

Lecture 39

Relevant sections in text: §5.6

Example: Auto-ionization of Helium (cont.)

We want to see how to compute the transition rate for auto-ionization of Helium using Fermi's Golden Rule:

$$w = \int d\alpha \int_{\mathcal{E}} dE \rho(E) \frac{2\pi}{\hbar} |V_{\gamma i}|^2 \delta(E - E_i) = \frac{2\pi}{\hbar} \rho(E_i) \int d\alpha |V_{\gamma i}|^2.$$

We take the initial state to be of the form

$$|\text{initial}\rangle = |2, 0, 0\rangle \otimes |2, 0, 0\rangle.$$

(We are ignoring spin here, but since this part of the state vector is symmetric under particle interchange the symmetrization postulate would demand that the total spin state be a singlet.) The final state is of the form

$$|\text{final}\rangle = |1, 0, 0\rangle \otimes |E, l, m\rangle,$$

where $|E, l, m\rangle$ is an energy eigenket in the continuum with E being the (unperturbed) energy difference between the initial state and the energy of the electron in the 1S state. (If we were worried about spin, we would have to symmetrize (anti-symmetrize) this state if the final spin state were a singlet (triplet). As we shall see, only the singlet case is relevant.) Because the ejected electron can have a continuous range of energies, the final state of the system lies in the continuum.

Viewing the inter-electron repulsion as the perturbation:

$$V = \frac{e^2}{|\vec{X}_1 - \vec{X}_2|},$$

we need to compute the matrix elements:

$$\langle \text{initial} | V | \text{final} \rangle = \int d^3x_1 d^3x_2 \psi_{200}^*(r_1) \psi_{200}^*(r_2) \psi_{100}(r_1) \psi_{E,l,m}(\vec{r}_2) \left(\frac{e^2}{|\vec{r}_1 - \vec{r}_2|} \right).$$

(Note that the initial state wave functions' contribution to the integral is symmetric under interchange of particles. This symmetrizes the final state wave functions' contribution. If we were taking account of spin, this matrix element would therefore vanish if the final state was anti-symmetrized, as would occur in the triplet spin state. The matrix element

forces the final state to be symmetric, hence a singlet, and is correct as it stands.) This matrix element can be simplified by using the familiar multipole expansion:

$$\frac{1}{|\vec{r}_1 - \vec{r}_2|} = 4\pi \sum_{l,m} \frac{1}{2l+1} \frac{r_{<}^l}{r_{>}^{l+1}} Y_{lm}^*(\theta_2, \phi_2) Y_{lm}(\theta_1, \phi_1),$$

where $r_{>}$ ($r_{<}$) is the greater (smaller) of r_1 and r_2 . Because the \vec{r}_1 wave functions are spherically symmetric, the matrix element vanishes for all the terms in the expansion except the $l = 0$ term. This then gives a vanishing matrix element unless $l = 0$ in the wave function for the ejected electron. Thus the transitions go from S states to S states. This is an example of a *selection rule*. Roughly speaking, you can interpret this selection rule as saying the ejected electron moves off in a radial direction only. Using the spherically symmetric (delta-function normalized) hydrogenic wave function for an unbound electron of energy E the integrations can be performed. I will not bother to write it all down here, but we denote the result by $\mathcal{V}(E)$.

Next, let's turn to the computation of the density of states factor which counts the number of final states with the indicated energy. To keep things simple, we can approximate the final state wave function for the ejected electron as that of a free particle with zero angular momentum. It is not hard to check that the position wave function for a free particle with energy E and $l = 0$ is of the form

$$\psi_{k00}(\vec{r}) = \frac{1}{\pi\sqrt{2}} \frac{\sin(kr)}{r}, \quad E = \frac{\hbar^2 k^2}{2m}.$$

This is a simultaneous eigenfunction of (P^2, L^2, L_z) with eigenvalues $(2mE, 0, 0)$ and is normalized so that

$$\int d^3x \psi_{k'00}^* \psi_{k00} = \delta(k - k').$$

Summing over states with a given range of final energies can be accomplished by making a change of variables $k = \frac{1}{\hbar} \sqrt{2mE}$ so that

$$dk = \frac{m}{\hbar\sqrt{2mE}} dE = \rho(E) dE.$$

Putting all this together, the transition rate w from the initial state to the final state characterized by an ejected electron with energy E (determined as the difference between the initial energy of the system and the energy of the bound electron in the ground state) is given by

$$w = \frac{2\pi m}{\hbar^2 \sqrt{2mE}} \mathcal{V}(E).$$