Coursework 1 - 2011 - Solution

(Atom - Photon physics)

1. We are interested in the matrix element

$\boxed{1}$ $$\langle n_2, l_2, m_2 | \, x z \, | n_1, l_1, m_1 \rangle =$$

$$= \int d^3r \, \Psi^*_{n_2 l_2 m_2}(\vec{r}) \, x z \, \Psi_{n_1, l_1, m_1}(\vec{r}) = I$$

Separation of angular and radial parts:

We will use

$\boxed{1}$ $$z = r\cos\theta = r 2\sqrt{\frac{\pi}{3}} \, Y_1^0(\theta,\varphi)$$

$\boxed{1}$ $$x = r\sin\theta\cos\varphi = r\sqrt{\frac{2\pi}{3}} \left[Y_1^{-1}(\theta,\varphi) - Y_1^1(\theta,\varphi) \right]$$

$$\Rightarrow \quad x z = r^2 \, 2\sqrt{2}\,\frac{\pi}{3} \left[Y_1^0 Y_1^{-1} - Y_1^0 Y_1^1 \right]$$

$\boxed{1}$ and $$\Psi_{nlm}(\vec{r}) = R_{nl}(r) \, Y_l^m(\theta,\varphi)$$

$\boxed{1}$ Angular ~~Radial~~ Integrals $\Rightarrow$ provide the selection rules

$$\Rightarrow \quad I \propto \underbrace{\int_0^\infty r^4 R_{n_1 l_1}(r) R_{n_2 l_2}(r)\, dr}_{\boxed{1} \text{ Radial integral} \Rightarrow \text{non-vanishing}} \times \left[\iint \left[Y^{*m_2}_{l_2}(\theta,\varphi) \, Y_1^0(\theta,\varphi) \times \underbrace{Y_1^{-1}(\theta,\varphi) \, Y^{m_1}_{l_1}(\theta,\varphi)}_{I_1} - \underbrace{Y^{*m_2}_{l_2}(\theta,\varphi) \, Y_1^0(\theta,\varphi) Y_1^1(\theta,\varphi) \, Y^{m_1}_{l_1}(\theta,\varphi)}_{I_2} \right] d\Omega \right.$$

$\boxed{2}$

$I_\phi \neq 0$ if $-m_2 \pm 1 + m_1 = 0 \Rightarrow m_2 - m_1 = \pm 1$

$$\boxed{\Delta m = \pm 1}$$

$I_\theta \neq 0$?

$$I_\theta = \int_{-1}^{1} P_{\ell_1}^{m_1}(\cos\theta) \cos\theta \sin\theta \, P_{\ell_2}^{m_2}(\cos\theta) \, d\cos\theta$$

we will apply the relations

$\boxed{1}$ $(2\ell+1)\cos P_\ell^m(\cos\theta) = (\ell+1-m) P_{\ell+1}^m(\cos\theta) + P_{\ell-1}^m(\cos\theta)$

and

$\boxed{1}$ $\sin\theta \, P_\ell^m(\cos\theta) = \dfrac{1}{(2\ell+1)} \left[P_{\ell+1}^{m+1}(\cos\theta) - P_{\ell-1}^{m+1}(\cos\theta) \right]$

in the above-stated integral, we find

$\boxed{1}$ $\sin\theta\cos\theta \, P_{\ell_2}^{m_2}(\cos\theta) = \dfrac{\sin\theta}{(2\ell_2+1)} \left[(\ell_2+1-m_2) P_{\ell_2+1}^{m_2}(\cos\theta) + P_{\ell_2-1}^{m_2}(\cos\theta) \right]$

$\boxed{1}$ $\sin\theta \, P_{\ell_2+1}^{m_2}(\cos\theta) = \dfrac{1}{[2(\ell_2+1)+1]} \left[P_{\ell_2+2}^{m_2+1}(\cos\theta) + P_{\ell_2}^{m_2+1}(\cos\theta) \right]$

$\boxed{1}$ $\sin\theta \, P_{\ell_2-1}^{m_2}(\cos\theta) = \dfrac{1}{[2(\ell_2-1)+1]} \left[P_{\ell_2}^{m_2+1}(\cos\theta) + P_{\ell_2-2}^{m_2+1}(\cos\theta) \right]$

In terms of spherical coordinates,

$$Y_1^0(\theta,\varphi)\,Y_1^1(\theta,\varphi) = -\frac{1}{4\sqrt{2}}\cdot\frac{3}{\pi}\sin\theta\cos\theta\, e^{i\varphi}$$

$\boxed{2}$ $\Rightarrow$ proportional to Y_2^1

Check: $Y_2^1 = -\frac{1}{2}\sqrt{\frac{15}{2\pi}}\sin\theta\cos\theta\, e^{i\phi}$

Similarly,

$\boxed{1}$ $Y_1^{-1}(\theta,\varphi)\,Y_1^0(\theta,\varphi) = \frac{1}{4\sqrt{2}}\times\frac{3}{\pi}\sin\theta\cos\theta\, e^{-i\phi} \Rightarrow$ proportional to Y_2^{-1}

$\boxed{1}$ $\Rightarrow I_{I,2} \propto \int Y_{\ell_2}^{*m_2}\, Y_2^{\pm1}\, Y_{\ell_1}^{m_1}\, d\Omega$

Possibilities: either $I_{1,2}$ can be solved employing Clebsch Gordan coefficients and properties of spherical harmonics (acceptable if steps are well justified), or the properties of Legendre polynomials discussed in class. A marking scheme is provided for the latter.

$\boxed{1}$ Using $Y_\ell^m(\theta,\varphi) = e^{im\varphi}P_\ell^m(\cos\theta)$ the integral over the solid angle may be written as

$$I_{1,2} \propto \underbrace{\int_0^{2\pi} e^{im_2\varphi}\, e^{\pm i\varphi}\, e^{im\varphi}\, d\varphi}_{I_\varphi\text{: gives the selection rule upon } m}\ \underbrace{\int_{-1}^{1} P_{\ell_1}^{m_1}(\cos\theta)\cos\theta\sin\theta\, P_{\ell_2}^{m_2}(\cos\theta)\, d\theta}_{I_\theta\text{: gives the selection rule upon } \ell}$$

$\boxed{2}$

$$\Rightarrow I_\theta = \int_{-1}^{1} P_{\ell_1}^{m_1}(\cos\theta)\,\frac{1}{2\ell_2+1}\left[\frac{(\ell_2+1-m_2)}{2(\ell_2+1)+1}\left[P_{\ell_2+2}^{m_2+1}(\cos\theta) + P_{\ell_2}^{m_2+1}(\cos\theta)\right] + \frac{P_{\ell_2}^{m_2+1}(\cos\theta) + P_{\ell_2-2}^{m_2+1}(\cos\theta)}{2(\ell_2-1)}\right] d\cos\theta$$

$$\int_{-1}^{1} P_{\ell_1}^{m_1}(\cos\theta)\, P_{\ell_2+2}^{m_2+1}(\cos\theta)\, d\cos\theta \propto \delta_{\ell_1,\ell_2+2}$$

$$\int_{-1}^{1} P_{\ell_1}^{m_1}(\cos\theta)\, P_{\ell_2-2}^{m_2+1}(\cos\theta)\, d\cos\theta \propto \delta_{\ell_1,\ell_2-2}$$

$$\int_{-1}^{1} P_{\ell_1}^{m_1}(\cos\theta)\, P_{\ell_2}^{m_2+1}(\cos\theta)\, d(\cos\theta) \propto \delta_{\ell_1,\ell_2}$$

(note that the condition upon m_1, m_2 for the above-stated identities to be employed have already been met by I_ϕ)

$\Rightarrow \boxed{\Delta\ell = 0, \pm 2}$

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2 Transition $3P_{1/2} \to 4f_{5/2}$; electric quadrupole, components x^2, xz and z^2 of the quadrupole operator

$\boxed{1}$ initial state: $j = 1/2$, $l = 1$; final state: $j = 5/2$, $l = 3$

For the above-stated transition,

$\boxed{1}$ $\Delta j = 2$, $\Delta l = 0$ (transition allowed by the electric quadrupole selection rules)

- m sublevels:

$\boxed{2}$ $3P_{1/2} \to m = -1/2, +1/2$ (2 sublevels)

$4f_{5/2} \to m = -\frac{5}{2}, -\frac{3}{2}, -1/2, +1/2, +3/2, +5/2)$ (6 sublevels)

In order to determine which m sublevels are coupled, we will write the operators in spherical harmonics and inspect the integrals in ϕ.

$\boxed{1}$ $$Y_l^m = e^{im\phi} P_l^m(\cos\theta)$$

- Component xz:

$\boxed{1}$ $$xz = r^2 \frac{\pi}{3} [\underbrace{Y_1^0 Y_1^{-1}}_{e^{-i\phi} P_1^0(\cos\theta) P_1^{-1}(\cos\theta)} - \underbrace{Y_1^0 Y_1^1}_{e^{i\phi} P_1^0(\cos\theta) P_1^{-1}(\cos\theta)}]$$

Matrix element:

$\boxed{1}$ $\langle n' l' m' | xz | n l m \rangle$ = radial integral $\times$ integral in θ $\times$
$$\times \left[\int_0^{2\pi} e^{i\phi - im'\phi + im\phi} \, d\phi - \int_0^{2\pi} e^{-im'\phi - i\phi + im\phi} \, d\phi \right]$$

$\boxed{1}$ $\langle n' \ell' m' | xz | n \ell m \rangle \neq 0$ for $\Delta m = \pm 1$

$\boxed{2}$

$3P_{1/2}\ (m=-1/2) \rightarrow 4f_{5/2}\ (m=-3/2)$

$3P_{1/2}\ (m=-1/2) \rightarrow 4f_{5/2}\ (m=+1/2)$

$3P_{1/2}\ (m=+1/2) \rightarrow 4f_{5/2}\ (m=-1/2)$ are coupled

$3P_{1/2}\ (m=+1/2) \rightarrow 4f_{5/2}\ (m=+3/2)$

Component $x^2 \propto r^2 \underbrace{\left[Y_1^{-1}(\theta,\phi) - Y_1^{1}(\theta,\varphi)\right]^2}$

$\boxed{1}$

$$= \left[Y_1^{-1}(\theta,\varphi)\right]^2 + \left[Y_1^{1}(\theta,\varphi)\right]^2 + - 2Y_1^{-1}(\theta,\varphi)\, Y_1^{1}(\theta,\varphi)$$

$\boxed{1}$ $\left[Y_1^{-1}(\theta,\varphi)\right]^2 \propto e^{-2i\varphi}\left[P_1^{-1}(\cos\theta)\right]^2$

$\boxed{1}$ $\left[Y_1^{1}(\theta,\varphi)\right]^2 \propto e^{i2\varphi}\left[P_1^{1}(\cos\theta)\right]^2$

$\boxed{1}$ $\left[Y_1^{-1}(\theta,\varphi)\, Y_1^{1}(\theta,\varphi)\right] \propto \underbrace{e^{i\varphi}\cdot e^{-i\varphi}}_{1}\left[P_1^{1}(\cos\theta)\, P_1^{-1}(\cos\theta)\right]$

$\boxed{2}$ Azimuthal integrals: $I_{\varphi_1} = \int_0^{2\pi} e^{\pm i2\varphi}\, e^{i(m-m')\varphi}\, d\varphi$

$$I_{\varphi_2} = \int_0^{2\pi} e^{i(m-m')\varphi}\, d\varphi$$

$\Rightarrow \Delta m = 0, \pm 2$

$\boxed{2}$

$3P_{1/2}\ (m=-1/2) \rightarrow 4f_{5/2}\ (m=-5/2)$

$3P_{1/2}\ (m=-1/2) \rightarrow 4f_{5/2}\ (m=-1/2)$

$3P_{1/2}\ (m=-1/2) \rightarrow 4f_{5/2}\ (m=+3/2)$ are coupled

$3P_{1/2}\ (m=+1/2) \rightarrow 4f_{5/2}\ (m=+1/2)$

$3P_{1/2}\ (m=+1/2) \rightarrow 4f_{5/2}\ (m=-3/2)$

$3P_{1/2}\ (m=+1/2) \rightarrow 4f_{5/2}\ (m=+5/2)$

Component $z^2 \propto r^2 (Y_i^0)^2 \Rightarrow$ no dependence in ϕ (7)

$\boxed{1}$ $\Rightarrow \Delta m = 0$

$\boxed{1}$ $3P_{1/2}\ (m = -1/2) \rightarrow 4f_{S1/2}\ (m = -1/2)$
$3P_{1/2}\ (m = +1/2) \rightarrow 4f_{S1/2}\ (m = 1/2)$ are coupled

(20)

(b) $\boxed{1}$ Electric dipole transitions $\Delta l = \pm 1$, $\Delta m = 0, \pm 1$ → $\sigma+$, $\sigma-$, linearly polarized light $\boxed{1}$

If we take the total angular momentum quantum number j for the initial and final states, we can see that, in principle, all transitions are allowed as $\Delta j = +1$ $(\frac{3}{2} - 1)$. This cannot be verified by taking the orbital quantum number l without spin-orbit coupling $\boxed{5}$

Missing polarizations:

(i) σ^+. The transition from the initial state to a virtual intermediate level increased m by $+1$. In order to increase m once more by $+1$ and reach the indicated final level ($m_{Final} - m_{initial} = +2$), the system must absorb another σ^+ photon. $\boxed{5}$

$\boxed{2}$ (ii) linearly polarized, as there is no increase in the magnetic quantum number ($m_{Final} - m_{initial} = 0$)

$\boxed{1}$ (iii) $\sigma -$, as $m_{Final} - m_{initial} = -1$ (15)

(c) None. The magnetic dipole operator couples levels with the same principal quantum number only. This is not the case for the transition provided as $n_{initial} = 2$ and $n_{final} = 3$. From the selection rules, one may show that the radial integral will vanish in this case due to the orthogonality of the wavefunctions involved.

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(a)

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(a)

$\boxed{1}$ Expectation value of the dipole operator

$e\langle\Psi(t)|\hat{z}|\Psi(t)\rangle$:

Using $|\Psi(t)\rangle = |\Psi_0\rangle + \sum_{m\neq 0} \frac{eE_0\omega_{no}}{2\hbar\omega}\langle\Psi_m|\hat{z}|\Psi_0\rangle F(\omega,\omega_0)|\Psi_m\rangle$

we find

$$\langle\Psi(t)|\hat{z}|\Psi(t)\rangle = \left[\langle\Psi_0| + \sum \frac{eE_0\omega_{no}}{2\hbar\omega}\langle\Psi_0|\hat{z}|\Psi_m\rangle \cdot F^*(\omega,\omega_0)\langle\Psi_m|\right] z \left[|\Psi_0\rangle + \sum \frac{eE_0\omega_{no}}{2\hbar\omega}\langle\Psi_m|\hat{z}|\Psi_0\rangle F(\omega,\omega_0)|\Psi_m\rangle\right]$$

$\boxed{2}$

$$= \underbrace{\langle\Psi_0|z|\Psi_0\rangle}_{=0\text{ as}} + \sum \frac{eE_0\omega_{no}}{2\hbar\omega} F^*(\omega,\omega_0)\langle\Psi_0|\hat{z}|\Psi_n\rangle\langle\Psi_n|\hat{z}|\Psi_0\rangle$$

$\boxed{2}$ the dipole operator only couples states of different parity

$\boxed{1}$

$$+\sum \frac{eE_0\omega_{no}}{2\hbar\omega} F(\omega,\omega_0)\underbrace{\langle\Psi_0|\hat{z}|\Psi_n\rangle\langle\Psi_n|\hat{z}|\Psi_0\rangle}_{=|\langle\Psi_0|z|\Psi_n\rangle|^2} +$$

$$+ O(E_0^2)$$

can be neglected $\boxed{2}$ because is quadratic with regard to the field strength

$\boxed{1}$ $$\langle\Psi(t)|\hat{z}|\Psi(t)\rangle = \sum \frac{eE_0\omega_{no}}{2\hbar\omega}\left[F^*(\omega,\omega_0) + F(\omega,\omega_0)\right]|\langle\Psi_0|z|\Psi_n\rangle|^2$$

$\boxed{2}$ $F^*(\omega,\omega_0) + F(\omega,\omega_0) = 2\,\mathrm{Re}[F(\omega,\omega_0)]$ (*)

$\boxed{2}$
$$e^{\pm i\omega_{no}t} = \cos(\omega_{no}t) \pm i\sin(\omega_{no}t)$$
$$e^{\pm i\omega t} = \cos(\omega t) \pm i\sin(\omega t)$$

$$\Rightarrow (*) = 2\left[\frac{\cos(\omega_{no}t) - \cos(\omega t)}{\omega_{no}+\omega} - \frac{(\cos(\omega_{no}t) - \cos\omega t)}{\omega_{no}-\omega}\right] =$$

$\boxed{2}$
$$= 2[\cos(\omega_{no}t) - \cos(\omega t)]\left[\frac{\cancel{\omega_{no}} - \omega - \cancel{\omega_{no}} - \omega}{\omega_{no}^2 - \omega^2}\right] =$$

$$= \frac{-2\omega}{\omega_{no}^2 - \omega^2}[2\cos[\omega_{no}t] - 2\cos[\omega t]]$$

We can neglect the term in $\cos[\omega_{no}t]$ because it $\boxed{3}$ will lead to a nonlinear temporal dependence with regard to the field. This means that

$\boxed{1}$
$$(*) \simeq \frac{4\omega}{\omega_{no}^2 - \omega^2}\cos\omega t \;\Rightarrow\; \boxed{\begin{aligned}\langle D(z)\rangle &= e\langle\Psi(t)|\hat{z}|\Psi(t)\rangle \\ &= 2e^2 E_0 \cos\omega t \sum_{n\neq 0} \frac{\cancel{2\omega}}{2\omega}\frac{\omega_{no}}{\hbar}|\langle\Psi_0|z|\Psi_n\rangle|^2\end{aligned}}\;\boxed{1}$$

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(b)

Forced harmonic oscillator: equation of motion

$$m\ddot{z} + m\omega_0^2 z = -eE_0\cos(\omega t)$$

The above-stated equation exhibits a general solution, of the form $C_1 e^{-i\omega_0 t} + C_2 e^{i\omega_0 t}$ and a particular

Solution $z_p = C\exp[i\omega t] + c.c.$. This particular solution oscillates with the frequency of the field, while the general solution oscillates with the natural frequency of the system, i.e., ω_0. As we are interested in the solution that "follows" the field, we will only take into account the particular solution.

Stating the general solution: 2 marks
Stating the particular solution: 2 marks
Giving a Reason for the general solution to be neglected: 2 marks

In order to find C, we insert z_p and $\ddot{z}_p$ in the differential equation

$\boxed{1}$ $\dot{z}_p = -\omega C \sin\omega t$

$\boxed{1}$ $\ddot{z}_p = -\omega^2 C \cos\omega t$ $\Rightarrow$ $m[-\omega^2 + \omega_0^2]C \cos\omega t = -eE_0 \cos\omega t$

$\boxed{1}$ $\Rightarrow C = \dfrac{+eE_0}{(\omega^2 - \omega_0^2)m}$

$\boxed{1}$ $z_p = \dfrac{+eE_0}{m(\omega^2 - \omega_0^2)} \cos\omega t$

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(c) The above-stated results show that, under the influence of an external electric field, a quantum mechanical atom behaves as if it were an ensemble of classical forced harmonic oscillators (2 marks). Each "atom" in the ensemble has a natural frequency ω_{n0}, which corresponds to the transition frequency of the transitions from a level n to a level 0 or vice versa, and the statistical weight in the ensemble is given by the oscillator strength (3 marks).

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