric field $\mathcal{E}$ is turned on. The interaction term is $V = -e\boldsymbol{\mathcal{E}} \cdot \mathbf{r}$. The spin of the electron can be ignored.

(1) Calculate the matrix elements of V in the standard basis for $\mathcal{E}$ that points in the Z direction.

(2) Calculate the matrix elements of V in the standard basis for $\mathcal{E}$ that points in the X direction.

(3) Repeat the derivation in the latter case using coordinates such that $\mathcal{B}$ points in the X direction, and $\mathcal{E}$ in the Z direction.

(4) Explain what are the selection rules of transitions in the following cases:
$\mathcal{E} = (0, 0, cos(\Omega t))$
$\mathcal{E} = (cos(\Omega t), 0, 0)$
$\mathcal{E} = (cos(\Omega t), sin(\Omega t), 0)$
Assume that Ω is comparable to the Zeeman splitting.

The solution:

(1) We use the standard basis $|nlm>$ and write
$\mathcal{V} =< nlm|V|n'l'm' >= - < nlm|ez\mathcal{E}|n'l'm' >$
We note that in spherical coordinates $z = rcos\theta$ and get
$\mathcal{V} = -e\mathcal{E} \int_0^{\pi} \int_0^{\infty} \int_0^{2\pi} \Psi^{nlm*} rcos\theta \Psi^{n'l'm'} r^2 dr d\phi d\theta$,
we use $\Psi^{nlm} = R^{nl} Y^{lm}$, where R^{nl} are the Laguerre polynomials and Y^{lm} are the Spherical harmonics.

We note that $cos(\theta) = \sqrt{\frac{4\pi}{3}} Y^{10}$

And write the radial part as $S_{nln'l'} = \int_0^{\infty} R^{nl^*} r R^{n'l'} r^2 dr$ so that

$\mathcal{V} = -\sqrt{\frac{4\pi}{3}} e\mathcal{E} S_{nln'l'} \int_0^{4\pi} Y^{lm^*} Y^{10} Y^{l'm'} d\Omega$

It is known that the spherical harmonics' parity is given by $Y^{lm}(-\vec{r}) = (-1)^l Y^{lm}(\vec{r})$ which means the spherical harmonics are even when l is even and odd when l is odd.

From here we deduce that the condition for l and l' so that the integral won't vanish is that $l - l' = \Delta l$ has to be an odd number.
Angular momentum considerations allow us to further limit Δl so that $|\Delta l| \leq 1$ (see last paragraph for detailed explanation).
So finally we get $\Delta l = \pm 1$.

In order to find the condition on m, let us look at the ϕ component:
$\mathcal{V} \propto \int_0^{2\pi} e^{-i\phi m} e^{i\phi m'} d\phi$
Since complex exponentials are orthogonal, the condition on m so that $\mathcal{V}$ won't vanish is $m = m'$.

So in total we got the selection rules:
$\Delta l = \pm 1, \Delta m = 0$
and the matrix elements:
$$V = \begin{cases} -\sqrt{\frac{4\pi}{3}} e\mathcal{E} S_{nln'l'} \int_0^{4\pi} Y^{lm^*} Y^{10} Y^{l'm} d\Omega, & \text{for } \Delta m = 0 \text{ and } \Delta l = \pm 1 \\ 0, & \text{otherwise} \end{cases}$$
Where $S_{nln'l'}$ and the angular integral are easily calculated given particular n, m, l.

(2) Same as (1) but now we take $x = rsin(\theta)cos(\phi) = rsin(\theta)(e^{-i\phi} + e^{i\phi})$

We note that $sin(\theta)e^{\pm i\phi} = \sqrt{\frac{2\pi}{3}} Y^{1\pm 1}$

So now we get:
$\mathcal{V} = -e\mathcal{E} < nlm|x|n'l'm' >= -\sqrt{\frac{2\pi}{3}} e\mathcal{E} S_{nln'l'} (\int_0^{4\pi} Y^{lm^*} Y^{11} Y^{l'm'} d\Omega + \int_0^{4\pi} Y^{lm^*} Y^{1-1} Y^{l'm'} d\Omega)$.
$Y^{1\pm 1}$ are both odd, so from parity we get again $\Delta l = \pm 1$.

For the condition on m, we again look at the ϕ component:
$\mathcal{V} \propto \int_0^{2\pi} e^{-i\phi m} e^{i\phi} e^{i\phi m'} d\phi + \int_0^{2\pi} e^{-i\phi m} e^{-i\phi} e^{i\phi m'} d\phi$
we get that $m - m' = \Delta m = \pm 1$ in order that $\mathcal{V}$ won't vanish.
Hence:

$$\mathcal{V} = \begin{cases} -\sqrt{\frac{2\pi}{3}} e\mathcal{E} S_{nln'l'} \int_0^{4\pi} Y^{lm^*} Y^{11} Y^{l'm-1} d\Omega, & \text{for } \Delta m = 1 \text{ and } \Delta l = \pm 1 \\ -\sqrt{\frac{2\pi}{3}} e\mathcal{E} S_{nln'l'} \int_0^{4\pi} Y^{lm^*} Y^{1-1} Y^{l'm+1} d\Omega, & \text{for } \Delta m = -1 \text{ and } \Delta l = \pm 1 \\ 0, & \text{otherwise} \end{cases}$$
(3) Now the magnetic field lies in the x direction, so the natural basis for the problem would be:
$|nlm_x >$
Where m_x are the eigenvalues of L_x.
We can represent m_x by the standard basis as follows:
$|nlm_x >= R^l(\frac{\pi}{2}\hat{n_y})|nlm >$
Where $R^l(\frac{\pi}{2}\hat{n_y})$ is the rotation matrix for 90 degrees around the y axis.
Using this, we can now find the matrix elements:
$\mathcal{V} = - < nlm_x|e\mathcal{E}z|nlm_x >= -e\mathcal{E} < R^l(\frac{\pi}{2}\hat{n_y})nlm|zR^l(\frac{\pi}{2}\hat{n_y})|n'l'm' >$
$\mathcal{V} = -e\mathcal{E} < nlm|R^{l^{-1}}(\frac{\pi}{2}\hat{n_y})zR(\frac{\pi}{2}\hat{n_y})|n'l'm' >$
From the algebraic characteristics of rotations (see chapter 6.4 in the lecture notes):
$R^{l^{-1}}(\frac{\pi}{2}\hat{n_y})zR(\frac{\pi}{2}\hat{n_y}) = x$
Plugging this into the former equation we get:
$V = -e\mathcal{E} < nlm|x|n'l'm' >$
Which is exactly the same as in section (2)! So the selection rules are also the same:
$\Delta l = \pm 1, \Delta m = \pm 1$

(4) Given that Ω is comparable to the Zeeman splitting, we can use the Fermi golden rule. Hence transitions that have $\Gamma \neq 0$ are ones that have $|V_{ij}| \neq 0$, so for the first and second cases, the selection rules are simply those found in (1) and (2). That is, $\Delta m = 0, \Delta l = \pm 1$ and $\Delta m = \pm 1, \Delta l = \pm 1$ respectively.
For the last case we can represent the electric field as follows:
$\mathcal{E}(t) = \frac{\mathcal{E}}{\sqrt{2}} Re[(\hat{x} + i\hat{y})e^{i\Omega t}]$
Now,
$V \propto \mathcal{E} \int e^{im\phi}(x + iy)e^{-im'\phi} d\phi = \mathcal{E} rsin\theta \int e^{im\phi} e^{-i\phi} e^{-im'\phi} d\phi$

The above integral vanishes for $m-1-m' \neq 0$ so we get the selection rule $\Delta m = m - m' = 1$, and $\Delta l = \pm 1$ as before.

* Note that the selection rules derived from the integral over three spherical harmonics,
$\int (Y^{l_1 m_1})^* Y^{l_2 m_2} Y^{l_3 m_3} d\Omega$
are identical to the rules for addition of angular momentum. Consider the product $Y^{l_2 m_2} Y^{l_3 m_3}$, which is analogous to the tensor product $|l_2 m_2 > \otimes |l_3 m_3 >$ so the above integral can be written as $< l_1 m_1 | (|l_2 m_2 > \otimes |l_3 m_3 >)$.
We can now use the addition of angular momentum theorem, from which we ascertain that the tensor product decomposes into states $|j, m_j >$ such that $|l_3 - l_2| \leq j \leq l_2 + l_3$, and $m_j = m_2 + m_3$. In this basis, the bra $< l_1 m_1 |$ stays the same since nothing is added to it.
The product then becomes $< l_1 m_1 | j, m_2 + m_3 >$ and the selection rules become evident since l_1 has to be in the decomposition of $l_2 \otimes l_3$ so $|l_3 - l_2| \leq l_1 \leq l_2 + l_3$ and the m's have to match: $m_1 = m_2 + m_3$.

Notice that this is compatible with the results obtained through manual inspection of the integrals as done in the previous sections, when $l_2 = 1$ and $m_2 = 0, \pm 1$ as is the case for $x, y, z \propto Y^{1m}$. The exclusion of $\Delta l = 0$ is based on the parity of the spherical harmonics as is explained above.