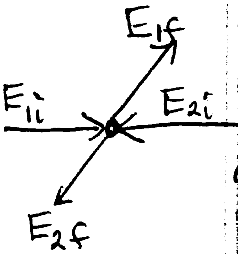
8.2. Fermi's Golden Rule

As time increases, for time independent H' or very slowly varying, we certainly expect the probability of transition to grow as well. Indeed from our Dirac perturbation formula (page -1143-), we might expect that for approximately equal initial and final energies that $P_{fi}(t,t_0)$ may grow like $|t-t_0|^2$ so that the rate of transition

$$R_{fi} \equiv \frac{P_{fi}(t,t_0)}{|t-t_0|} \quad \text{grows in time!}$$

However, it is precisely the transitions to the states $E_f \simeq E_i$ that can occur below the energy resolution limits that temper this growth of the rate so that in fact the transition rate R_{fi} is constant in time. This property is known as Fermi's Golden Rule for time-dependent perturbation theory.

To be more precise, as well as to determine the conditions for the validity of the rule, let's first consider the example of scattering from a time-independent potential i.e. H' is constant in time $H' = H'(\vec{r})$. We will consider the transition probability to scatter from some initial energy eigenstate to some final energy eigenstate. $|\varphi_i\rangle$ is the sum of 2 plane waves, say $|\varphi_f\rangle$ also, but now of different energy for the "incoming" particle E_i and E_f. That is $|\varphi_i\rangle$ describes the incoming particle as well as target and $|\varphi_f\rangle$ the scattered particle, now with different energy and the different state of the target particle. So the incoming particle interacts with the target, exchanges energy and scatters. The transition probability is given to lowest order by the Dirac perturbation theory expression



$E_{\substack{i\\f}} = E_{1\substack{i\\f}} + E_{2\substack{i\\f}}$

$E_i = E_f$ conservation of energy as we shall see.

$$P_{fi}(t,t_0) = \left|\frac{1}{i\hbar}\int_{t_0}^{t} dt_1 \langle\varphi_f|H'|\varphi_i\rangle e^{\frac{i}{\hbar}(E_f-E_i)t_1}\right|^2,$$

just as previously.

Defining the transition frequency

$$\omega_{fi} \equiv \frac{E_f-E_i}{\hbar},$$

and using the fact that H' is time independent yields

$$P_{f_i}(t,t_0)=\frac{1}{\hbar^2}\,|\langle\varphi_f|H'|\varphi_i\rangle|^2\left|\frac{\sin\left(\frac{1}{2}\omega_{fi}(t-t_0)\right)}{\frac{1}{2}\omega_{fi}}\right|^2$$

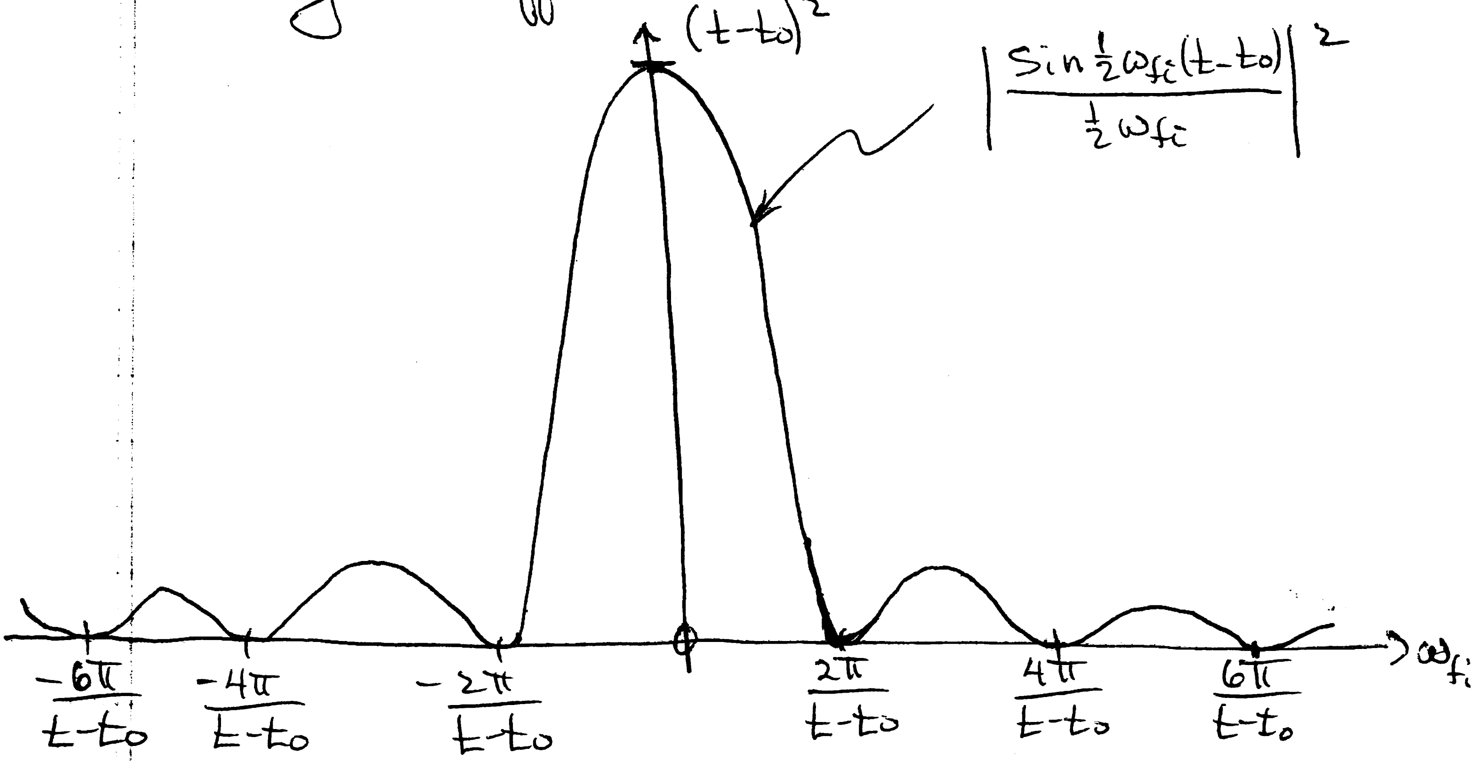
since

$$\int_{t_0}^{t}dt_1\,e^{i\omega_{fi}t_1}=\frac{e^{i\omega_{fi}t}-e^{i\omega_{fi}t_0}}{i\omega_{fi}}$$

$$=\frac{e^{i\omega_{fi}\left(\frac{t+t_0}{2}\right)}}{\frac{1}{2}\omega_{fi}}\left[\frac{e^{i\omega_{fi}\left(\frac{t-t_0}{2}\right)}-e^{-i\omega_{fi}\left(\frac{t-t_0}{2}\right)}}{2i}\right]$$

$$=e^{i\omega_{fi}\left(\frac{t+t_0}{2}\right)}\;\frac{\sin\omega_{fi}\left(\frac{t-t_0}{2}\right)}{\frac{1}{2}\omega_{fi}}\,.$$

Plotting this diffraction function



we see that it is strongly peaked about $\omega_{fi}=0$, i.e. $E_f = E_i$. The larger $t-t_0$ the more sharply peaked. It decreases rapidly for increasing $|\omega_{fi}|$, vanishing at frequencies $\omega_{fi} = \pm\frac{2\pi n}{t-t_0}$ with $n=1,2,3,\ldots$, typical of diffraction patterns.

So defining the total time T over which the interaction occurs as

$$T \equiv t-t_0,$$

The transition rate is given by

$$R_{fi} \equiv \frac{P_{fi}(t,t_0)}{|t-t_0|} = \frac{P_{fi}(t,t_0)}{T}$$

$$= \frac{1}{\hbar^2}|\langle\varphi_f|H'|\varphi_i\rangle|^2 T \left[\frac{\sin(\frac{1}{2}\omega_{fi}T)}{(\frac{1}{2}\omega_{fi}T)}\right]^2$$

$$\equiv \frac{1}{\hbar^2}|\langle\varphi_f|H'|\varphi_i\rangle|^2 f(T,\omega_{fi}) .$$

The function $f(T,\omega_{fi}) \equiv T\left[\frac{\sin(\frac{1}{2}\omega_{fi}T)}{(\frac{1}{2}\omega_{fi}T)}\right]^2$ has the properties

1) $f(T,0) = T$

2) $f(T,\omega_{fi}) \longrightarrow 0$ as $T\to\infty$ for any $\omega_{fi} \neq 0$.

This implies that $f(T,\omega_{fi})$ for large T is very peaked at $\omega_{fi} = 0$.

3) $$\int_{-\infty}^{+\infty} d\omega_{fi}\, f(T,\omega_{fi}) = T\int_{-\infty}^{+\infty} d\omega_{fi} \left[\frac{\sin(\frac{1}{2}\omega_{fi}T)}{(\frac{1}{2}\omega_{fi}T)}\right]^2$$

(let $s \equiv \frac{1}{2}\omega_{fi}T$) $$= 2\int_{-\infty}^{+\infty} ds\, \frac{\sin^2 s}{s^2} = 2\pi$$

Thus, these properties imply that

$$f(T, \omega_{fi}) \xrightarrow[T\to\infty]{} 2\pi\,\delta(\omega_{fi}) = 2\pi\hbar\,\delta(E_f - E_i),$$

expressing the conservation of energy in a scattering process. Thus ~~for~~ sufficiently large T (to be quantified next) we ~~have~~ have that

$$R_{fi} = \frac{2\pi}{\hbar} |\langle\varphi_f|H'|\varphi_i\rangle|^2\,\delta(E_f - E_i),$$

a form of Fermi's Golden Rule, the transition rate is a constant in time.

In this discrete energy case, we have that

$$P_{fi}(t, t_0)\Big|_{E_i = E_f} = T R_{fi}\Big|_{\omega_{fi}=0}$$

$$= \frac{T^2}{\hbar^2} |\langle\varphi_f|H'|\varphi_i\rangle|^2.$$

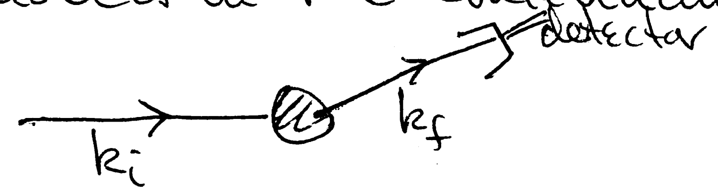
Thus, for $P_{fi}(t, t_0)\Big|_{E_i = E_f} < 1$, we must have that $\frac{1}{\hbar^2} |\langle\varphi_f|H'|\varphi_i\rangle|^2 < \frac{1}{T^2}$.

However, we must also have $(\omega_{fi} T)$ large so that $f(T, \omega_{fi})$ can be approximated by $2\pi\delta(\omega_{fi})$ in order to obtain Fermi's Golden Rule. Hence the region of validity for Fermi's Golden Rule is when the transition rates are small. That is just the condition for the validity for the use of first order perturbation theory. This was just equivalent to approximating $b_i(t)$ for $t > t_0$ by $b_i(t_0)$ in the Schrödinger equation for $b_i(t)$. Then there is very little depletion in the initial state, i.e. the transition rates are small.

When one of the particles in the final state has energy in the continuum, we can observe more carefully the cancellation of the T^2 growth of the $\omega_{fi} = 0$ channel against the oscillation of the $\omega_{fi} \neq 0$ but E_f in the continuum, channels, resulting in a constant R_{fi} rate and Fermi's Golden Rule. As well this continuum case describes very important realistic examples of actual scattering experiments.

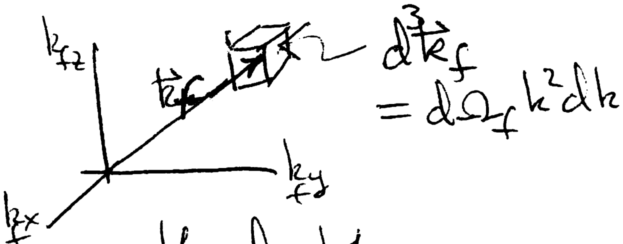
In particular we will ~~be~~ able to apply the golden rule to the cases of

1) Elastic & Inelastic Scattering in which the detector observes a scattered particle with energy $\frac{\hbar^2 k_f^2}{2m}$ which is in the continuum

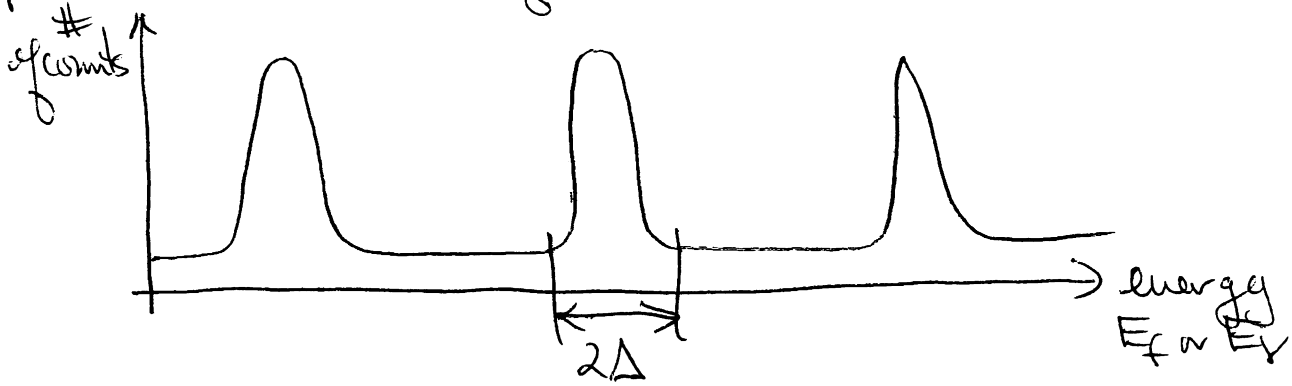


2) Photoemission in which the detector observes an emitted photon with energy $\hbar\omega$ which is in the continuum

In reality all detectors have a finite energy resolution Δ, hence we cannot measure the probability of detecting the system in the distinct state $|\psi_f\rangle$ if the energy of this state lies in the continuum. ~~Thus~~ all physical predictions involve an integration over a group of final states depending on the particular measurement being made. The detector signals when it detects a particle with momentum in the domain D_f of momentum space



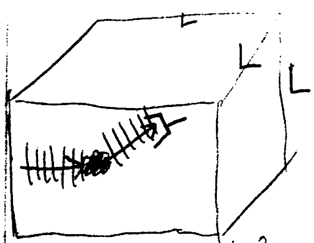
centered about $\vec{p}_f = \hbar \vec{k}_f$ so that the energy is in the interval Δ centered about $E_f = \frac{\hbar^2 k_f^2}{2m}$ for a massive (non-relativistic) particle or $E_\gamma = \hbar k_f c$ for a photon. Hence the detector records a series of peaks (excitations of the target)



where the detector energy resolution Δ is small enough to resolve the individual peaks while large enough to contain an entire peak. Thus we need to count the number of states in $\mathcal{D}_f$. This is easily done by placing the system in a box of side length L and volume $\Omega = L^3$. The normalized final state plane wave is then

$$\varphi_{\vec{k}}(\vec{r}) = \langle \vec{r} | \varphi_f \rangle = \frac{1}{\sqrt{\Omega}} e^{i\vec{k}\cdot\vec{r}}$$

with energy $E_f = \frac{\hbar^2 k^2}{2m}$. Imposing periodic boundary conditions on the plane



wave, the components of $\mathbf{k}$ are given by

$$k_i = \frac{2\pi n_i}{L} \quad , n_i = 0, \pm 1, \pm 2, \ldots$$
$$i = 1, 2, 3.$$

Thus $\Delta n_i = \frac{L}{2\pi}\Delta k_i$ and the number of states in D_f is simply

$$\Delta n = \Delta n_x \Delta n_y \Delta n_z = \frac{L^3}{(2\pi)^3}\Delta k_x \Delta k_y \Delta k_z$$
$$= \frac{\Omega}{(2\pi)^3}\Delta k_x \Delta k_y \Delta k_z \quad .$$

As $L \to \infty$, the energy levels become continuously close and $\Delta n \to \infty$, but for L large we write this as

$$dn = \frac{\Omega}{(2\pi)^3} d^3k \quad .$$

In addition there may be additional degeneracy associated with each energy eigenvalue labelled by other quantum numbers (besides the momentum). As usual, denote the degree of degeneracy by $g(E)$ (for photons for example, there are 2 polarization states for each energy), Thus

$$dn = \frac{\Omega}{(2\pi)^3} g(E) d^3k$$ is the

number of states in D_f when $\vec{k}$ is restricted to lie in the domain D_f centered about $\vec{k}_f$.

The transition rate to any of these states is given by (recall they are centered about E_f)

$$\delta R_{fi}(E_f) = \int_{D_f} dn\, R_{fi}(E)$$

where

$$R_{fi}(E) = \frac{1}{\hbar^2} |\langle \varphi_f | H' | \varphi_i \rangle|^2 f(T, \frac{E - E_i}{\hbar})$$

is the transition rate to final states $|\varphi_f\rangle$ with energy E instead of E_f. Of course $E_f - \Delta \le E \le E_f + \Delta$ in the integral. Hence we have

$$\delta R_{fi}(E_f) = \frac{\Omega}{(2\pi)^3} \int_{E_f - \Delta \le \frac{\hbar^2 k^2}{2m} \le E_f + \Delta} d^3k\, g(E) R_{fi}(E)$$

$$= \frac{\Omega}{(2\pi)^3} \int_{\delta\Omega_f} d\Omega_k \int_{E_f - \Delta \le E \le E_f + \Delta} dk\, k^2 g(E) R_{fi}(E)$$

This we write as

$$\delta R_{fi}(E_f) = \int_{E_f-\Delta}^{E_f+\Delta} dE \left(\frac{\partial n(E)}{\partial E}\right) R_{fi}(E)$$

with $\frac{\partial n(E)}{\partial E}$ the <u>density of final states</u> (sometimes $\rho(E) = n(E)$ is used)

$$\boxed{\frac{\partial n(E)}{\partial E} \equiv \delta\Omega_f \, g(E) \frac{\Omega}{(2\pi)^3} k^2 \frac{dk}{dE}}.$$

Thus we find

$$\delta R_{fi}(E_f) = \int_{E_f-\Delta}^{E_f+\Delta} dE \frac{\partial n(E)}{\partial E} \frac{1}{\hbar^2} |\langle \varphi_f | H' | \varphi_i \rangle|^2 f(T, \tfrac{E-E_i}{\hbar}).$$

$f(T, \frac{E-E_i}{\hbar})$ is sharply peaked about $E=E_i$, and since $E_f-\Delta \le E \le E_f+\Delta$, the integral is dominated by the contribution from $E \approx E_i \approx E_f$. Since $\frac{\partial n(E)}{\partial E}$ and $\langle \varphi_f | H' | \varphi_i \rangle$ are slowly varying functions of E, we can evaluate them at $E=E_f=E_i$, and so pull them out of the integral

$$\delta R_{fi}(E_f) = \left[\frac{\partial n(E_f)}{\partial E_f}\frac{1}{\hbar^2}|\langle\varphi_f|H'|\varphi_i\rangle|^2\right]\Bigg|_{E_f=E_i} \times$$

$$\times \int_{E_f-\Delta}^{E_f+\Delta} dE\, f\left(T, \frac{E-E_i}{\hbar}\right).$$

The integral can be performed, recall

$$\int_{E_f-\Delta}^{E_f+\Delta} dE\, f\left(T, \frac{E-E_i}{\hbar}\right) = \int_{E_f-\Delta}^{E_f+\Delta} dE\; T\left[\frac{\sin\frac{1}{2\hbar}(E-E_i)T}{\frac{1}{2\hbar}(E-E_i)T}\right]^2$$

(letting $s = \frac{1}{2\hbar}(E-E_i)T$)

$$= 2\hbar \int_{\frac{(E_f-E_i)T}{2\hbar}-\frac{\Delta T}{2\hbar}}^{\frac{(E_f-E_i)T}{2\hbar}+\frac{\Delta T}{2\hbar}} ds\, \frac{\sin^2 s}{s^2}$$

Now if $\Delta T \gg \hbar$ this becomes

$$= 2\hbar\int_{-\infty}^{+\infty} ds\, \frac{\sin^2 s}{s^2} = 2\pi\hbar.$$

Thus we find

$\left(\begin{array}{l} E_i = \text{total initial energy} \\ E_f = \text{total final energy} \end{array}\right)$

for $T\Delta \gg \hbar$

$$\delta R_{fi}(E_f) = \left[\frac{2\pi}{\hbar}\frac{\partial n(E_f)}{\partial E_f}|\langle\varphi_f|H'|\varphi_i\rangle|^2\right]\Bigg|_{E_i=E_f},$$

This is Fermi's Golden Rule for the transition rate when one particle is in the final state continuum. Note this is independent of T and Δ. We can obtain this result directly from our previous form of Fermi's Golden Rule by summing over all states in D_f:

$$\delta R_{fi}(E_f) = \int_{D_f} dn\, R_{fi}(E)$$

$$= \int_{E_f-\Delta}^{E_f+\Delta} dE\, \frac{\partial n(E)}{\partial E} R_{fi}(E)$$

$$= \int_{E_f-\Delta}^{E_f+\Delta} dE\, \frac{\partial n(E)}{\partial E}\frac{2\pi}{\hbar}|\langle\varphi_f|H'|\varphi_i\rangle|^2\delta(E-E_i)$$

$$= \frac{2\pi}{\hbar}\left[\frac{\partial n(E_f)}{\partial E_f}|\langle\varphi_f|H'|\varphi_i\rangle|^2\right]\Bigg|_{E_f=E_i}.$$

cannot prepare system & immediately probe it — uncertainty principle.

Fermi's Golden Rule is valid for $T\Delta \gg \hbar$ while in order to insure that probability was less than one we had

$$\frac{1}{\hbar}|\langle\varphi_f|H'|\varphi_i\rangle| \ll \frac{1}{T}.$$

Combining these conditions results in

$$\frac{\hbar}{\Delta} \ll T \ll \frac{\hbar}{|\langle\varphi_f|H'|\varphi_i\rangle|}.$$

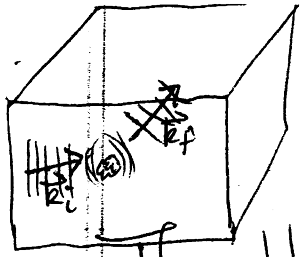
These inequalities can be satisfied for some T provided $|\langle\varphi_f|H'|\varphi_i\rangle|$ is sufficiently small. Thus again Fermi's Golden Rule is valid for calculating small transition rates.

Example: Elastic Scattering of a spinless particle from a potential $V(\vec{R})$

The full (time-independent) Hamiltonian is

$$H = \frac{1}{2m}\vec{P}^2 + V(\vec{R}) \equiv H_0 + H'$$

with $H_0 = \frac{1}{2m}\vec{P}^2$ and $H' = V(\vec{R})$.



The H_0 eigenstates are given by the normalized plane waves

initial state: $\varphi_i(\vec{r}) = \langle \vec{r} | \varphi_i \rangle = \frac{1}{\sqrt{\Omega}} e^{i\vec{k}_i \cdot \vec{r}}$

final state: $\varphi_f(\vec{r}) = \langle \vec{r} | \varphi_f \rangle = \frac{1}{\sqrt{\Omega}} e^{i\vec{k}_f \cdot \vec{r}}$

with $|\vec{k}_i| = |\vec{k}_f| = k$ for elastic scattering, with initial and final energies

$$E_i = \frac{\hbar^2 k^2}{2m} = E_f .$$

Since $k \in \mathbb{R}^+$, the final state plane wave has its energy in the continuum. Applying Fermi's Golden Rule we first evaluate the matrix element

$$\langle \varphi_f | H' | \varphi_i \rangle = \frac{1}{\Omega} \int d^3r \, e^{-i\vec{k}_f \cdot \vec{r}} V(\vec{r}) e^{+i\vec{k}_i \cdot \vec{r}}$$

$$= \frac{1}{\Omega} \int d^3r \, e^{-i\vec{q} \cdot \vec{r}} V(\vec{r})$$

where $\vec{q} \equiv \vec{k}_f - \vec{k}_i$ is the momentum transfer. Next we must evaluate the density of states from $E_f = \frac{\hbar^2 k^2}{2m}$

$\Rightarrow \; = \frac{2m}{2\hbar^2 k} = \frac{m}{\hbar^2 k}$

$$\frac{\partial n(E_f)}{\partial E_f} = \delta\Omega_f \underbrace{g(E_f)}_{=1} \frac{\Omega}{(2\pi)^3} k^2 \underbrace{\frac{dk}{dE_f}}$$

$$= \delta\Omega_f \frac{\Omega}{(2\pi)^3} \frac{mk}{\hbar^2}$$

$$= \delta\Omega_f \frac{\Omega}{(2\pi\hbar)^3} m\hbar k$$

Hence we find from page -1167-

$$\delta R_{fi}(E_f) = \left(\delta\Omega_f \frac{\Omega}{(2\pi\hbar)^3} m\hbar k\right) \frac{2\pi}{\hbar} \left| \frac{1}{\Omega} \int d^3r \, e^{-i\vec{q}\cdot\vec{r}} V(\vec{r}) \right|$$

Recall that the elastic cross-section is defined as

$$J_{in} \delta\sigma_{el}(\theta,\varphi) = \frac{\# \text{ of transitions } |\varphi_i\rangle \to |\varphi_f\rangle}{\text{unit time}}\Bigg|_{E_f = E_i}$$

$$= \text{transition Rate for } |\varphi_i\rangle \to |\varphi_f\rangle \text{ with } E_f = E_i$$

$$\Rightarrow \delta\sigma_{el}(\theta,\varphi) = \frac{\delta R_{fi}(E_f)}{J_{in}}$$

Letting $\vec{k}_i = k\hat{z}$, the incident flux is simply

$$J_{in} = \vec{J}_{in} \cdot \hat{z}$$

$$= \frac{\hbar}{2mi}\left[\varphi_i^*(\vec{r})\vec{\nabla}\varphi_i(\vec{r}) - (\vec{\nabla}\varphi_i(\vec{r}))^*\varphi_i(\vec{r})\right] \cdot \hat{z}$$

$$= \frac{1}{\Omega}\frac{\hbar k}{m} .$$

Thus

$$\delta\sigma_{el}(\theta,\varphi) = \frac{1}{\frac{1}{\Omega}\frac{\hbar k}{m}}\left(\delta\Omega_f \frac{\Omega}{(2\pi\hbar)^3} m\hbar k\right)\frac{2\pi}{\hbar}\frac{1}{\Omega^2} \times$$

$$\times\left|\int d^3r\, e^{-i\vec{q}\cdot\vec{r}} V(\vec{r})\right|^2$$

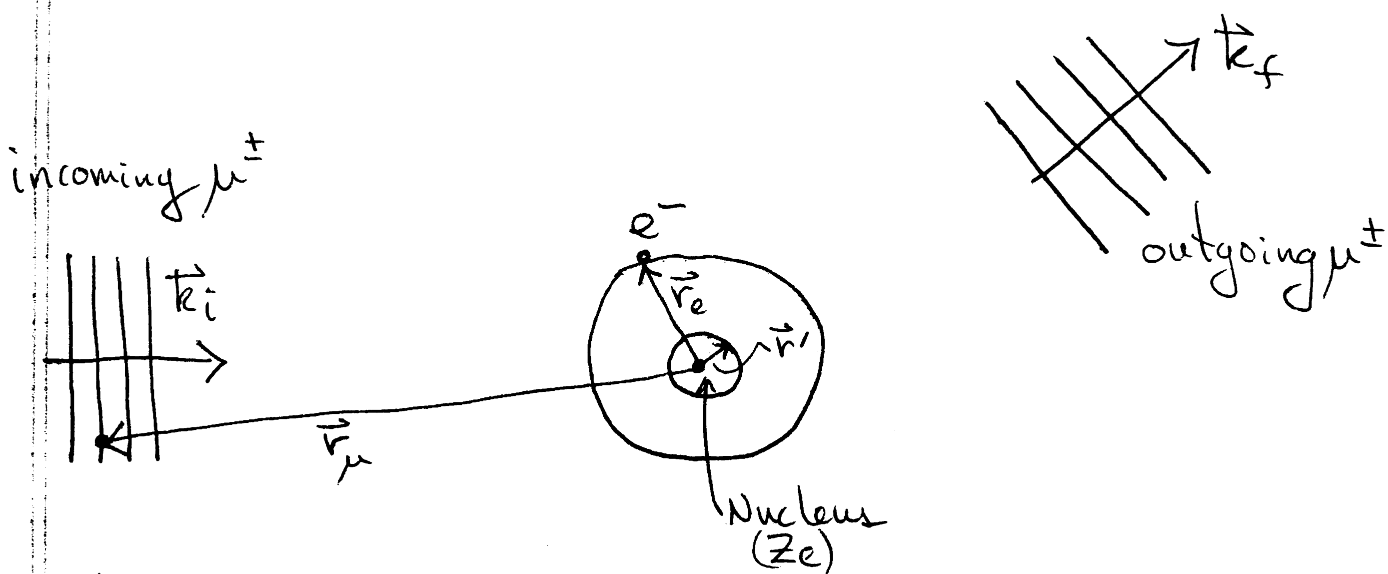
$\Rightarrow$

$$\sigma_{el}(\theta,\varphi) \equiv \boxed{\frac{d\sigma_{el}}{d\Omega_f} = \left|\frac{-1}{4\pi}\int d^3r\, e^{-i\vec{q}\cdot\vec{r}} \underbrace{\frac{2m}{\hbar^2}V(\vec{r})}_{=U(\vec{r})}\right|^2}$$

Precisely the same result we obtained for elastic scattering in the Born approximation (page -1034-).

As well we can apply Fermi's Golden Rule to inelastic scattering processes

Example: Scattering of spin $\frac{1}{2}$ muons ($\mu^\pm$) from single electron (e^-) atoms



The full (time-independent) Hamiltonian is

$$H = H_0 + H'$$

where

$$H_0 = \underbrace{\frac{1}{2m_\mu}\vec{P}_\mu^{\,2}}_{\text{KE of } \mu^\pm} + \underbrace{\frac{1}{2m_e}\vec{P}_e^{\,2} - \frac{Ze^2}{r_e}}_{\text{KE of } e^- \text{ and Coulomb interaction of Bound } e^- \text{ and nucleus } (Ze)}$$

$$H' = \underbrace{Z z_\mu e^2 \int d^3r' \frac{\rho_N(r')}{|\vec{r}_\mu - \vec{r}'|}}_{\text{Coulomb interaction of } \mu^\pm \text{ with nucleus}} - \underbrace{\frac{z_\mu e^2}{|\vec{r}_\mu - \vec{r}_e|}}_{\text{Coulomb interaction of } \mu^\pm \text{ with } e^-}$$

We assume the ~~nucleus~~ nucleus is at rest since it is much more massive than e or μ. For μ^-, $z_\mu = -1$, for μ^+, $z_\mu = +1$ and $\rho_N(r')$ is the nuclear charge density normalized so that $\int d^3r' \rho_N(r') = 1$.

The initial and final states are eigenstates of H_0. For the incoming state we have the non-interacting $\mu^\pm$ plane wave and single e^- atom

$$\varphi_i(\vec{r}_e, \vec{r}_\mu) = \underbrace{\psi_i(\vec{r}_e)}_{\substack{\text{initial boundstate} \\ e^- \text{ wavefunction}}} \underbrace{\frac{1}{\sqrt{\Omega}} e^{i\vec{k}_i \cdot \vec{r}_\mu} \chi(\sigma_i)}_{\substack{\text{incident } \mu^\pm \text{ plane wave with spinor} \\ \text{wavefunction for spin } \pm\frac{1}{2} \text{ particle}}}$$

with initial energy

$$E_i = \underbrace{\varepsilon_i^0}_{\substack{\text{atomic}\\ \text{bound state}\\ \text{energy of } e^-}} + \underbrace{\frac{\hbar^2 k_i^2}{2m_\mu}}_{\text{KE of incoming } \mu^\pm} .$$

Likewise the final outgoing state is comprised of the non-interacting $\mu^\pm$ plane wave and single e^- atom wavefunctions

$$\varphi_f(\vec{r}_e, \vec{r}_\mu) = \underbrace{\psi_f(\vec{r}_e)}_{\substack{\text{final boundstate}\\ e^- \text{ wavefunction}}} \underbrace{\frac{1}{\sqrt{\Omega}}\, e^{i\vec{k}_f \cdot \vec{r}_\mu}\, \chi(\sigma_f)}_{\substack{\text{outgoing } \mu^\pm \text{ plane wave}\\ \text{with spinor wavefunction}}}$$

with final energy

$$E_f = \underbrace{\varepsilon_f^0}_{\substack{\text{atomic}\\ \text{boundstate}\\ \text{energy of } e^-}} + \underbrace{\frac{\hbar^2 k_f^2}{2m_\mu}}_{\text{KE of outgoing } \mu^\pm} .$$

For single electron Coulomb atoms the bound state energies are given by

$$\varepsilon_n^0 = -\frac{m_e c^2 (Z\alpha)^2}{2n^2}, \quad n = 1, 2, \ldots .$$

Overall energy conservation demands that (H is time independent)

$$E_i = E_f \quad \Rightarrow$$

$$\varepsilon_i^0 + \frac{\hbar^2 k_i^2}{2m_\mu} = \varepsilon_f^0 + \frac{\hbar^2 k_f^2}{2m_\mu} .$$

According to Fermi's Golden Rule we must calculate the initial and final state matrix element of H'

$$\langle \varphi_f | H' | \varphi_i \rangle = \chi^\dagger(\sigma_f)\chi(\sigma_i)\frac{1}{\Omega}\int d^3r_e\, d^3r_\mu \,\times$$

$$\times\, \psi_f^*(\vec{r}_e)\, e^{-i\vec{k}_f\cdot\vec{r}_\mu}\left[Z z_\mu e^2 \int d^3r' \frac{\rho_N(r')}{|\vec{r}_\mu - \vec{r}'|} - \frac{z_\mu e^2}{|\vec{r}_\mu - \vec{r}_e|}\right] \times$$

$$\times\, \psi_i(\vec{r}_e)\, e^{+i\vec{k}_i\cdot\vec{r}_\mu}$$

Since the spinor wavefunctions are orthonormal

$$\chi^\dagger(\sigma_f)\chi(\sigma_i) = \delta_{\sigma_f \sigma_i} ,$$

as well, the e^- bound state wavefunctions are orthonormal

$$\int d^3r_e\, \psi_f^*(\vec{r}_e)\psi_i(\vec{r}_e) = \delta_{fi}$$

hence we find

$$\langle\varphi_f|H'|\varphi_i\rangle = \delta_{\sigma_f\sigma_i}\frac{1}{\Omega}\Big\{\delta_{fi}\, z_\mu Z e^2\int d^3r'\,\rho_N(r')\,\times$$

$$\times\int d^3r_\mu \frac{e^{-i\vec{q}\cdot\vec{r}_\mu}}{|\vec{r}_\mu-\vec{r}'|}$$

$$-z_\mu e^2\int d^3r_e\,\psi_f^*(\vec{r}_e)\psi_i(\vec{r}_e)\int d^3r_\mu\frac{e^{-i\vec{q}\cdot\vec{r}_\mu}}{|\vec{r}_\mu-\vec{r}_e|}\Big\}$$

where the momentum transfer $\vec{q} \equiv \vec{k}_f - \vec{k}_i$.

Hence we must evaluate the Fourier transform of the Coulomb potential

$$\int d^3r_\mu \frac{e^{-i\vec{q}\cdot\vec{r}_\mu}}{|\vec{r}_\mu-\vec{r}|} = \int d^3\xi\, \frac{e^{-i\vec{q}\cdot(\vec{\xi}+\vec{r})}}{|\vec{\xi}|}$$

where $\vec{\xi} = \vec{r}_\mu - \vec{r}$

$$= e^{-i\vec{q}\cdot\vec{r}}\int d^3\xi\, \frac{e^{-i\vec{q}\cdot\vec{\xi}}}{|\vec{\xi}|}$$

But $\int d^3\xi \, \frac{e^{-i\vec{q}\cdot\vec{\xi}}}{|\vec{\xi}|} = \frac{4\pi}{\vec{q}^{\,2}}$, hence

$$\int d^3r_\mu \frac{e^{-i\vec{q}\cdot\vec{r}_\mu}}{|\vec{r}_\mu - \vec{r}|} = \frac{4\pi\, e^{-i\vec{q}\cdot\vec{r}}}{\vec{q}^{\,2}} .$$

Substituting into the matrix element yields

$$\langle\varphi_f|H'|\varphi_i\rangle = \delta_{\sigma_f\sigma_i}\left(\frac{Z_\mu e^2}{\Omega}\right)\frac{4\pi}{\vec{q}^{\,2}} \times$$

$$\times\Big[Z\delta_{fi}\int d^3r'\, e^{-i\vec{q}\cdot\vec{r}'}\rho_N(r') - \int d^3r_e\, \psi_f^*(\vec{r}_e)\psi_i(\vec{r}_e)\, e^{-i\vec{q}\cdot\vec{r}_e}\Big]$$

Defining

$F_N(q) \equiv \int d^3r'\, e^{-i\vec{q}\cdot\vec{r}'}\rho_N(r')$ = Nuclear (charge) form factor

$F_{fi}(q) \equiv \int d^3r_e\, e^{-i\vec{q}\cdot\vec{r}_e}\psi_f^*(\vec{r}_e)\psi_i(\vec{r}_e)$ = Atomic form factor

This becomes

$$\boxed{\langle \varphi_f | H' | \varphi_i \rangle = \delta_{\sigma_f \sigma_i} \left(\frac{Z_\mu e^2}{\Omega} \right) \frac{4\pi}{\vec{q}^{\,2}} \left[Z F_N(q) \delta_{fi} - F_{fi}(q) \right]}$$

Recall that ρ_N is normalized to 1 so

$$F_N(0) = \int d^3r' \rho_N(r') = 1$$

and $F_{fi}(0) = \int d^3r_e \, \psi_f^*(\vec{r}_e) \psi_i(\vec{r}_e) = \delta_{fi}$.

The next quantity we need in the golden rule is the density of final states,

$$\frac{\partial n(E_f)}{\partial E_f} = \delta\Omega_f \, g(E_f) \frac{\Omega}{(2\pi)^3} k_f^2 \frac{dk_f}{dE_f} .$$

Now the final state energy is

$$E_f = \varepsilon_f^0 + \frac{\hbar^2 k_f^2}{2m_\mu}, \quad k_f \text{ is in the continuum.}$$

Thus $\dfrac{\partial E_f}{\partial k_f} = \dfrac{\hbar^2 k_f}{m_\mu}$. Since the $\mu^\pm$ can be spin up or down, $\sigma_f = \pm 1$, E_f has an additional 2-fold spin degeneracy so we must sum over these spin states in $\dfrac{\partial n}{\partial E}$.

Putting this altogether, we get

$$\frac{\partial n(E_f)}{\partial E_f} = \delta\Omega_f \sum_{\sigma_f=\pm1}' \frac{\Omega}{(2\pi)^3} k_f^2 \frac{m_\mu}{\hbar^2 k_f}$$

$$= \delta\Omega_f \frac{\Omega}{(2\pi\hbar)^3} m_\mu \hbar k_f \sum_{\sigma_f=\pm1}' .$$

Applying Fermi's Golden Rule for the case of the final particle in the continuum we find (-page -116-)

$$\delta R_{fi}(E_f) = \frac{2\pi}{\hbar} \frac{\partial n(E_f)}{\partial E_f} |\langle\varphi_f| H' |\varphi_i\rangle|^2 \Big|_{E_f=E_i}$$

$$= \frac{2\pi}{\hbar}\left(\delta\Omega_f \frac{\Omega}{(2\pi\hbar)^3} m_\mu \hbar k_f \sum_{\sigma_f=\pm1}'\right) \times$$

$$\times\left(\delta_{\sigma_f\sigma_i} \left|\frac{Z_\mu e^2}{\Omega} \frac{4\pi}{\vec{q}^{\,2}} [Z F_N(q)\delta_{fi} - F_{fi}(q)]\right|^2\right)$$

$$= \delta\Omega_f \frac{1}{\Omega} \frac{4}{(\vec{q}^{\,2})^2} \left(\frac{e^2}{\hbar c}\right)^2 \frac{m_\mu c^2}{\hbar} k_f \times$$

$$\times |Z F_N(q)\delta_{fi} - F_{fi}(q)|^2 ,$$

where $Z_\mu^2 = 1$ and $\sum_{\sigma_f=\pm1}' \delta_{\sigma_f \sigma_i} = 1$.

Since the incident muons have spin, we can prepare the initial state as polarized or unpolarized depending on the experimental situation. To be concrete, let's take our initial beam of muons as unpolarized, so we can average over the spins. Since there are $2s+1 = 2$ spin states we sum over $\sigma_i = \pm 1$ and divide by 2 for the average

$$\frac{1}{2}\sum_{\sigma_i=\pm1}' .$$

So doing, we can define the initial spin averaged differential cross section as the spin averaged transition rate divided by the incident flux

$$d\sigma_{fi} = \frac{1}{2}\sum_{\sigma_i=\pm1}' \frac{\delta R_{fi}(E_f)}{J_{in}} .$$

From our expression for δR_{fi} we see it is independent of σ_i hence the initial spin average just gives 1

$$\frac{1}{2}\sum_{\sigma_i=\pm1}' 1 = 1 .$$

So the spin averaged cross-section is

$$d\sigma_{fi} = \frac{\delta R_{fi}(E_f)}{J_{in}}.$$

(Since H' is independent of spin, the average over the initial $\mu^\pm$ spin and sum over the final $\mu^\pm$ spin just yields a factor of 1

$$\frac{1}{2}\sum_{\sigma_i=\pm 1}\sum_{\sigma_f=\pm 1} \delta_{\sigma_f\sigma_i} = 1,$$

hence we could have neglected spin altogether (in the wavefunction as well as in the density of states).) If the initial beam of muons ~~was~~ spin-polarized, i.e. say $\sigma_i=+1$, the mu's stay in that spin state since H' is independent of spin, again the cross-section would simply be

$$d\sigma_{fi} = \frac{\delta R_{fi}(E_f)}{J_{in}}.$$

As usual for plane waves the incident flux is

$$J_{in} = \frac{\hbar k_i}{m_\mu}\frac{1}{\Omega}, \quad \text{so}$$

we find

$$d\sigma_{fi} = \delta\Omega_f \left(\frac{\Omega m_\mu}{\hbar k_i}\right)\left(\frac{1}{\Omega}\frac{4}{(\vec{q}^{\,2})^2}\underbrace{\left(\frac{e^2}{\hbar c}\right)}_{\alpha}^2 \frac{m_\mu c^2}{\hbar} k_f\right)$$

$$\left|Z F_N(q)\delta_{fi} - F_{fi}(q)\right|^2$$

$\Rightarrow$

$$\sigma_{fi}(\theta,\varphi) = \boxed{\frac{d\sigma_{fi}}{d\Omega_f} = \frac{4\alpha^2}{(\vec{q}^{\,2})^2}\left(\frac{m_\mu c^2}{\hbar c}\right)^2 \left|Z F_N(q)\delta_{fi} - F_{fi}(q)\right|^2 \left(\frac{k_f}{k_i}\right)}$$

Note, as required, all volume factors Ω cancel. Since $\alpha \approx \frac{1}{137}$, the transition rate is small, and so Fermi's Golden Rule is a sensible approximation. Our result is general, it applies to elastic as well as inelastic scattering.

Let's apply the above formula to the specific case of elastic scattering of $\mu^\pm$ off atomic hydrogen $(Z=1)$

Elastic scattering means $k_f = k_i \equiv k$

The momentum transfer $\vec{q} = \vec{k}_f - \vec{k}_i$ has magnitude

$$q^2 \equiv \vec{q}^{\,2} = 4k^2 \sin^2\frac{\theta}{2} \; ; \text{ with}$$

$$\cos\theta = \hat{k}_f \cdot \hat{k}_i \quad . \quad \text{Since } k_f = k_i \text{ we}$$

have that $E_f = E_i \Rightarrow \varepsilon_f^0 = \varepsilon_i^0$ the initial and final energy levels of the H-atom are the same. Let's choose it to be the H-ground state

$$\psi_i(\vec{r}_e) = \psi_{1,0,0}(\vec{r}_e) = \frac{1}{\sqrt{8\pi}}\left(\frac{2}{a_0}\right)^{3/2} e^{-\frac{r}{a_0}}$$

$$= \psi_f(\vec{r}_e)$$

with a_0 = Bohr radius and

$$\varepsilon_i^0 = -\frac{m_e c^2 \alpha^2}{2} = \varepsilon_f^0 \, .$$

The atomic elastic scattering form factor becomes

$$F_{ii}(q) = \int d^3r_e \, e^{-i\vec{q}\cdot\vec{r}_e} \, |\psi_i(\vec{r}_e)|^2$$

$$= \frac{1}{8\pi}\left(\frac{2}{a_0}\right)^3 \int d^3r_e \, e^{-i\vec{q}\cdot\vec{r}_e} \, e^{-\frac{2r_e}{a_0}}$$

$$= \frac{1}{8\pi}\left(\frac{2}{a_0}\right)^3 \int_0^{2\pi} d\varphi_e \int_0^\infty dr_e\, r_e^2\, e^{-\frac{2r_e}{a_0}} \underbrace{\int_{-1}^{+1} d(\cos\theta_e)\, e^{-iqr_e\cos\theta_e}}_{=\frac{i}{qr_e}\left(e^{-iqr_e}-e^{+iqr_e}\right)}$$

$$= \frac{1}{4}\left(\frac{2}{a_0}\right)^3 \frac{i}{q}\int_0^\infty dr_e\, r_e\left[e^{-\left(\frac{2}{a_0}+iq\right)r_e} - e^{-\left(\frac{2}{a_0}-iq\right)r_e}\right]$$

Now $\int_0^\infty ds\, s e^{-bs} = -\frac{d}{db}\int_0^\infty ds\, e^{-bs} = -\frac{d}{db}\frac{1}{b}$

$$= \frac{1}{b^2} \quad \Rightarrow$$

$$F_{ii}(q) = \frac{1}{4}\left(\frac{2}{a_0}\right)^3 \frac{i}{q}\left[\frac{1}{\left(\frac{2}{a_0}+iq\right)^2} - \frac{1}{\left(\frac{2}{a_0}-iq\right)^2}\right]$$

$$= \frac{1}{4}\left(\frac{2}{a_0}\right)^3 \frac{i}{q}\left[\frac{\left(\frac{2}{a_0}-iq\right)^2 - \left(\frac{2}{a_0}+iq\right)^2}{\left(\frac{4}{a_0^2}+q^2\right)^2}\right]$$

$$= \left(\frac{2}{a_0}\right)^4 \frac{1}{\left(\frac{4}{a_0^2}+q^2\right)^2}$$

$$= \left(\frac{2}{a_0}\right)^4 \frac{1}{\frac{16}{a_0^4}\left(1+\frac{(qa_0)^2}{4}\right)^2}$$

$$\Rightarrow \boxed{F_{ii}(q) = \frac{1}{\left(1+\frac{(qa_0)^2}{4}\right)^2}}$$

For Hydrogen the nucleus is just a single proton and so a point-like structure on the atomic scale, hence we have $\rho_N(r) = \delta^3(\vec{r})$ for hydrogen, this yields

$$F_N(q) = \int d^3r\, e^{-i\vec{q}\cdot\vec{r}} \rho_N(\vec{r})$$

$$= \int d^3r\, e^{-i\vec{q}\cdot\vec{r}} \delta^3(\vec{r})$$

$$= 1 \text{, for the nuclear form factor.}$$

Thus for elastic scattering ($\delta_{fi} = \delta_{ii} = 1$) the differential cross-section is

$$\frac{d\sigma_{el}}{d\Omega} = \frac{4\alpha^2}{q^4}\left(\frac{m_\mu c^2}{\hbar c}\right)^2 \left|1 - \frac{1}{\left(1+\frac{(qa_0)^2}{4}\right)^2}\right|^2 .$$

Now $\frac{4\alpha^2}{q^4}\left(\frac{m_\mu c^2}{\hbar c}\right)^2 = \left(\frac{2\alpha\, m_\mu c^2}{q^2\hbar c}\right)^2 = \left(\frac{2e^2 m_\mu}{q^2\hbar^2}\right)^2$

$$= \left(\frac{2e^2 m_\mu}{4\hbar^2 k^2 \sin^2\frac{\theta}{2}}\right)^2 = \left(\frac{e^2}{4\left(\frac{\hbar^2 k^2}{2m_\mu}\right)\sin^2\frac{\theta}{2}}\right)^2$$

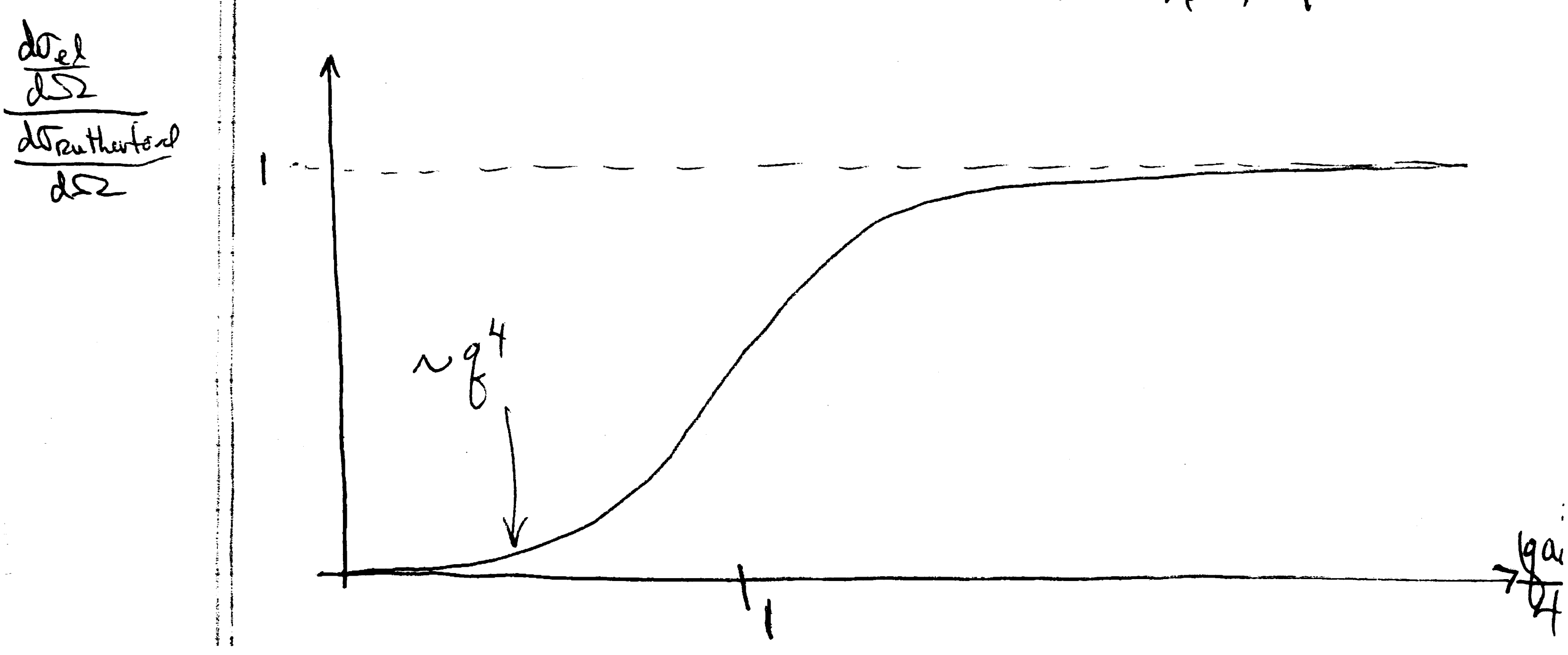
Recall that $\frac{\hbar^2 k^2}{2m_\mu} = E_\mu$, the incident and outgoing KE of the muon. So

$$\frac{4\alpha^2}{q^4}\left(\frac{m_\mu c^2}{\hbar c}\right)^2 = \left(\frac{e^2}{4E_\mu \sin^2\frac{\theta}{2}}\right)^2$$

$$\equiv \frac{d\sigma_{Rutherford}}{d\Omega}$$, this is just the Rutherford cross-section, that obtained from Coulomb scattering of a muon from a fixed point charge (page -1047-).

So we find

$$\frac{d\sigma_{el}}{d\Omega} = \frac{d\sigma_{Rutherford}}{d\Omega}\left|1 - \frac{1}{\left(1+\frac{(qa)^2}{4}\right)^2}\right|^2$$



Note that as $q \to 0$ we have in general

$$F_{ii}(q) = \int d^3r_e \, e^{-i\vec{q}\cdot\vec{r}_e} |\psi_i(\vec{r}_e)|^2$$

$$\underset{q\to 0}{\approx} \int d^3r_e |\psi_i(\vec{r}_e)|^2 + O(q^2)$$

$$\approx 1 + O(q^2), \text{ hence specifically}$$

$$\frac{d\sigma_{el}}{d\Omega} \underset{q\to 0}{\approx} \overbrace{\frac{d\sigma_{Rutherford}}{d\Omega}}^{\propto 1/q^4} \Big|\underbrace{1 - \left(1 - \tfrac{1}{2}(qa_0)^2\right)}_{\frac{1}{2}(a_0^2 q^2)}\Big|^2$$

$$\underset{q\to 0}{\sim} O(\alpha^2),$$

The incident $\mu^\pm$ sees an essentially neutral H-atom $F_{ii} \approx F_N \approx 1$, so there is very little low energy elastic scattering. As the (q^2) momentum transfer increases, the muon starts to probe the structure of the H-atom, it sees the difference between F_N and F_{ii}. For very large q^2 the muon misses the electron cloud completely and probes into the H-atom to see only the point like H-nucleus (i.e. the e^- cloud has charge $(-e)$ spread through volume a_0^3). Hence, we expect the cross section to describe scattering

So for ~~low~~ energy

$$\frac{d\sigma_{el}}{d\Omega} \underset{q\to 0}{\approx} \left(\frac{1}{4} a_0^4 q^4\right) \frac{d\sigma_{\text{Rutherford}}}{d\Omega}$$

$$\underset{q\to 0}{\approx} \frac{4\alpha^2}{q^4}\left(\frac{m_\mu c^2}{\hbar c}\right)^2 \left(\frac{1}{4} a_0^4 q^4\right)$$

$$\frac{d\sigma_{el}}{d\Omega} \underset{q\to 0}{\approx} \left(\frac{a_0^2 \alpha\, m_\mu c^2}{\hbar c}\right)^2 \quad \text{a constant}$$

The incident $\mu^\pm$ just sees a barrier at the origin!

from the point (proton) charge, this is precisely the Rutherford crossection result

$$\frac{d\sigma_{el}}{d\Omega} \xrightarrow[q^2\to 0]{} \frac{d\sigma_{Rutherford}}{d\Omega} .$$

Next consider elastic scattering from a large Z nucleus at high q. Since Z is large the ZF_N factor will overpower the F_{ii} atomic form factor, then

$$\frac{d\sigma_{el}}{d\Omega} = \frac{d\sigma_{Rutherford}}{d\Omega} Z^2 |F_N(q)|^2$$

with

$$F_N(q) = \int d^3r\, e^{-i\vec{q}\cdot\vec{r}} \rho_N(r)$$

(for spherically symmetric nucleus $\rho_N(\vec{r}) = \rho_N(r)$),

$$= 4\pi \int_0^\infty dr\, r^2 \rho_N(r) \left[\frac{\sin qr}{qr}\right]$$

and, as always, $F_N(0) = 1$. Thus we find

Finally let's consider *inelastic scattering* of $\mu^\pm$ from atomic hydrogen.

For inelastic scattering the initial and final states of the hydrogen atom are *different* so $\delta_{fi} = 0$. Hence from page -1182- we have

$$\frac{d\sigma_{fi}}{d\Omega} = \frac{4\alpha^2}{(\vec{q}^{\,2})^2}\left(\frac{m_\mu c^2}{\hbar c}\right)^2 |F_{fi}(q)|^2 \left(\frac{k_f}{k_i}\right), \quad f \neq i.$$

Defining $q_{el}^2 \equiv 4k_i^2 \sin^2\frac{\theta}{2}$ and recalling the Rutherford cross section

$$\frac{d\sigma_{\text{Rutherford}}}{d\Omega} \equiv \frac{4\alpha^2}{q_{el}^4}\left(\frac{m_\mu c^2}{\hbar c}\right)^2$$

we can write the inelastic cross section as

$$\boxed{\frac{d\sigma_{fi}}{d\Omega} = \frac{d\sigma_{\text{Rutherford}}}{d\Omega}\left(\frac{q_{el}^2}{q^2}\right)^2\left(\frac{k_f}{k_i}\right)\left|F_{fi}(q)\right|^2}$$

Now the momentum transfer $q^2 \equiv \vec{q}^{\,2} = (\vec{k}_f - \vec{k}_i)^2$

$q^2 = k_f^2 + k_i^2 - 2k_f k_i \cos\theta$. We can use the conservation of total energy to relate k_f to k_i

$$E_i = \mathcal{E}_i^0 + \frac{\hbar^2 k_i^2}{2m_\mu} = E_f = \mathcal{E}_f^0 + \frac{\hbar^2 k_f^2}{2m_\mu}$$

$$\Rightarrow \quad k_f^2 - k_i^2 = \frac{2m_\mu(\mathcal{E}_f^0 - \mathcal{E}_i^0)}{\hbar^2}$$

$$= \frac{2m_\mu}{\hbar^2}\left(\frac{-m_e c^2\alpha^2}{2}\right)\left(\frac{1}{n_f^2} - \frac{1}{n_i^2}\right).$$

Choosing the initial state of the H-atom to be ~~the~~ ground state $n_i = 1$,

we have
$$\psi_i(\vec{r}_e) = \psi_{100}(\vec{r}_e) = R_{10}(r_e)\, Y_0^0(\theta_e, \varphi_e)$$
while we choose the final state to be $n_f = n \neq 1$ so that
$$\psi_f(\vec{r}_e) = \sum_{l=0}^{n-1} \sum_{m=-l}^{+l} a_{nlm} R_{nl}(r_e)\, Y_l^m(\theta_e, \varphi_e) .$$

The muon energies are related by
$$k_f^2 - k_i^2 = \frac{m_\mu m_e c^2 \alpha^2}{\hbar^2 n^2}(n^2 - 1) .$$

It remains to evaluate the atomic (inelastic) form factor
$$F_{fi}(q) = \int d^3r_e\, e^{-i\vec{q}\cdot\vec{r}_e}\, \psi_f^*(\vec{r}_e)\, \psi_i(\vec{r}_e)$$
$$= \sum_{l=0}^{n-1} \sum_{m=-l}^{+l} a_{nlm} \int d^3r_e\, e^{-i\vec{q}\cdot\vec{r}_e}\, R_{nl}^*(r_e) R_{10}(r_e) \times$$
$$\times Y_l^{m*}(\theta_e, \varphi_e) \underbrace{Y_0^0(\theta_e, \varphi_e)}_{= \frac{1}{\sqrt{4\pi}}}$$

Choosing $\hat{q}\cdot\hat{r}_e = \cos\theta_e$, we can expand the plane wave in terms of the angular momentum basis

$$e^{-i\vec{q}\cdot\vec{r}_e} = \sum_{l'=0}^{\infty} (2l'+1)\, i^{l'} j_{l'}(qr_e) \underbrace{P_{l'}(\cos\theta_e)}_{\sqrt{\frac{4\pi}{2l'+1}}\, Y_{l'}^{0}(\theta_e,\varphi_e)}$$

$$= \sqrt{4\pi} \sum_{l'=0}^{\infty} \sqrt{2l'+1}\, i^{l'} j_{l'}(qr_e)\, Y_{l'}^{0}(\theta_e,\varphi_e),$$

substituting above $\Rightarrow$

$$F_{fi}(q) = \sum_{l=0}^{n-1} \sum_{m=-l}^{+l} a_{nlm} \sum_{l'=0}^{\infty} \sqrt{2l'+1}\, i^{l'} \times$$

$$\times \int_0^{\infty} dr_e\, r_e^2\, j_{l'}(qr_e)\, R^{*}_{nl}(r_e)\, R_{10}(r_e) \times$$

$$\times \underbrace{\int d\Omega_e\, Y_l^{m*}(\theta_e,\varphi_e)\, Y_{l'}^{0}(\theta_e,\varphi_e)}_{=\delta_{ll'}\delta_{m0}}$$

Hence

$$\boxed{F_{fi}(q) = \sum_{l=0}^{n-1} a_{nl0}\sqrt{2l+1}\, i^l \int_0^\infty dr\, r^2 j_l(qr) \times R^*_{nl}(r) R_{10}(r)}$$

8.3. Semi-Classical Treatment of Electromagnetic Radiation: The interaction of Bound states of charged particles with Photons

Up to present we have dealt with the interaction of matter with matter, we have not included the interaction of matter with electromagnetic radiation. For example the emission or absorption of photons by atoms. A consistent quantum mechanical treatment of the matter as well as electromagnetic radiation would require the generalization of our quantum mechanical postulates to the special relativistic Maxwell equations governing the time evolution of the E-M field as well as the generalization of the