The Ionization of Atomic Hydrogen

Again for simplicity, we will treat the case of atomic hydrogen. The initial state is an incoming photon with the electron in its ground state $|100\rangle$. The final state is the electron in one of the positive-energy ε-states of

$$H_0^{AT} = \frac{\vec{p}^{\,2}}{2m} - \frac{e^2}{r} \qquad (1)$$

labelled by momentum $\vec{p}_f = \hbar \vec{k}_f$. We shall approximate this state by a plane wave

$$\langle \vec{x} | k_f \rangle = \frac{e^{i k_f \cdot x}}{\sqrt{V}} \qquad (2)$$

where

$$\vec{k} = \frac{2\pi}{L} \vec{n} \qquad (3)$$

and

$$V = L^3. \qquad (4)$$

Once again

$$\langle k_f | 100, k_i \rangle_I = -\frac{i}{\hbar} \int_0^t \langle k_f | e^{iH_0 t'} \, -\frac{e}{mc} \vec{A}(x,0) \cdot \vec{p} \; e^{-iH_0 t'} | 100, k_i \rangle \, dt' \qquad (5)$$

in which

$$H_0 = H_0^{AT} + H_0^{EM} \qquad (6)$$

and

$$H_0 = \sum_{k,r} \hbar\omega \left(a_r^\dagger(k)a_r(k) + \tfrac{1}{2}\right). \qquad 7$$

Here

$$A(x,t) = e^{iH_0^{EM}t} A(x,0) e^{-iH_0^{EM}t}$$

$$= \sum_{k,r} \left(\frac{hc^2}{\omega_k V}\right)^{\frac{1}{2}} \left[e_r(k)a_r(k)e^{ik\cdot x - i\omega_k t} + e_r^*(k)a_r^\dagger(k)e^{-ik\cdot x + i\omega_k t}\right]. \qquad 8$$

So

$$\langle k_f | 100, k\rangle_I = \sum_{k,r} \frac{-i}{\hbar}\int_0^t \left(-\frac{e}{mc}\right)\langle k_f | e_r(k)\cdot p e^{ik\cdot x - i\omega_k t'} a_r(k)|100, k_i\rangle dt' \left(\frac{hc^2}{\omega_k V}\right)^{\frac{1}{2}} \times e^{i\frac{p_f^2}{2m}\frac{t'}{\hbar} - iE_{100}t'/\hbar}$$

$$= \frac{i}{\hbar}\left(\frac{e}{mc}\right)\left(\frac{hc^2}{\omega_{k_i}V}\right)^{\frac{1}{2}} \int_0^t \langle k_f | e_r(k)\cdot p e^{i\vec{k}_i\cdot\vec{x}} |100\rangle e^{i(E_f - E_{100})t'/\hbar - i\omega_{k_i}t'} dt'$$

$$= \left(\frac{e}{mc}\right)\left(\frac{hc^2}{\omega_{k_i}V}\right)^{\frac{1}{2}} \vec{e}_{r_i}(k_i)\cdot\langle k_f|\vec{p}e^{i\vec{k}_i\cdot\vec{x}}|100\rangle \frac{\left(e^{i(E_f - E_0 - \hbar\omega_{k_i})t/\hbar} - 1\right)}{E_f - E_{100} - \hbar\omega_{k_i}} \qquad 9$$

So the transition rate, as before, is

$$\hat{\omega}_{i\to f} = \frac{2\pi}{\hbar}\left(\frac{e}{mc}\right)^2\left(\frac{hc^2}{\omega_{k_i}V}\right) |\vec{e}_{r_i}(k_i)\cdot\langle k_f|\vec{p}e^{i\vec{k}_i\cdot\vec{x}}|100\rangle|^2 \delta(E_f - E_{100} - \hbar\omega_{k_i}). \qquad (10)$$

The matrix element is

$$\langle p_f | \vec{p}\cdot\vec{e}_{r_i}(k_i)\, e^{ik_i\cdot x} | 100\rangle$$

$$= \vec{p}_f\cdot\vec{e}_{r_i}(k_i)\ \langle p_f | e^{ik_i\cdot x} | 100\rangle. \qquad 11$$

The reduced matrix element then is

$$\langle p_f | e^{ik_i\cdot x} | 100\rangle = \int d^3x\, \langle p_f | x\rangle\langle x | e^{ik_i\cdot x} | 100\rangle$$

$$= \int d^3x\, \frac{e^{-ik_f\cdot x}}{\sqrt{V}}\, e^{ik_i\cdot x}\, R_{10}(x)\frac{1}{\sqrt{4\pi}} \qquad 12$$

since

$$\langle x | 100\rangle = R_{10}(r)\,Y_0^0(\Omega) = R_{10}(r)\frac{1}{\sqrt{4\pi}}$$

$$= \frac{1}{\sqrt{4\pi}}\left(\frac{Z}{a_0}\right)^{3/2} e^{-Zr/a_0}. \qquad 13$$

So with $\vec{q} = \vec{k}_f - \vec{k}_i$, the matrix element (11) is

$$\langle p_f | p\cdot e\, e^{ik_i\cdot x} | 100\rangle = \frac{p_f\cdot e_{r_i}(k_i)}{\sqrt{4\pi V}}\, 2\left(\frac{Z}{a_0}\right)^{3/2}\int d^3x\, e^{-iq\cdot x - Zr/a_0}$$

$$= 2\left(\frac{Z}{a_0}\right)^{\frac{3}{2}}\frac{p_f\cdot e_i\, 2\pi}{\sqrt{4\pi V}}\int_0^\infty dr\, r^2\int_{-1}^{1} d\cos\theta\, e^{-iqr\cos\theta - Zr/a_0} \qquad 14$$

in which we allow $Z > 1$.

So

$$\langle k_f | p\cdot e\, e^{i k_i\cdot x} | 100\rangle = \frac{\hbar k_f\cdot e\, 2\pi}{\sqrt{4\pi}\sqrt{V}}\, 2\left(\frac{Z}{a_0}\right)^{3/2}\int_0^\infty dr\, r^2 e^{-Zr/a_0}$$

$$\times\left(\frac{e^{-iqr}-e^{iqr}}{-iqr}\right)$$

$$= \sqrt{4\pi}\; p_f\cdot e\; 2\left(\frac{Z}{a_0}\right)^{3/2}\frac{1}{\sqrt{V}}\frac{1}{q}\int_0^\infty dr\; r\sin qr\, e^{-Zr/a_0}$$

$$= 2\sqrt{4\pi}\;\frac{p_f\cdot e_{n_i}(k_i)}{\sqrt{V}}\left(\frac{Z}{a_0}\right)^{3/2}\frac{1}{q}\;\frac{2qZa_0^3}{(Z^2+q^2a_0^2)^2} \quad (15)$$

So the rate is

$$\hat{W}_{i\to f} = \frac{2\pi}{\hbar}\left(\frac{e}{m}\right)^2\left(\frac{\hbar c^2}{\omega k_i V}\right)\frac{4\cdot 4\pi}{V}\left(\frac{Z}{a_0}\right)^3\frac{4Z^2a_0^6\,|p_f\cdot e_{n_i}(k_i)|^2}{(Z^2+q^2a_0^2)^4}$$

$$\times\,\delta(E_f-E_{100}-\hbar\omega_i). \quad (16)$$

We must integrate this over the final states of the electron: $\vec{k}_f = 2\pi\vec{n}/L$

(17)

$$\sum_n = \int\left(\frac{L}{2\pi}\right)^3 d^3k = V\int\frac{d^3k}{(2\pi)^3}$$ and also summing over the two spin states.

Now as long as the electron is non-relativistic

$$E = \frac{p_f^2}{2m} \quad \text{and} \quad dE = \frac{p_f}{m} dp_f = \frac{\hbar^2 k\, dk}{m} \qquad (18)$$

so

$$d^3k = d\phi\, d\cos\theta\, k^2 dk = d\Omega\, k \frac{m}{\hbar^2} dE\,. \qquad 19$$

So

$$w_{i\to f} = \sum_{s=1}^{2} \frac{2\pi}{\hbar}\left(\frac{e}{mc}\right)^2\left(\frac{hc^2}{\omega_{k_i} V}\right)\frac{16\pi}{V}\left(\frac{Z}{a_0}\right)^3 \frac{4Z^2 a_0^6 |p_f \cdot e_{r_i}(k_i)|^2}{(Z^2+q^2a_0^2)^4}$$

$$\cdot \quad V\int \frac{d^3k}{(2\pi)^3}\, \delta(E_f - E_{100} - \hbar\omega_1)$$

$$= \frac{4\pi}{\hbar}\left(\frac{e}{mc}\right)^2\left(\frac{hc^2}{\omega V}\right)64\pi\left(\frac{Z}{a_0}\right)^3 \frac{Z^2 a_0^6 |\vec{p}\cdot\vec{e}|^2}{(Z^2+q^2a_0^2)^4}\, \frac{d\Omega\, k_f\, m}{\hbar^2(2\pi)^3}$$

$$= \frac{32}{\pi\hbar}\left(\frac{e}{m\hbar c}\right)^2\left(\frac{hc^2}{\omega V}\right)\frac{Z^5 a_0^3 |p\cdot e|^2 k_f\, m\, d\Omega}{(Z^2+q^2a_0^2)^4} \qquad 20$$

Now $|\vec{p}\cdot\vec{e}|^2$ is to be averaged over the initial polarizations of the photon, so

$$\overline{|p\cdot e|^2} = \frac{1}{2}\sum_r p\cdot e\, e^\dagger \cdot p = \frac{1}{2} p\cdot\left(I - \hat{k}\hat{k}^T\right)\cdot p \qquad 21$$

$$\overline{|p\cdot e|^2} = \frac{1}{2}\left(\vec{p}^{\,2} - (\vec{p}\cdot\hat{k})^2\right). \qquad 22$$

So if $\vec{k}_i$ is in the z-direction with which the final-state electron makes polar angles θ, φ, then

$$\overline{|p\cdot e|^2} = \frac{1}{2} p_f^2 \left(1 - \cos^2\theta\right) = \frac{p_f^2}{2}\sin^2\theta \qquad 23$$

The incoming flux of photons is

$$F = \frac{nc}{V} \quad \text{with} \quad n = 1 \qquad 24$$

and so the cross-section is

$$\frac{d\sigma}{d\Omega} = \frac{32}{\pi\hbar}\left(\frac{e}{m\hbar c}\right)^2 \frac{hc^2}{\omega_k V} \frac{Z^5 a_0^3}{\frac{c}{V}} \frac{\frac{1}{2} p^2 \sin^2\theta \quad mp/\hbar}{\left(Z^2 + a_0^2 (k_f - k_i)^2\right)^4} \qquad (25)$$

Now $(k_f - k_i)^2 = k_f^2 + k_i^2 - 2k_f k_i \cos\theta$

$$= \left(p^2 + (\hbar\omega)^2 - 2p\hbar\omega\cos\theta\right)/\hbar^2. \qquad (26)$$

So

$$\frac{d\sigma}{d\Omega} = \frac{16}{\pi\hbar}\frac{e^2}{\hbar c}\frac{2\pi Z^5}{m\ \hbar\omega} \frac{a_0^3\, p^3 \sin^2\theta}{\left[Z^2 + a_0^2\left(p^2 + (\hbar\omega)^2 - 2\hbar\omega p\cos\theta\right)/\hbar^2\right]^4} \qquad (27)$$

in which ω refers to the photon and p to the electron.

So since $a_0 = \hbar^2/me^2$

$$\frac{d\sigma}{d\Omega} = 32\,\alpha\,\frac{a_0^2}{\hbar}\,\frac{\hbar^2 Z^5 p^3}{me^2\, m\,\hbar\omega}\,\frac{\sin^2\theta}{\left[Z^2 + a_0^2\left(p^2 + (\hbar\omega)^2 - 2\hbar\omega p\cos\theta\right)/\hbar^2\right]^4} \tag{28}$$

$$= 64\, a_0^2\, \frac{E_f}{mc^2}\,\frac{c\,p_f}{\hbar\omega}\,\frac{\sin^2\theta \quad Z^5}{\left[Z^2 + a_0^2\left(p_f^2 + (\hbar\omega)^2 - 2\hbar\omega p_f\cos\theta\right)/\hbar^2\right]^4}. \tag{29}$$

or in the form Sakurai used.

$$\frac{d\sigma}{d\Omega} = \frac{32\, e^2 k_f^3}{m c\,\omega_i}\,\frac{Z^5 \sin^2\theta}{a_0^5\left[Z^2/a_0^2 + q^2\right]^4} \tag{5.7.36}$$

where $\vec{q} = \vec{k}_f - \vec{k}_i$. I prefer (29) because it makes clear that the cross-section is a_0^2 reduced by $E_f/mc^2 < 1$ and modified by the other factors.