Exercise 4  The selection rules (electric dipole transitions)

The quantum state $|n, l, m_l\rangle$ of an electron in a hydrogen atom is characterised by the values of the principal quantum number $n$ ($n = 1, 2, \ldots$), the angular momentum quantum number $l$ ($l = 0, 1, \ldots, n - 1$) and the corresponding magnetic quantum number $m_l$ ($m_l = -l, -l + 1, \ldots, l - 1, l$). The level scheme for the states with $n = 2$ is shown in Fig. 1, with the quantization axis directed along the $z$-axis.

![Figure 1: Level scheme of a hydrogen atom for $n = 2$.](image)

The coordinate representation of these states reads

\[
\psi_g(\vec{r}) = \langle \vec{r} | g \rangle = \langle \vec{r} | 2, 0, 0 \rangle = R_{2,0}(r)Y_{0,0}(\theta, \varphi),
\]

\[
\psi_{e_1}(\vec{r}) = \langle \vec{r} | e_1 \rangle = \langle \vec{r} | 2, 1, -1 \rangle = R_{2,1}(r)Y_{1,-1}(\theta, \varphi),
\]

\[
\psi_{e_2}(\vec{r}) = \langle \vec{r} | e_2 \rangle = \langle \vec{r} | 2, 1, 0 \rangle = R_{2,1}(r)Y_{1,0}(\theta, \varphi),
\]

\[
\psi_{e_3}(\vec{r}) = \langle \vec{r} | e_3 \rangle = \langle \vec{r} | 2, 1, +1 \rangle = R_{2,1}(r)Y_{1,+1}(\theta, \varphi).
\]

The radial part $R_{n,l}(r)$ of the electronic wave function is normalised as

\[
\int_0^\infty dr \ r^2 R_{n,l}^2(r) = 1
\]

and given by

\[
R_{2,0}(r) = \frac{1}{\sqrt{2a_B^3}} \left( 1 - \frac{r}{2a_B} \right) e^{-\frac{r}{2a_B}},
\]

\[
R_{2,1}(r) = \frac{r}{2\sqrt{6a_B^3}} \frac{e^{-\frac{r}{2a_B}}}{a_B},
\]

where $a_B$ denotes the Bohr radius.
The angular part of the wave function is given by the spherical harmonics \( Y_{l,m_l}(\theta, \varphi) \), which are normalised and orthogonal to each other, that is

\[
\int_0^\pi d\theta \sin \theta \int_0^{2\pi} d\varphi \ Y_{l,m_l}^* (\theta, \varphi) Y_{l',m'_l}(\theta, \varphi) = \delta_{l,l'} \delta_{m_l,m'_l}.
\]

In particular, for the states under consideration

\[
Y_{0,0}(\theta, \varphi) = \sqrt{\frac{1}{4\pi}},
\]

\[
Y_{1,0}(\theta, \varphi) = i \sqrt{\frac{3}{4\pi}} \cos \theta,
\]

\[
Y_{1,\pm 1}(\theta, \varphi) = \mp i \sqrt{\frac{3}{8\pi}} \sin \theta e^{\pm i\varphi}.
\]

In the lecture we have defined the dipole matrix element for the transition between the ground \( |g\rangle \) and the exited \( |e\rangle \) states as

\[
\vec{d}_{eg} \equiv \langle e | \hat{d} | g \rangle \equiv \int \int \int d\vec{r} \psi_e^*(\vec{r}) (e\vec{r}) \psi_g(\vec{r}).
\]

a) Calculate the dipole matrix elements

\[
\vec{d}_{1g} = \langle e_1 | \hat{d} | g \rangle \text{ for } |e_1\rangle = |2, 1, -1\rangle
\]

\[
\vec{d}_{2g} = \langle e_2 | \hat{d} | g \rangle \text{ for } |e_2\rangle = |2, 1, 0\rangle
\]

\[
\vec{d}_{3g} = \langle e_3 | \hat{d} | g \rangle \text{ for } |e_3\rangle = |2, 1, +1\rangle
\]

for the transition between the ground state \( |g\rangle = |2, 0, 0\rangle \) and a given exited state \( |e_i\rangle \) with \( i = 1, 2, 3 \) (see Fig. 1).

(3 points)

b) What is the corresponding polarization of the electric field \( \vec{E} \) needed to induce each transition?

(1 point)