Department of Physics IIT-Madras PCD_STiAP_Self_Assesment_5 20 marks

- What are the parameters that can be measured in atomic photoionization process? Explain them briefly.
 3 marks
- a. Cross sections: The probability measure of a transition to take place during the process
- b. Angular distribution of photoelectrons: The direction in which the photoelectrons are ejected out with reference to the incident beam and polarization direction.
- c. Spin-polarization parameters of the photoelectrons: Gives the orientation of the angular momentum of the photoelectrons.
- 2. Consider a system of 20 electrons. Write down the relativistic configuration of the system and give the dipole transition from the valence subshell. 2marks

The relativistic Configuration:

$$1s_{1/2}^2 2s_{1/2}^2 2p_{1/2}^2 2p_{3/2}^4 3s_{1/2}^2 3p_{1/2}^2 3p_{3/2}^4 4s_{1/2}^2$$

The allowed dipole transition from 4s subshell is:

$$4s_{1/2} \rightarrow \varepsilon p_{1/2}$$
$$4s_{1/2} \rightarrow \varepsilon p_{3/2}$$

3. Determine the number of states within the solid angle $d\Omega$ in a cubical box of volume V and length L, with energy between E and E+dE. - 4 marks

The number of states in volume element is

$$n^{2}dnd\Omega = n^{2} \frac{dn}{dE} dEd\Omega \qquad n = \frac{L}{2\pi} k \Rightarrow dn = \frac{L}{2\pi} dk$$

$$= n^{2} \frac{dk}{dE} \frac{L}{2\pi} dEd\Omega \qquad \text{[mul and div by L/2]]}$$

$$= n^{2} \frac{dk}{dE} \left(\frac{L}{2\pi}\right)^{2} \frac{2\pi}{L} dEd\Omega \qquad \frac{dk}{dE} = \frac{m}{\hbar^{2}k}$$

$$= \left(\frac{L}{2\pi}k\right)^{2} \left(\frac{m}{\hbar^{2}}\frac{1}{k}\right) \left(\frac{L}{2\pi}\right)^{2} \frac{2\pi}{L} dEd\Omega$$

$$= \left(\frac{L}{2\pi}\right)^{3} \frac{mk}{\hbar^{2}} dEd\Omega$$

Number of states within the solid angle $d\Omega$ in a cubical box with energy between E and E+dE is given by:

$$\rho(E)d\Omega = \left(\frac{1}{2\pi}\right)^3 \frac{mk}{\hbar^2} V$$
; Where L³ = V

4. a. What is Born approximation. Show that $\frac{v_f}{2c} <<<1$. - 2+1 marks

Born approximation is a high energy approximation. The incident photon energy is very high compared to the $|E_{1s}|$ i.e $\hbar \omega \gg |E_{1s}|$. So we have

$$\hbar \omega = \frac{\hbar^2 k_f^2}{2m} + I.P \approx \frac{\hbar^2 k_f^2}{2m} \qquad E = \hbar \omega = \hbar kc$$

$$kc = \frac{\hbar k_f^2}{2m} \Longrightarrow \frac{k}{k_f} = \frac{\hbar k_f}{2mc} = \frac{p_f}{2mc} = \frac{v_f}{2c}$$

$$\frac{v_f}{2c} <<<1$$

b. Under Born approximation in what powers of energy and atomic number do the photoionization cross section depends on?

$$\sigma \rightarrow E^{-7/2}, Z^5$$

5. Given the matrix element $\langle f | e^{i\vec{k} \cdot \vec{r}} \hat{\epsilon} \cdot \vec{\nabla} | i \rangle$ where $|i\rangle$ represents initial bound state and $|f\rangle$ represents final continuum state, under dipole approximation, determine the momentum and length form of the matrix elements.

- 5 marks

$$\langle f | e^{i\vec{k}\cdot\vec{r}} \hat{\varepsilon} \cdot \vec{\nabla} | i \rangle = \frac{1}{(-i\hbar)} \langle f | e^{i\vec{k}\cdot\vec{r}} \hat{\varepsilon} \cdot (-i\hbar\vec{\nabla}) | i \rangle$$

$$= \frac{i}{\hbar} \langle f | e^{i\vec{k}\cdot\vec{r}} \hat{\varepsilon} \cdot \vec{p} | i \rangle ; \text{ In dipole approximation } e^{+i(\vec{k}\cdot\vec{r})} \approx 1$$

$$\langle f | e^{i\vec{k}\cdot\vec{r}} \hat{\varepsilon} \cdot \vec{\nabla} | i \rangle = \frac{i}{\hbar} \langle f | p_x | i \rangle$$

$$[r_k, p_k^2] = r_k r_k p_k - p_k p_k r_k$$

$$= r_k p_k p_k - p_k r_k p_k + p_k r_k p_k - p_k p_k r_k$$

$$= [r_k, p_k] p_k + p_k [r_k, p_k]$$

$$= 2i\hbar p_k \qquad [r_k, H_0] = [r_k, \frac{p^2}{2m}] = \frac{i\hbar}{m} p_k$$

$$\langle f | e^{i\vec{k}\cdot\vec{r}} \hat{\varepsilon} \cdot \vec{\nabla} | i \rangle = \frac{i}{\hbar} \langle f | \frac{m}{i\hbar} [x, H_0] | i \rangle$$

$$\langle f | e^{i\vec{k}\cdot\vec{r}} \hat{\varepsilon} \cdot \vec{\nabla} | i \rangle = \frac{i}{\hbar} \langle f | \frac{m}{i\hbar} [xH_0 - H_0 x] | i \rangle$$

$$\langle f | e^{i\vec{k}\cdot\vec{r}} \hat{\varepsilon} \cdot \vec{\nabla} | i \rangle = \frac{m}{\hbar^2} (E_i - E_f) \langle f | x | i \rangle$$

$$\langle f | p_x | i \rangle = \frac{im}{\hbar} (E_i - E_f) \langle f | x | i \rangle$$

$$\langle f | p_x | i \rangle = im\omega_{fi} \langle f | x | i \rangle$$

$$\Rightarrow \vec{p}_{fi} = im\omega_{fi} \vec{r}_{fi}$$

6. Given the differential cross section equation $\begin{bmatrix} \frac{d\sigma}{d\Omega} \end{bmatrix}_{\hat{k}_{f}}^{\hat{\varepsilon}} = \frac{\sigma_{Total}}{4\pi} [1 + \beta P_{2} \cos \Theta] \text{ where}$ $P_{2} \cos \Theta = \frac{1}{2} (3\cos^{2} \Theta - 1) \text{. Find the range of } \beta \text{ . } -3 \text{ marks}$ Since cross section cannot go negative $1 + \frac{\beta}{2} (3\cos^{2} \Theta - 1) \ge 0$ $\frac{\beta}{2} (3\cos^{2} \Theta - 1) \ge -1 \qquad 0 \le \Theta \le \pi$ $0 \le \Theta \le \pi$ $0 \le \cos^{2} \Theta \le 1$ $[\cos^{2} \Theta]_{max} = 1 \Rightarrow \beta \ge -1$ $[\cos^{2} \Theta]_{min} = 0 \Rightarrow \beta \le 2$ $\Rightarrow -1 \le \beta \le 2$