The Ionization of Atomic Hydrogen

We'll take the initial state to be the ground state plus one incident photon of wave vector $\vec{k}$

$$|100, k\rangle . \tag{1}$$

The final state will be an electron of momentum $\vec{p}$

$$|\vec{p}\rangle . \tag{2}$$

We'll use box quantization so that

$$\vec{k} = \frac{2\pi}{L}\vec{n}_k \quad \text{and} \quad \vec{p} = \frac{2\pi\hbar}{L}\vec{n}_p . \tag{3}$$

with $V = L^3$.

The hamiltonian of the H-atom is

$$H_{0a} = \frac{p^2}{2m} - \frac{e^2}{4\pi\epsilon_0 r} = \frac{p^2}{2m} - \frac{\alpha\hbar c}{r} \tag{4}$$

where $\alpha = 1/137.036$, and that of the photons is

$$H_{0F} = \sum_{k,r} \hbar\omega_k \left(a_r^\dagger(k) a_r(k) + \tfrac{1}{2}\right) . \tag{5}$$

As before

$$\langle p|S(t,0)|100,k\rangle = -\frac{i}{\hbar}\int_0^t \langle p|e^{i(H_{om}+H_{oF})t'/\hbar}\left(-\frac{q}{m}\vec{p}\cdot\vec{A}\right)e^{-i(H_{om}+H_{oF})t'/\hbar}|100,k\rangle\, dt' \quad (6)$$

in which $\vec{A}$ is

$$\vec{A}(\vec{x},0) = \sum_{k,r}\left(\frac{\hbar}{2\epsilon_0 V\omega_k}\right)^{\frac{1}{2}}\left[\epsilon_r(k)a_r(k)e^{ik\cdot x} + \epsilon_r^*(k)a_r^\dagger(k)e^{-ik\cdot x}\right] \quad (7)$$

So

$$\langle p|e^{i(H_{om}+H_{oF})t'/\hbar}\left(-\frac{q}{m}p\cdot A\right)e^{-i(H_{om}+H_{oF})t'/\hbar}|100,k\rangle = e^{i(E_p-E_{100}-\hbar\omega)t'/\hbar}\left(-\frac{q}{m}\right)\langle p|p\cdot A|100,k\rangle \quad (8)$$

and since $a_{r'}(k')|kr\rangle = \delta_{rr'}\delta_{kk'}|0\rangle$

$$\langle p|p\cdot A|100,k\rangle = \sum_r\left(\frac{\hbar}{2\epsilon_0 V\omega_k}\right)^{\frac{1}{2}} p\cdot\epsilon_r(k)\langle p|e^{ik\cdot x}|100\rangle. \quad (9)$$

The atomic matrix element $\langle p|e^{ik\cdot x}|100\rangle$ involves the wave function

$$\langle x|100\rangle = \frac{1}{\sqrt{4\pi}}R_{10}(r) = \frac{2}{\sqrt{4\pi}}\left(\frac{Z}{a_0}\right)^{3/2}e^{-Zr/a_0} \quad (10)$$

in which $a_0 = 4\pi\epsilon_0\hbar^2/mq^2 = (\hbar/mc)1/\alpha = 0.53\,\mathring{A}$.

The atomic matrix element $\langle p|e^{ik\cdot x}|100\rangle$ is a Fourier transform of $\langle x|100\rangle$:

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

$$= \int \frac{d^3x}{\sqrt{\pi}} \frac{e^{i(k - p/\hbar)\cdot x}}{\sqrt{V}} \left(\frac{Z}{a_0}\right)^{3/2} e^{-Zr/a_0} . \tag{11}$$

We set $\vec{s} = \vec{k} - \vec{p}/\hbar$ and choose the z-axis of $\vec{x}$-space to lie in the $\vec{s}$-direction, so that

$$\langle p| e^{ik\cdot x} |100\rangle = \frac{1}{\sqrt{4\pi V}} \left(\frac{Z}{a_0}\right)^{3/2} 2\pi \int_0^\infty dr \int_{-1}^{1} dx \; r^2 e^{isrx - Zr/a_0}$$

$$= \frac{2\pi}{\sqrt{\pi V}} \left(\frac{Z}{a_0}\right)^{3/2} \int_0^\infty dr \; r^2 \left(\frac{e^{isr} - e^{-isr}}{isr}\right) e^{-Zr/a_0}$$

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

$$= 4\sqrt{\frac{\pi}{V}} \left(\frac{Z}{a_0}\right)^{3/2} \frac{2 Z a_0^3}{\left(Z^2 + s^2 a_0^2\right)^2} . \tag{12}$$

So using (6) and (8), we have

$$\langle p| S(t,0) |100, k\rangle = -\frac{i}{\hbar} \int_0^t dt' \, e^{i(E_p - E_{100} - \hbar\omega_k)t'/\hbar} \left(-\frac{q}{m}\right) \langle p| p\cdot A |100, k\rangle$$

$$= \frac{q}{m} \frac{\left(e^{i(E_p - E_{100} - \hbar\omega_k)t/\hbar} - 1\right)}{\left(E_p - E_{100} - \hbar\omega_k\right)} \langle p| p\cdot A |100, k\rangle$$

or

$$|\langle p|S(t,0)|100,k\rangle|^2 = \frac{4q^2}{m^2}\frac{\sin^2\left((E_p - E_{100} - \hbar\omega_k)t/2\hbar\right)}{(E_p - E_{100} - \hbar\omega_k)^2}|\langle p|p\cdot A|100,k\rangle|^2.$$

As $t \to \infty$, this becomes

$$|\langle p|S(t,0)|100,k\rangle|^2 = \frac{4q^2}{m^2}|\langle p|p\cdot A|100,k\rangle|^2 \frac{\pi t}{2\hbar}\delta(E_p - E_{100} - \hbar\omega_k).$$

So the rate $\hat{w}$ apart from the sum over final states (and the average over initial states) is

$$\hat{w} = \frac{d}{dt}|\langle p|S(t,0)|100,k\rangle|^2$$

$$= \frac{2q^2\pi}{m^2\hbar}|\langle \vec{p}|\vec{p}\cdot A|100,k\rangle|^2 \delta(E_p - E_{100} - \hbar\omega_k)$$

Now using (9) and (12), we get for the rate

$$\hat{w} = \frac{q^2\pi}{m^2\hbar}\frac{\hbar}{2\epsilon_0 V\omega_k}|p\cdot\epsilon_n(k)|^2\frac{16\pi}{V}\left(\frac{Z}{a_0}\right)^3\frac{4Z^2a_0^6\,\delta(E_p - E_{100} - \hbar\omega_k)}{(Z^2 + s^2a_0^2)^4},$$

To sum over final states, we use

$$E_p = \frac{p^2}{2m} \quad \text{so that} \quad dE_p = \frac{p\,dp}{m}.$$

Also, since the ejected electron has 2 spin states

$$\sum_{n_p} = \frac{2V}{(2\pi\hbar)^3} d^3p = \frac{2V}{(2\pi\hbar)^3} p^2 dp\, d\Omega$$

so

$$w = \frac{2V}{(2\pi\hbar)^3} \int p^2 dp\, d\Omega\ \hat{w}$$

$$= \frac{2V\, m}{(2\pi\hbar)^3} \int p\, dE_p\, d\Omega\, \hat{W}$$

$$= \frac{32 q^2 \pi^2}{m\,(2\pi\hbar)^3} \frac{p\,|p\cdot\epsilon_r(k)|^2}{\epsilon_0 V \omega_k} \left(\frac{Z}{a_0}\right)^3 \frac{4 Z^2 a_0^6}{(Z^2 + s^2 a_0^2)^4}\, d\Omega$$

Now the average over the polarizations of the initial photon gives

$$\frac{1}{2}\sum_{r=1}^{2} |p\cdot\epsilon_r(k)|^2 = \frac{1}{2}\sum_{r=1}^{2} p\cdot\epsilon_r(k)\, \epsilon_r^\dagger(k)\cdot p$$

$$= \frac{1}{2}\, p\cdot\left(I - \hat{k}\hat{k}^T\right)\cdot p$$

$$= \frac{1}{2}\left(p^2 - (\hat{k}\cdot p)^2\right).$$

Let $\hat{k}\cdot p = p\cos\theta$. Then

$$\frac{1}{2}\sum_r |p\cdot\epsilon_r(k)|^2 = \frac{1}{2}p^2(1-\cos^2\theta) = \frac{1}{2}p^2\sin^2\theta.$$

The initial flux of photons is

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

so

$$\frac{d\sigma}{d\Omega} = \frac{W}{F} = \frac{WV}{c} = \frac{64\pi^2 q^2}{m(2\pi\hbar)^3}\frac{V}{c}\left(\frac{Z}{a_0}\right)^3 \frac{Z^2 a_0^6 \, p^3 \sin^2\theta}{2\epsilon_0 V \omega_k \left(Z^2 + s^2 a_0^2\right)^4}$$

$$= \frac{8 Z^5 a_0^3 q^2}{m \pi \hbar^3 c \epsilon_0 \omega_k} \frac{p^3 \sin^2\theta}{\left(Z^2 + s^2 a_0^2\right)^4}.$$

Now $q^2 = 4\pi\epsilon_0 \alpha \hbar c$, so

$$\frac{d\sigma}{d\Omega} = \frac{8 Z^5 a_0^3 \, 4\pi \epsilon_0 \alpha \hbar c}{m \pi \hbar^3 c \epsilon_0 \omega_k} \frac{p^3 \sin^2\theta}{\left(Z^2 + s^2 a_0^2\right)^4}$$

$$= \frac{32 Z^5 a_0^3 \alpha}{m \hbar^2 \omega_k} \frac{p^3 \sin^2\theta}{\left(Z^2 + s^2 a_0^2\right)^4}$$

$$= 32 Z^5 \frac{p^2/2m}{\hbar\omega_k} \frac{a_0^3 \alpha}{\hbar} \frac{p \sin^2\theta}{\left(Z^2 + s^2 a_0^2\right)^4}$$

$$= 32 a_0^2 Z^5 \frac{E_p}{mc^2} \frac{cp}{\hbar\omega_k} \frac{\sin^2\theta}{\left(Z^2 + s^2 a_0^2\right)^4}$$

An equivalent expression for $d\sigma/d\Omega$ is

$$\frac{d\sigma}{d\Omega} = 32 \frac{E_p}{mc^2} \frac{cp}{\hbar\omega_k} \frac{Z^5 \sin^2\theta}{a_0^6 \left(s^2 + Z^2/a_0^2\right)^4}$$

$$= 32 \frac{E_p}{mc^2} \frac{cp\, mc\alpha}{\hbar\omega_k\, \hbar} \frac{Z^5 \sin^2\theta}{a_0^5 \left(s^2 + Z^2/a_0\right)^4}$$

$$= 32\, E_p \frac{p\alpha}{\hbar^2\omega_k} \frac{Z^5 \sin^2\theta}{a_0^5 \left(s^2 + Z^2/a_0^2\right)^4}$$

$$= 16 \frac{p^3\alpha}{m\hbar^2\omega_k} \frac{Z^5 \sin^2\theta}{a_0^5 \left(s^2 + Z^2/a_0^2\right)^4}.$$

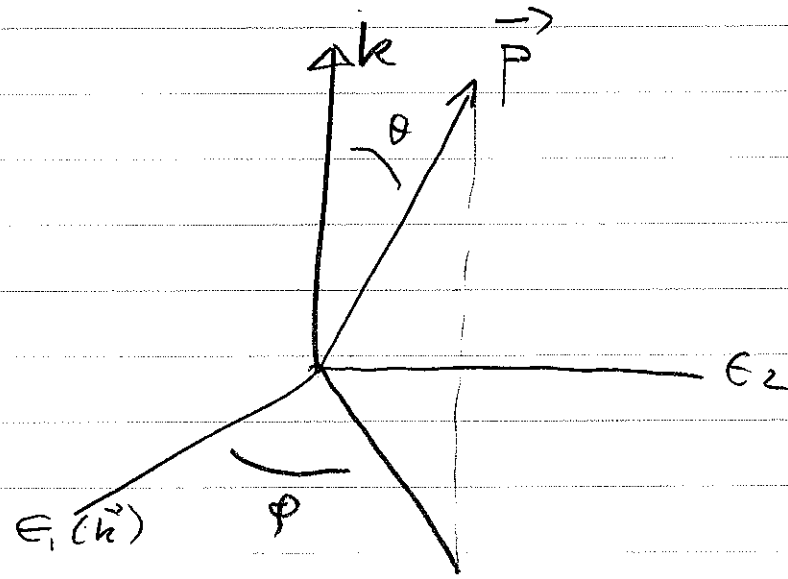
If the initial photon has a specific polarization, represented by $\epsilon_n(k)$, then we must replace

$$\frac{p^2}{2} \sin^2\theta \quad \text{by} \quad |p \cdot \epsilon_n(k)|^2$$

so that

$$\frac{d\sigma}{d\Omega} = 32 \frac{|p \cdot \epsilon_n(k)|^2\, p\alpha}{m\hbar^2\omega_k} \frac{Z^5}{a_0^5 \left(s^2 + Z^2/a_0^2\right)^4}.$$

If we take the polarization vector $\vec{\epsilon}_r(\vec{k}) = \vec{\epsilon}_1(\vec{k})$ point in the x-direction and let θ, ϕ be the polar angles of the ejected electron



Then
$$|p \cdot \epsilon_1(k)|^2 = p^2 \sin^2\theta \cos^2\phi$$

and

$$\frac{d\sigma}{d\Omega} = \frac{32\, p^3 \alpha \, \sin^2\theta \cos^2\phi}{m\, \hbar^2 \omega_k \, a_0^5 \left(s^2 + Z^2/a_0^2\right)^4}$$

where
$$s^2 = \left(k - \frac{p}{\hbar}\right)^2 = k^2 + \frac{p^2}{\hbar^2} - 2\frac{p \cdot k}{\hbar}$$

$$= k^2 + \frac{p^2}{\hbar^2} - 2\frac{pk}{\hbar}\cos\theta .$$