Recap:

We found the photo-ionization cross-section

$$\sigma(\theta) = \frac{\frac{32a_0^3e^2p_f^3}{m\omega e\hbar^3}(\cos^2\theta)}{\left[1+(\frac{p_fa_0}{\hbar})^2\right]^4} \tag{1}$$

Dimensional Analysis:

Note that the we can re-write equation (1) as (ignoring constant and dimensional less quantities)

$$\frac{e^2}{\hbar c}a_0^2\frac{p_fa_0}{\hbar}\left(\frac{E_f}{\hbar\omega}\right) \tag{2}$$

Note that equation (2) written in this way clearly has cross-section unit L^3 .

Angle part (from last lecture)

We know that

$$\cos^2\theta \sim (\vec{A}_0\cdot\vec{p}_f)^2 \tag{3}$$

where the direction of $\vec{A}_0$ determines the polarization of the $\vec{E}$ field because $\vec{E}=\frac{1}{c}\frac{\partial\vec{A}}{\partial t}$. This means that equation (3) is maximized when $\vec{p}_f \mid\mid \vec{E}$, and it is min when $\vec{p}_f \perp \vec{E}$.

Denominator

Note that the denominator of (1)

$$\frac{1}{\left[1+(\frac{p_fa_0}{\hbar})^2\right]^4} \sim |\langle\vec{p}_f|\psi_{100}\rangle|^2$$

This is because

$$\begin{aligned}&\langle\vec{p}_f|H_1|\psi_{100}\rangle\\&\sim \vec{A}_0\cdot\langle\vec{p}_f|\vec{\nabla}|\psi_{100}\rangle\\&\sim \vec{A}_0\vec{p}_f\,\langle\vec{p}_f|\psi_{100}\rangle\\\implies&\langle\vec{p}_f|\psi_{100}\rangle \sim \frac{1}{\left[1+(\frac{p_fa_0}{\hbar})^2\right]^2}\end{aligned}$$

Note that the overlap integral between $\langle\vec{p}|\psi_{100}\rangle$ is nothing but imaging the ground state wave function in $\vec{p}$ space. Specifically, we are probing $\vec{p}_f$ in ψ_{100}.

Electric Dipole Approximation

We have the set-up

$$\vec{E} = -\frac{1}{c}\frac{\partial\vec{A}}{\partial t} = \frac{i\omega}{c}\vec{A}_0e^{-i\omega t}e^{i\vec{k}\cdot\vec{r}} + \text{c.c} \tag{4}$$

where the absorption $e^{-i\omega t}$ dominates, and $e^{i\vec{k}\cdot\vec{r}}\approx 1$ because $\lambda=\frac{2\pi}{k}\gg a_0$

This indicates that equation (4) is almost spatially invariant as the main contribution comes from resonant absorption.
Because $\vec{E}$ couples to the electric dipole $|e|\vec{R}$ where $\vec{R}$ is the position vector of e^- , we have:

$$H_{\rm dip} = -|e|\vec{R}\cdot\vec{E} = -i\frac{\omega}{2c}|e|\vec{A}_0\cdot\vec{R}e^{-i\omega t} \tag{5}$$

However, what we did instead for the dipole approximation is

$$H_1 = \frac{-|e|}{2mc}\vec{A}_0\cdot\vec{p}e^{-i\omega t} \tag{6}$$

This is rather strange, because equation (6) is independent of the position vector $\vec{R}$, but equation (5) couples vector potentials to position. This is what we are trying to understand.

Let us start considering this with a unperturbed hydrogen atom $H_0 = \frac{p^2}{2m} + V(R)$
We observe that

$$[\vec{R}, H_0] = \frac{i\hbar}{m}\vec{p} \tag{7}$$

Note that our because equation (7) relate $\vec{R}$ and $\vec{p}$, let us start from this. Sand-witching equation (7) gets:

$$\begin{aligned}
\langle f\rangle[\vec{R}, H_0]|i\rangle &= \frac{i\hbar}{m}\langle f|\vec{p}|i\rangle \\
\implies -(E_f - E_i)\langle f|\vec{R}|i\rangle &= \frac{i\hbar}{m}\langle f|\vec{p}|i\rangle \\
\implies \langle f|H_1|i\rangle &= \frac{-|e|}{2mc}\vec{A}_0\cdot\langle f\rangle\vec{p}|i\rangle e^{-i\omega t} \\
&= \frac{-|e|}{2mc}(im\omega_{fi})\vec{A}_0\cdot\langle f|\vec{R}|i\rangle e^{-i\omega t} \\
&= \frac{\omega_{fi}}{\omega}\langle f|H_{dip}|i\rangle
\end{aligned}$$

Because we are near resonance, so we have $\omega \approx \omega_{fi}$, we have $H_1 \approx H_{dip}$.

Selection Rules:

(pp 458-459 Shankar in time-independent P.T.)

Q. When does $\langle f|H_1|i\rangle = 0$ for a given perturbation H_1?

Let us exploit symmetry. First, symmetry is something that **commutes with the Hamiltonian**, let's call this symmetry operator Λ.By the definition of symmetry, we have

$$[\Lambda, H_0] = [\Lambda, H_1] = [\Lambda, H] = 0$$

and let us consider the eigenstates of Λ

$$\Lambda|\alpha_i, \lambda_i\rangle = \lambda_i|a_i, \lambda_i\rangle$$

this implies:

$$\langle\alpha_2, \lambda_2|H_1|\alpha_1, \lambda_1\rangle = 0 \quad \text{unless} \quad \lambda_2 = \lambda_1 \tag{8}$$

Proof of (8)

$$\begin{aligned}
\langle\alpha_2, \lambda_2|[\Lambda, H_1]|\alpha_1, \lambda_1\rangle &= 0 \\
(\lambda_2 - \lambda_1)\langle\alpha_2, \lambda_2|H_1|\alpha_1, \lambda_1\rangle &= 0 \\
\text{if} \quad \lambda_2 \neq \lambda_1 \implies \langle\alpha_2, \lambda_2|H_1|\alpha_1, \lambda_1\rangle &= 0
\end{aligned}$$

Example 1: Parity

Let $\Lambda = \text{parity}$
if $[H_1, \Lambda] = 0$, then:

$$\begin{aligned}
\langle\text{odd}|H_1|\text{even}\rangle = 0 \\
\langle\text{even}|H_1|\text{odd}\rangle = 0
\end{aligned}$$

In this case, we cut the amount of calculation by a factor of 2!

Example 2: Dipole Selection Rule

Let us use angular momentum states:

$$\langle \alpha_2, j_2, m_2 | z | \alpha_1, j_1, m_1 \rangle = 0 \quad \text{unless} \quad j_{2=} \begin{cases} j_1 + 1 \\ j_1 \\ j_1 - 1 \end{cases} \quad \text{and} \quad m_2 = m_1$$

Let us focus on a special case where $\vec{S} = 0$, this gives $\vec{J} = \vec{L}$

Then, the matrix element becomes:

$$\int_0^{2\pi} \int_{-1}^{1} Y^*_{l_2 m_2}(\theta, \phi) \cos\theta Y_{l_1, m_1} \, d(\cos\theta) \, d\phi$$

Note that the condition for $m_2 = m_1$ is clear, as the $e^{-im_2\phi}$ and $e^{-m_1\phi}$ should cancel each other.