

Fermi's Two Golden Rules

Golden Rule Number 2

Light and Atoms:

Absorption

Stimulated Emission

Spontaneous Emission

Photo-ionization

$$H_1 = \vec{d} \cdot \vec{E}$$

$$\vec{d} = e \vec{r}$$

$$\vec{E} = \hat{\epsilon} E_0 e^{i(\vec{k} \cdot \vec{r} + \omega t)}$$

$$\langle f | \hat{\epsilon} \cdot \vec{r} e E_0 e^{i \vec{k} \cdot \vec{r}} | i \rangle$$

$$e^{i \vec{k} \cdot \vec{r}} = 1 + i \vec{k} \cdot \vec{r} + \frac{1}{2!} (i \vec{k} \cdot \vec{r})^2 + \dots$$

Selection Rules

Selection Rules for Electronic Transitions

In spectral phenomena such as the [Zeeman effect](#) it becomes evident that transitions are not observed between all pairs of energy levels. Some transitions are "forbidden" (i.e., highly improbable) while others are "allowed" by a set of selection rules. The number of split components observed in the Zeeman effect is consistent with the selection rules:

$$\Delta \ell = \pm 1 \text{ (not zero)}$$

$$\Delta m_{\ell} = 0, \pm 1$$

These are the selection rules for an electric dipole transition. One can say that the oscillating electric field associated with the transitions resembles an oscillating electric dipole. When this is expressed in quantum terms, photon emission is always accompanied by a change of 1 in the orbital [angular momentum quantum number](#). The [magnetic quantum number](#) can change by zero or one unit.

Another approach to the selection rules is to note that any electron transition which involves the emission of a [photon](#) must involve a change of 1 in the angular momentum. The photon is said to have an intrinsic angular momentum or "spin" of one, so that conservation of angular momentum in photon emission requires a change of 1 in the atom's angular momentum. The [electron spin quantum number](#) does not change in such transitions, so an additional selection rule is:

$$\Delta m_s = 0$$

The [total angular momentum](#) may change be either zero or one:

$$\Delta j = 0, \pm 1$$

An exception to this last selection rule is that you cannot have a transition from $j=0$ to $j=0$; i.e., since the vector angular momentum must change by one unit in an electronic transition, $j=0 \rightarrow 0$ can't happen because there is no total angular momentum to re-orient to get a change of 1.

Conservation of Angular Momentum

Photon spin = 1

Therefore $\Delta\ell = -1$ or $+1$

**Photon Propagation Direction Can Be
parallel**

anti-parallel

perpendicular

to the L quantization axis

Therefore $\Delta m = -1, 0, +1$

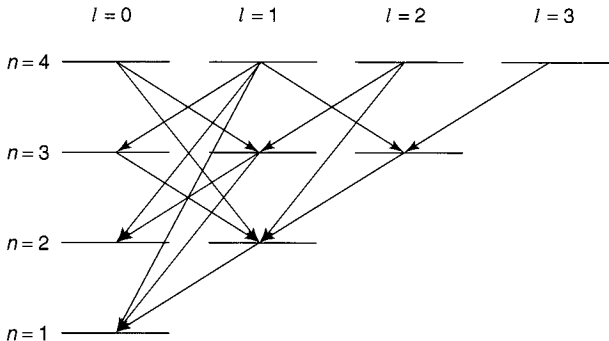


FIGURE 9.6: Allowed decays for the first four Bohr levels in hydrogen.

Summary table

		Electric dipole (E1)	Magnetic dipole (M1)	Electric quadrupole (E2)	Magnetic quadrupole (M2)	Electric octupole (E3)	Magnetic octupole (M3)
Rigorous rules	(1)	$\Delta J = 0, \pm 1$ ($J = 0 \not\leftrightarrow 0$)		$\Delta J = 0, \pm 1, \pm 2$ ($J = 0 \not\leftrightarrow 0, 1; \frac{1}{2} \not\leftrightarrow \frac{1}{2}$)		$\Delta J = 0, \pm 1, \pm 2, \pm 3$ ($0 \not\leftrightarrow 0, 1, 2; \frac{1}{2} \not\leftrightarrow \frac{1}{2}, \frac{3}{2}; 1 \not\leftrightarrow 1$)	
	(2)	$\Delta M_J = 0, \pm 1$		$\Delta M_J = 0, \pm 1, \pm 2$		$\Delta M_J = 0, \pm 1, \pm 2, \pm 3$	
	(3)	$\pi_f = -\pi_i$	$\pi_f = \pi_i$		$\pi_f = -\pi_i$		$\pi_f = \pi_i$
LS coupling	(4)	One electron jump $\Delta l = \pm 1$	No electron jump $\Delta l = 0,$ $\Delta n = 0$	None or one electron jump $\Delta l = 0, \pm 2$	One electron jump $\Delta l = \pm 1$	One electron jump $\Delta l = \pm 1, \pm 3$	One electron jump $\Delta l = 0, \pm 2$
	(5)	If $\Delta S = 0$ $\Delta L = 0, \pm 1$ ($L = 0 \not\leftrightarrow 0$)	If $\Delta S = 0$ $\Delta L = 0$	If $\Delta S = 0$ $\Delta L = 0, \pm 1, \pm 2$ ($L = 0 \not\leftrightarrow 0, 1$)		If $\Delta S = 0$ $\Delta L = 0, \pm 1, \pm 2, \pm 3$ ($L = 0 \not\leftrightarrow 0, 1, 2; 1 \not\leftrightarrow 1$)	
Inter- mediate coupling	(6)	If $\Delta S = \pm 1$ $\Delta L = 0, \pm 1, \pm 2$		If $\Delta S = \pm 1$ $\Delta L = 0, \pm 1,$ $\pm 2, \pm 3$ ($L = 0 \not\leftrightarrow 0$)	If $\Delta S = \pm 1$ $\Delta L = 0, \pm 1$ ($L = 0 \not\leftrightarrow 0$)	If $\Delta S = \pm 1$ $\Delta L = 0, \pm 1,$ $\pm 2, \pm 3, \pm 4$ ($L = 0 \not\leftrightarrow 0, 1$)	If $\Delta S = \pm 1$ $\Delta L = 0, \pm 1,$ ± 2 ($L = 0 \not\leftrightarrow 0$)

S selection rules

when are the matrix elements zero?

$$\text{If } [\Omega, H_1] = 0$$

then $\langle \alpha_2 \omega_2 | H_1 | \alpha_1 \omega_1 \rangle = 0$ unless $\omega_1 = \omega_2$

$$0 = \langle \alpha_2 \omega_2 | \Omega H_1 - H_1 \Omega | \alpha_1 \omega_1 \rangle$$

$$= (\omega_2 - \omega_1) \langle \alpha_2 \omega_2 | H_1 | \alpha_1 \omega_1 \rangle$$

PARITY OPERATOR

$$P|+\rangle = +|+\rangle$$

$$P|-\rangle = -|-\rangle$$

$$[P, H] = 0$$

$$P\psi(\vec{r}) = \pm\psi(\vec{r})$$

The Dipole Allowed Decays of $n=2$ States

Time-Dependent Perturbation Theory: Solved Problems

1. Consider a hydrogen atom in a time-dependent electric field $\mathbf{E} = E(t) \mathbf{k}$. Calculate all ten of the dipole matrix elements between the $n = 1$ ground state and the four $n = 2$ excited states. Also calculate the five expectation values of the dipole operator for these five states. Note that “calculate” here means show that fourteen out of the fifteen are zero with a clever argument, so that you only need to do one integral!

First, do the calculation using the even-odd symmetry with respect to z of the three ingredients, namely: (1) the wavefunctions, (2) the dipole term, and (3) the limits of integration. Show which matrix elements must vanish and which ones can survive:

- (a) Write down the $n = 1$ ground state wavefunction, and the four $n = 2$ excited state wavefunctions in spherical coordinates:

$$\psi_{nlm}(\mathbf{r}) = \langle r, \theta, \phi | n, l, m \rangle = R_{nl}(r) Y_{lm}(\theta, \phi).$$

- (b) Show that these five wavefunctions squared $|\psi_{nlm}(x, y, z)|^2$ are all even functions of z .
 (c) Use your result from part b to show that the matrix elements

$$\langle n, l, m | z | n, l, m \rangle = \int_{-\infty}^{\infty} z |\psi(x, y, z)|^2 dx dy dz = 0.$$

- (d) Show that four of these five states are even functions of z , namely that ψ_{100} , ψ_{200} , ψ_{211} and ψ_{21-1} are all even functions of z , and that ψ_{210} is an odd function of z .
 (e) Use your result from part d to show that all the following dipole matrix elements between pairs of the even states are zero, *i.e.*, show that

$$\langle 1, 0, 0 | z | 2, 0, 0 \rangle = \langle 1, 0, 0 | z | 2, 1, 1 \rangle = \langle 1, 0, 0 | z | 2, 1, -1 \rangle = 0,$$

$$\langle 1, 0, 0 | z | 2, 1, 0 \rangle = \langle 2, 1, 1 | z | 2, 1, 0 \rangle = \langle 2, 1, -1 | z | 2, 1, 0 \rangle = 0,$$

$$\langle 2, 0, 0 | z | 2, 1, 1 \rangle = \langle 2, 0, 0 | z | 2, 1, -1 \rangle = \langle 2, 1, 1 | z | 2, 1, -1 \rangle = 0.$$

- (f) Use the even and odd argument in z to explain why the only non-zero matrix elements are

$$\langle 1, 0, 0 | z | 2, 1, 0 \rangle = \int_{-\infty}^{\infty} \psi_{200}^*(x, y, z) z \psi_{210}(x, y, z) dx dy dz,$$

and

$$\langle 2, 0, 0 | z | 2, 1, 0 \rangle = \int_{-\infty}^{\infty} \psi_{100}^*(x, y, z) z \psi_{210}(x, y, z) dx dy dz.$$

- (g) Put in the wavefunctions and calculate the two non-zero $H_1 = -eEz$ integrals from part f, *i.e.*, do the integrals. For example, calculate

$$\langle 1, 0, 0 | H_1 | 2, 1, 0 \rangle = -eE \frac{1}{\sqrt{\pi a^3}} \frac{1}{\sqrt{32\pi a^3}} \frac{1}{a} \int_{-\infty}^{\infty} e^{-r/a} e^{-r/2a} z d^3r$$

or

$$\langle 1, 0, 0 | z | 2, 1, 0 \rangle = -eE \frac{1}{\sqrt{\pi a^3}} \frac{1}{\sqrt{32\pi a^3}} \frac{1}{a} \int_{-\infty}^{\infty} e^{-r/a} e^{-r/2a} (r \cos \theta) \sin \theta d\theta d\phi r^2 dr.$$

You should find that

$$\langle 1, 0, 0 | H_1 | 2, 1, 0 \rangle = -(2^8/3^5\sqrt{2}) eEa \simeq -0.7449 eEa,$$

and that

$$\langle 2, 0, 0 | z | 2, 1, 0 \rangle = -3 eEa.$$

Second, do the calculation using the orthonormality of the spherical harmonics and the addition rules for angular momentum:

- (h) First show that $z = r \cos \theta \simeq Y_{10}(\theta, \phi)$. Then use the angular momentum addition rules to add Y_{10} to one (or the other) Y_{lm} under the integral. Finally, use the orthonormality of the Y_{lm} 's to show that all the matrix elements except $\langle 1, 0, 0 | z | 2, 1, 0 \rangle$ must vanish.
- (i) Which method do you prefer? Explain why you prefer it! It is very important that you fully understand both methods: they are both extremely powerful and extremely useful!!!

1. The wave function expressed in spherical coordinates is given by

$$\psi_{nlm}(\vec{r}) = \langle r, \theta, \phi | n, l, m \rangle R_{nl}(r) Y_{lm}(\theta, \phi).$$

Using the functional forms of the R_{nl} s and of the spherical harmonics, we find

$$\psi_{100} = R_{10} Y_{00} = 2a^{-3/2} e^{-r/a} \left(\frac{1}{4\pi} \right)^{1/2} = \frac{1}{\sqrt{\pi}} a^{-3/2} e^{-r/a},$$

$$\psi_{200} = R_{20} Y_{00} = \frac{1}{\sqrt{2}} a^{-3/2} \left(1 - \frac{r}{2a} \right) e^{-r/2a} \left(\frac{1}{4\pi} \right)^{1/2} = \frac{1}{2\sqrt{2\pi}} a^{-3/2} \left(1 - \frac{r}{2a} \right) e^{-r/2a},$$

$$\psi_{210} = R_{21}Y_{10} = \frac{1}{\sqrt{24}}a^{-3/2} \left(\frac{r}{a}\right) e^{-r/2a} \left(\frac{3}{4\pi}\right)^{1/2} \cos(\theta) = \frac{1}{4\sqrt{2\pi}}a^{-3/2} \left(\frac{r}{a}\right) e^{-r/2a} \cos(\theta),$$

$$\psi_{211} = R_{21}Y_{11} = \frac{1}{\sqrt{24}}a^{-3/2} \left(\frac{r}{a}\right) e^{-r/2a} \left[-\left(\frac{3}{8\pi}\right)^{1/2} \sin(\theta)e^{i\phi}\right] = -\frac{1}{8\sqrt{\pi}}a^{-3/2} \left(\frac{r}{a}\right) e^{-r/2a} \sin(\theta)e^{i\phi},$$

$$\psi_{21,-1} = R_{21}Y_{1,-1} = \frac{1}{\sqrt{24}}a^{-3/2} \left(\frac{r}{a}\right) e^{-r/2a} \left(\frac{3}{8\pi}\right)^{1/2} \sin(\theta)e^{-i\phi} = \frac{1}{8\sqrt{\pi}}a^{-3/2} \left(\frac{r}{a}\right) e^{-r/2a} \sin(\theta)e^{-i\phi}.$$

1.(b) Remember, an even function is one for which $f(-x) = f(x)$. If there is more than one independent variable, as we have here, the function may be even with respect to one or more of the variables. Even with respect to z for the function $f(x, y, z)$ means that $f(x, y, -z) = f(x, y, z)$. The wave functions are currently in spherical coordinates $\psi(r, \theta, \phi)$. We need to find their symmetries in Cartesian coordinates

$$r = (x^2 + y^2 + z^2)^{1/2}, \quad \cos \theta = \frac{z}{(x^2 + y^2 + z^2)^{1/2}}, \quad \sin \theta = \frac{(x^2 + y^2)^{1/2}}{(x^2 + y^2 + z^2)^{1/2}}, \quad \text{and} \quad \phi = \tan^{-1} \left(\frac{y}{x}\right).$$

We actually only need to do enough examination to determine the symmetry with respect to z and not a complete change of variables. Using the ψ_{nlm} 's from part a, we find

$$|\psi_{100}(x, y, z)|^2 = \frac{1}{\pi}a^{-3}e^{-2(x^2+y^2+z^2)^{1/2}/a}, \quad \text{where} \quad (-z)^2 = z^2$$

$$\Rightarrow |\psi_{100}(x, y, -z)|^2 = |\psi_{100}(x, y, z)|^2 \quad \text{so} \quad |\psi_{100}|^2 \quad \text{is even wrt } z.$$

$$|\psi_{200}(x, y, z)|^2 = \frac{1}{8\pi}a^{-3} \left(1 - \frac{(x^2 + y^2 + z^2)^{1/2}}{2a}\right)^2 e^{-(x^2+y^2+z^2)^{1/2}/a} \quad \text{and} \quad (-z)^2 = z^2 \quad \text{in both places}$$

$$\Rightarrow |\psi_{200}(x, y, -z)|^2 = |\psi_{200}(x, y, z)|^2 \quad \text{so} \quad |\psi_{200}|^2 \quad \text{is even wrt } z.$$

$$|\psi_{210}(x, y, z)|^2 = \frac{1}{32\pi}a^{-3} \left(\frac{(x^2 + y^2 + z^2)^{1/2}}{a^2}\right) e^{-(x^2+y^2+z^2)^{1/2}/a} \frac{z^2}{(x^2 + y^2 + z^2)}$$

and $(-z)^2 = z^2$ in all four places

$$\Rightarrow |\psi_{210}(x, y, -z)|^2 = |\psi_{210}(x, y, z)|^2 \quad \text{so} \quad |\psi_{210}|^2 \quad \text{is even wrt } z.$$

$$|\psi_{211}(x, y, z)|^2 = \frac{1}{64\pi} a^{-3} \left(\frac{(x^2 + y^2 + z^2)}{a^2} \right) e^{-(x^2 + y^2 + z^2)^{1/2}/a} \frac{x^2 + y^2}{(x^2 + y^2 + z^2)} e^{i\phi(x, y)}$$

and $(-z)^2 = z^2$ in all three places

$$\Rightarrow |\psi_{211}(x, y, -z)|^2 = |\psi_{211}(x, y, z)|^2 \quad \text{so} \quad |\psi_{211}|^2 \quad \text{is even wrt } z.$$

$$|\psi_{21,-1}(x, y, z)|^2 = \frac{1}{64\pi} a^{-3} \left(\frac{(x^2 + y^2 + z^2)}{a^2} \right) e^{-(x^2 + y^2 + z^2)^{1/2}/a} \frac{x^2 + y^2}{(x^2 + y^2 + z^2)} e^{-i\phi(x, y)}$$

and $(-z)^2 = z^2$ in all three places

$$\Rightarrow |\psi_{211}(x, y, -z)|^2 = |\psi_{211}(x, y, z)|^2 \quad \text{so} \quad |\psi_{211}|^2 \quad \text{is even wrt } z.$$

1.(c) Here we use the facts that the product of an even function is an odd function, and that an odd function integrated between symmetric limits is zero. The expectation values of z are given by

$$\langle n, l, m | z | n, l, m \rangle = \int_{-\infty}^{\infty} z |\psi(x, y, z)|^2 dx dy dz = \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy \int_{-\infty}^{\infty} z |\psi(x, y, z)|^2 dz,$$

but z is an odd function, and all of the $|\psi_{nlm}(x, y, z)|^2$ are even functions, so all of the $z|\psi_{nlm}(x, y, z)|^2$ are odd functions. The integral with respect to z is between symmetric limits. Therefore

$$\langle n, l, m | z | n, l, m \rangle = \left(\int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy \right) \cdot 0 = 0.$$

1.(d) Referring to wave functions of part (a) and the Cartesian/spherical relations of part (b),

$$\psi_{100} = \frac{1}{\sqrt{\pi}} a^{-3/2} e^{-(x^2 + y^2 + z^2)^{1/2}/a}, \quad \text{and} \quad (-z)^2 = z^2$$

$$\Rightarrow \psi_{100}(x, y, -z) = \psi_{100}(x, y, z) \quad \text{so} \quad \psi_{100} \quad \text{is even wrt } z.$$

$$\psi_{200}(x, y, z) = \frac{1}{2\sqrt{2\pi}} a^{-3/2} \left(1 - \frac{(x^2 + y^2 + z^2)^{1/2}}{2a} \right) e^{-(x^2 + y^2 + z^2)^{1/2}/2a},$$

and $(-z)^2 = z^2$ in both places

$$\Rightarrow \psi_{200}(x, y, -z) = \psi_{200}(x, y, z) \quad \text{so} \quad \psi_{200} \quad \text{is even wrt } z.$$

$$\psi_{210} = \frac{1}{4\sqrt{2\pi}} a^{-3/2} \left(\frac{(x^2 + y^2 + z^2)^{1/2}}{a} \right) e^{-(x^2 + y^2 + z^2)^{1/2}/2a} \frac{z}{(x^2 + y^2 + z^2)^{1/2}},$$

This is an odd function. In the three places where $(x^2 + y^2 + z^2)^{1/2}$ is substituted for r , $(-z)^2 = z^2$. This portion of the wave function is even. The remaining factor is z , which is an odd function. The product of an even and an odd function is an odd function

$$\Rightarrow \psi_{210}(x, y, -z) = -\psi_{210}(x, y, z) \quad \text{so} \quad \psi_{210} \quad \text{is odd wrt } z.$$

$$\psi_{211} = -\frac{1}{8\sqrt{\pi}} a^{-3/2} \left(\frac{(x^2 + y^2 + z^2)^{1/2}}{a} \right) e^{-(x^2 + y^2 + z^2)^{1/2}/2a} \frac{(x^2 + y^2)^{1/2}}{(x^2 + y^2 + z^2)^{1/2}} e^{i\phi(x, y)},$$

where $(-z)^2 = z^2$ in all three places, and $\phi = \phi(x, y)$ is independent of z ,

$$\Rightarrow \psi_{211}(x, y, -z) = \psi_{211}(x, y, z) \quad \text{so} \quad \psi_{211} \quad \text{is even wrt } z.$$

$$\psi_{21,-1} = -\frac{1}{8\sqrt{\pi}} a^{-3/2} \left(\frac{(x^2 + y^2 + z^2)^{1/2}}{a} \right) e^{-(x^2 + y^2 + z^2)^{1/2}/2a} \frac{(x^2 + y^2)^{1/2}}{(x^2 + y^2 + z^2)^{1/2}} e^{-i\phi(x, y)},$$

where $(-z)^2 = z^2$ in all three places, and $\phi = \phi(x, y)$ is again independent of z ,

$$\Rightarrow \psi_{21,-1}(x, y, -z) = \psi_{21,-1}(x, y, z) \quad \text{so} \quad \psi_{21,-1} \quad \text{is even wrt } z.$$

1.(e) From part (d), ψ_{100} , ψ_{200} , ψ_{211} , and $\psi_{21,-1}$ are even functions with respect to z . Using the same argument as in part (c),

$$\begin{aligned} \langle \psi_{\text{even wrt } z} | z | \psi_{\text{even wrt } z} \rangle &= \int_{-\infty}^{\infty} (\psi_{\text{even wrt } z})^* z (\psi_{\text{even wrt } z}) dx dy dz \\ &= \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy \int_{-\infty}^{\infty} (\psi_{\text{even wrt } z})^* z (\psi_{\text{even wrt } z}) dz. \end{aligned}$$

Again, z is an odd function. The product of an even and odd function is odd; this odd function multiplied by another even function yields an odd function overall. The integral with respect to z is between symmetric limits, and an integral of an odd function between symmetric limits is zero. Therefore

$$\begin{aligned} \langle 1, 0, 0 | z | 2, 0, 0 \rangle &= \langle 1, 0, 0 | z | 2, 1, 1 \rangle = \langle 1, 0, 0 | z | 2, 1, -1 \rangle = 0 \\ \langle 2, 0, 0 | z | 2, 1, 1 \rangle &= \langle 2, 0, 0 | z | 2, 1, -1 \rangle = \langle 2, 1, 1 | z | 2, 1, -1 \rangle = 0. \end{aligned}$$

1.(f) The remaining matrix elements are given by

$$\langle 1, 0, 0 | z | 2, 1, 0 \rangle, \quad \langle 2, 0, 0 | z | 2, 1, 0 \rangle, \quad \langle 2, 1, 1 | z | 2, 1, 0 \rangle \quad \text{and} \quad \langle 2, 1, -1 | z | 2, 1, 0 \rangle.$$

These integrals all have the form $\int_{-\infty}^{\infty} (\text{even function}) (\text{odd function}) (\text{odd function})$ with respect to z , which we would expect to be non-zero. We can examine two at once, using $z = r \cos \theta$, and the volume element in spherical coordinates which is $dv = r^2 \sin \theta dr d\theta d\phi$,

$$\begin{aligned} \langle 2, 1, \pm 1 | z | 2, 1, 0 \rangle &= \int_{-\infty}^{\infty} \left(\frac{\mp 1}{8\sqrt{\pi}} a^{-3/2} \left(\frac{r}{a} \right) e^{-r/2a} \sin(\theta) e^{\pm i\phi} \right)^* r \cos \theta \frac{1}{4\sqrt{2\pi}} a^{-3/2} \left(\frac{r}{a} \right) e^{-r/2a} \cos(\theta) dV \\ &= \frac{\mp 1}{32\pi\sqrt{2}} \frac{1}{a^5} \int_0^{\infty} dr r^5 e^{-r/a} \int_0^{\pi} d\theta \sin^2 \theta \cos^2 \theta \int_0^{2\pi} d\phi e^{\mp i\phi} \end{aligned}$$

Examining just the azimuthal integral, we find

$$\begin{aligned} \int_0^{2\pi} d\phi e^{\mp i\phi} &= \int_0^{2\pi} d\phi \cos \phi \mp i \sin \phi \\ &= \int_0^{2\pi} d\phi \cos \phi \mp i \int_0^{2\pi} d\phi \sin \phi \\ &= \sin \phi \Big|_0^{2\pi} \pm i \cos \phi \Big|_0^{2\pi} \\ &= (0 - 0) \pm i(1 - 1) = 0, \end{aligned}$$

therefore, the integral over all space will be zero regardless of the values of the radial and polar integrals, *i.e.*,

$$\langle 2, 1, 1 | z | 2, 1, 0 \rangle = \langle 2, 1, -1 | z | 2, 1, 0 \rangle = 0.$$

1.(g) We have been examining expectation values of z because $H_1 = -eEz$, where $-eE$ is a constant. If the expectation value is non-zero, the value of the integral multiplied by $-eE$ will express the result in energy units.

There are two remaining integrals. Using $z = r \cos \theta$ and $dV = r^2 \sin \theta dr d\theta d\phi$, the integral

$$\begin{aligned}
\langle 2, 0, 0 | z | 2, 1, 0 \rangle &= \int_{-\infty}^{\infty} \left(\frac{1}{2\sqrt{2\pi}} a^{-3/2} \left(1 - \frac{r}{2a}\right) e^{-r/2a} \right)^* r \cos \theta \frac{1}{4\sqrt{2\pi}} a^{-3/2} \left(\frac{r}{a}\right) e^{-r/2a} \cos(\theta) dV \\
&= \frac{1}{16\pi a^4} \int_0^{\infty} dr \left(1 - \frac{r}{2a}\right) r^4 e^{-r/a} \int_0^{\pi} d\theta \cos^2 \theta \sin \theta \int_0^{2\pi} d\phi \\
&= \frac{1}{16\pi a^4} \int_0^{\infty} dr \left(1 - \frac{r}{2a}\right) r^4 e^{-r/a} \int_0^{\pi} d\theta \cos^2 \theta \sin \theta [2\pi] \\
&= \frac{1}{8a^4} \int_0^{\infty} dr \left(1 - \frac{r}{2a}\right) r^4 e^{-r/a} \left[-\frac{\cos^3 \theta}{3} \right]_0^{\pi} \\
&= \frac{1}{8a^4} \int_0^{\infty} dr \left(1 - \frac{r}{2a}\right) r^4 e^{-r/a} \left[\frac{2}{3} \right] \\
&= \frac{1}{12a^4} \int_0^{\infty} dr \left(1 - \frac{r}{2a}\right) r^4 e^{-r/a} \\
&= \frac{1}{12a^4} \left[\int_0^{\infty} dr r^4 e^{-r/a} - \frac{1}{2a} \int_0^{\infty} dr r^5 e^{-r/a} \right].
\end{aligned}$$

These integrals are evaluated using

$$\int_0^{\infty} x^n e^{-\mu x} dx = n! \mu^{-n-1}, \quad \text{Re } \mu > 0,$$

with $\mu = 1/a$ for both, and with $n = 4$ and 5 respectively, so we find

$$\begin{aligned}
\langle 2, 0, 0 | z | 2, 1, 0 \rangle &= \frac{1}{12a^4} \left[4! \left(\frac{1}{a}\right)^{-4-1} - \frac{1}{2a} 5! \left(\frac{1}{a}\right)^{-5-1} \right] \\
&= \frac{1}{12a^4} \left[\frac{4 \cdot 3 \cdot 2}{(1/a)^5} - \frac{1}{2a} \left(\frac{5 \cdot 4 \cdot 3 \cdot 2}{(1/a)^6} \right) \right] \\
&= \frac{1}{12a^4} \left[24a^5 - \frac{1}{2a} 120a^6 \right] = \frac{1}{12a^4} [24a^5 - 60a^5] \\
&= \frac{1}{12a^4} (-36a^5) = -3a.
\end{aligned}$$

Since $H_1 = -eEz$, we find

$$\Rightarrow \langle 2, 0, 0 | z | 2, 1, 0 \rangle = 3eEa.$$

The last integral is $\langle 1, 0, 0 | z | 2, 1, 0 \rangle$ which in energy units is given by

$$\begin{aligned}
\langle 1, 0, 0 | H_1 | 2, 1, 0 \rangle &= \langle 1, 0, 0 | -eEz | 2, 1, 0 \rangle \\
&= -eE \langle 1, 0, 0 | z | 2, 1, 0 \rangle \\
&= -eE \int_{-\infty}^{\infty} (\psi_{100})^* z \psi_{210} dV \\
&= -eE \int_{-\infty}^{\infty} \frac{1}{\sqrt{\pi}} a^{-3/2} e^{-r/a} z \frac{1}{4\sqrt{2\pi}} a^{-3/2} \left(\frac{r}{a}\right) e^{-r/2a} \cos(\theta) dV \\
&= -\frac{eE}{4\pi\sqrt{2}a^4} \int_{-\infty}^{\infty} r e^{-3r/2a} z \cos(\theta) dV.
\end{aligned}$$

Using $z = r \cos \theta$ and $dV = r^2 \sin \theta dr d\theta d\phi$, we find

$$\begin{aligned}
\langle 1, 0, 0 | H_1 | 2, 1, 0 \rangle &= -\frac{eE}{4\pi\sqrt{2}a^4} \int_{-\infty}^{\infty} r^4 e^{-3r/2a} \cos^2 \theta \sin \theta dr d\theta d\phi \\
&= -\frac{eE}{4\pi\sqrt{2}a^4} \int_0^{\infty} dr r^4 e^{-3r/2a} \int_0^{\pi} d\theta \cos^2 \theta \sin \theta \int_0^{2\pi} d\phi \\
&= -\frac{eE}{4\pi\sqrt{2}a^4} \int_0^{\infty} dr r^4 e^{-3r/2a} \int_0^{\pi} d\theta \cos^2 \theta \sin \theta (2\pi) \\
&= -\frac{eE}{2\sqrt{2}a^4} \int_0^{\infty} dr r^4 e^{-3r/2a} \left[-\frac{\cos^3 \theta}{3} \right]_0^{\pi} \\
&= -\frac{eE}{2\sqrt{2}a^4} \int_0^{\infty} dr r^4 e^{-3r/2a} \left[-\frac{-1-1}{3} \right]_0^{\pi} \\
&= -\frac{eE}{3\sqrt{2}a^4} \int_0^{\infty} dr r^4 e^{-3r/2a}.
\end{aligned}$$

As before, using

$$\int_0^{\infty} x^n e^{-\mu x} dx = n! \mu^{-n-1}, \quad \text{Re } \mu > 0,$$

with $\mu = 3/2a$ and $n = 4$ we find

$$\begin{aligned}
\langle 1, 0, 0 | H_1 | 2, 1, 0 \rangle &= -\frac{eE}{3\sqrt{2}a^4} 4! \left(\frac{3}{2a}\right)^{-5} \\
&= -\frac{eE}{3\sqrt{2}a^4} \frac{4 \cdot 3 \cdot 2 (2a)^5}{3^5} \\
&= -\frac{eE}{3\sqrt{2}a^4} \frac{3 \cdot 2^3 \cdot 2^5 \cdot a^5}{3^5}
\end{aligned}$$

$$\Rightarrow \langle 1, 0, 0 | H_1 | 2, 1, 0 \rangle = -\frac{eE}{\sqrt{2}} \frac{2^8 \cdot a}{3^5} = -0.7449eEa.$$

1.(h) The wave functions under consideration are $\psi_{nlm} = R_{nl}(r)Y_{lm}(\theta, \phi)$, which are explicitly

$$\psi_{100} = R_{10}Y_{00}, \quad \psi_{200} = R_{20}Y_{00}, \quad \psi_{210} = R_{21}Y_{10}, \quad \psi_{211} = R_{21}Y_{11}, \quad \psi_{21,-1} = R_{21}Y_{1,-1}.$$

The integrals for the expectation values of z are given by

$$\begin{aligned} \langle n, l, m | z | n', l', m' \rangle &= \langle n, l, m | r \cos \theta | n', l', m' \rangle \\ &= \int_{-\infty}^{\infty} \psi_{nlm}^* r \cos \theta \psi_{n'l'm'} dV \\ &= \int_{-\infty}^{\infty} R_{nl}^* Y_{lm}^* r \cos \theta R_{n'l'} Y_{l'm'} dV \\ &= \int_0^{\infty} R_{nl}^* R_{n'l'} r^3 dr \int Y_{lm}^* \cos \theta Y_{l'm'} d\Omega, \end{aligned}$$

where the factor of r^2 in the radial integral comes from the volume element. The angular momentum addition rules and the integration can be summarized by

$$\int Y_{lm}^* \cos \theta Y_{l'm'} d\Omega, = \left[\frac{(l' - m' + 1)(l' + m' + 1)}{(2l' + 1)(2l' + 3)} \right]^{1/2} \delta_{mm'} \delta_{l, l'+1} + \left[\frac{(l' - m')(l' + m')}{(2l' - 1)(2l' + 1)} \right]^{1/2} \delta_{mm'} \delta_{l, l'-1}.$$

For this integral to be non-zero, l' must differ from l by ± 1 . This means that

$$\begin{aligned} \langle 1, 0, 0 | z | 1, 0, 0 \rangle &= \langle 2, 0, 0 | z | 2, 0, 0 \rangle = \langle 2, 1, 0 | z | 2, 1, 0 \rangle = \langle 2, 1, 1 | z | 2, 1, 1 \rangle = \langle 2, 1, -1 | z | 2, 1, -1 \rangle \\ &= \langle 1, 0, 0 | z | 2, 0, 0 \rangle = \langle 2, 1, 0 | z | 2, 1, 1 \rangle = \langle 2, 1, 0 | z | 2, 1, -1 \rangle = \langle 2, 1, 1 | z | 2, 1, -1 \rangle = 0. \end{aligned}$$

Also, m must equal m' for the integral to be non-zero, so

$$\langle 1, 0, 0 | z | 2, 1, 1 \rangle = \langle 1, 0, 0 | z | 2, 1, -1 \rangle = \langle 2, 0, 0 | z | 2, 1, 1 \rangle = \langle 2, 0, 0 | z | 2, 1, -1 \rangle = 0.$$

Only $\langle 1, 0, 0 | z | 2, 1, 0 \rangle$ and $\langle 2, 0, 0 | z | 2, 1, 0 \rangle$ remain as non-zero possibilities. Knowing that $z = r \cos \theta \sim Y_{10}$, we can see that these two integrals have the form

$$\int Y_{00} Y_{10} Y_{10} d\Omega.$$

Parity conservation in angle space can be summarized by $l_1 + l_2 + l_3 + m_1 + m_2 + m_3 = \text{even integer}$. For our two integrals, this condition is satisfied for the integer 2. For both $\langle 1, 0, 0 | z | 2, 1, 0 \rangle$ and $\langle 2, 0, 0 | z | 2, 1, 0 \rangle$, the integral over solid angle can now be evaluated using

$$\int Y_{00}^* \cos \theta Y_{10} d\Omega, = \left[\frac{(1 - 0 + 1)(1 + 0 + 1)}{(2 \cdot 1 + 1)(2 \cdot 1 + 3)} \right]^{1/2} \delta_{00} \delta_{0, 1+1} + \left[\frac{(1 - 0)(1 + 0)}{(2 \cdot 1 - 1)(2 \cdot 1 + 1)} \right]^{1/2} \delta_{00} \delta_{0, 1-1}.$$

Here, the first expression on the right side of the equation will be zero because the indices on the second Kronecker δ are not identical. Both sets of indices on the Kronecker δ of second expression on the right are identical, so we find

$$\int Y_{00}^* \cos \theta Y_{10} d\Omega, = \frac{1}{\sqrt{3}}.$$

Next, we will evaluate the radial integrals using this angular factor. We find

$$\begin{aligned}
\langle 1, 0, 0 | z | 2, 1, 0 \rangle &= \frac{1}{\sqrt{3}} \int_0^\infty R_{10} r R_{21} r^2 dr \\
&= \frac{1}{\sqrt{3}} \int_0^\infty \left(2a^{-3/2} e^{-r/a} \right) \left(\frac{1}{\sqrt{24}} a^{-3/2} \frac{r}{a} e^{-r/2a} \right) r^3 dr \\
&= \frac{1}{3\sqrt{2}a^4} \int_0^\infty r^4 e^{-3r/2a} dr
\end{aligned}$$

This integral can be evaluated using

$$\int_0^\infty x^n e^{-\mu x} dx = n! \mu^{-n-1}, \quad \text{Re } \mu > 0,$$

with $\mu = 3/2a$ and $n = 4$, so we find

$$\begin{aligned}
\langle 1, 0, 0 | z | 2, 1, 0 \rangle &= \frac{1}{3\sqrt{2}a^4} 4 \cdot 3 \cdot 2 \left(\frac{3}{2a} \right)^{-5} \\
&= \frac{1}{3\sqrt{2}a^4} \frac{3 \cdot 2^3 \cdot 2^5 \cdot a^5}{3^5} \\
\Rightarrow \langle 1, 0, 0 | z | 2, 1, 0 \rangle &= \frac{2^8}{\sqrt{2} \cdot 3^5} a
\end{aligned}$$

$$\Rightarrow \langle 1, 0, 0 | H_1 | 2, 1, 0 \rangle = -eE \frac{2^8}{\sqrt{2} \cdot 3^5} a = -0.7449eEa, \quad \text{which is the same as part (g).}$$

The other integral is given by

$$\begin{aligned}
\langle 2, 0, 0 | z | 2, 1, 0 \rangle &= \frac{1}{\sqrt{3}} \int_0^\infty R_{20} r R_{21} r^2 dr \\
&= \frac{1}{\sqrt{3}} \int_0^\infty \left(\frac{1}{\sqrt{2}} a^{-3/2} \left(1 - \frac{r}{2a} \right) e^{-r/2a} \right) \left(\frac{1}{\sqrt{24}} a^{-3/2} \frac{r}{a} e^{-r/2a} \right) r^3 dr \\
&= \frac{1}{\sqrt{3}\sqrt{2}\sqrt{24}a^4} \int_0^\infty \left(1 - \frac{r}{2a} \right) r^4 e^{-r/a} dr \\
&= \frac{1}{12a^4} \int_0^\infty r^4 e^{-r/a} dr - \frac{1}{24a^5} \int_0^\infty r^5 e^{-r/a} dr.
\end{aligned}$$

We can evaluate this integral using the same procedure, with $\mu = 1/a$ and $n = 4$ and 5 respectively. We find

$$\begin{aligned}
\langle 2, 0, 0 | z | 2, 1, 0 \rangle &= \frac{1}{12a^4} \frac{4 \cdot 3 \cdot 2}{(1/a)^5} - \frac{1}{24a^5} \frac{5 \cdot 4 \cdot 3 \cdot 2}{(1/a)^6} \\
&= \frac{24a^5}{12a^4} - \frac{120a^6}{24a^4}
\end{aligned}$$

$$\Rightarrow \langle 2, 0, 0 | z | 2, 1, 0 \rangle = 2a - 5a = -3a, \quad \text{which is the same as part (g)}$$

$$\text{and } \langle 2, 0, 0 | H_1 | 2, 1, 0 \rangle = 3eEa.$$

1.(i) .. Wow! That spherical harmonic stuff does seem to be a lot less work...

The Dipole Allowed Decays of $|3\ 0\ 0\rangle$

4. An electron in the $n = 3, l = 0, m = 0$ state of hydrogen decays by a sequence of electric dipole transitions to the ground state. The selection rules for electric dipole transitions are that $\Delta m = \pm 1$ or 0 and that $\Delta l = \pm 1$. In this problem you are only asked to consider the transitions where n changes, so the nine possible transitions are:

$$| 3, 0, 0 \rangle \Rightarrow | 2, 1, 1 \rangle$$

$$| 3, 0, 0 \rangle \Rightarrow | 2, 1, 0 \rangle$$

$$| 3, 0, 0 \rangle \Rightarrow | 2, 1, -1 \rangle$$

$$| 3, 0, 0 \rangle \Rightarrow | 2, 0, 0 \rangle$$

$$| 3, 0, 0 \rangle \Rightarrow | 1, 0, 0 \rangle$$

$$| 2, 1, 1 \rangle \Rightarrow | 1, 0, 0 \rangle$$

$$| 2, 1, 0 \rangle \Rightarrow | 1, 0, 0 \rangle$$

$$| 2, 1, -1 \rangle \Rightarrow | 1, 0, 0 \rangle$$

$$| 2, 0, 0 \rangle \Rightarrow | 1, 0, 0 \rangle$$

- (a) Which of these nine transitions obey the $\Delta m = \pm 1$ or 0 dipole selection rule?
 (b) Which of these nine transitions obey the $\Delta l = \pm 1$ dipole selection rule?
 (c) The dipole allowed transitions must obey both rules. Which six of the nine transitions are dipole allowed?
 (d) List all of the allowed dipole transition routes, which pass through the $n = 2$ states, from the $| 3, 0, 0 \rangle$ state to the $| 1, 0, 0 \rangle$ state, *i.e.*, list the three dipole allowed routes which have the form:

$$| 3, 0, 0 \rangle \Rightarrow | 2, ?, ? \rangle \Rightarrow | 1, 0, 0 \rangle .$$

- (e) Write down the integral for the dipole matrix element from the $| 3, 0, 0 \rangle$ state to the $| 2, 1, 0 \rangle$ state. Show that this matrix element only depends on the z component of the \mathbf{r} operator, *i.e.*, show that

$$\langle 2, 1, 0 | \mathbf{r} | 3, 0, 0 \rangle = \langle 2, 1, 0 | z | 3, 0, 0 \rangle \mathbf{k} .$$

- (f) Do the integral that you wrote down in part e. You should find $\langle 2, 1, 0 | z | 3, 0, 0 \rangle =$

$$\left[\sqrt{\frac{3}{4\pi}} \sqrt{\frac{1}{24}} a^{-\frac{3}{2}} \right] \left[\sqrt{\frac{1}{4\pi}} \frac{2}{\sqrt{27}} a^{-\frac{3}{2}} \right] \int_0^\infty \left[r \cos(\theta) \exp\left(\frac{-r}{2a}\right) \left(1 - \frac{2r}{3a} + \frac{2r^2}{27a^2} \right) \right]$$

$$\times \left[r \cos(\theta) \exp\left(\frac{-r}{3a}\right) \right] r^2 dr \sin\theta d\theta d\phi$$

so

$$\langle 2, 1, 0 | z | 3, 0, 0 \rangle = - \left[\frac{2^8 3^4}{5^6 \sqrt{6}} \right] a.$$

- (g) Write down the integrals for the dipole matrix elements from the $| 3, 0, 0 \rangle$ state to the $| 2, 1, \pm 1 \rangle$ states. Show that these matrix elements only depend on the x and y components of the \mathbf{r} operator, *i.e.*, show that

$$\langle 2, 1, \pm 1 | \mathbf{r} | 3, 0, 0 \rangle = \langle 2, 1, \pm 1 | x | 3, 0, 0 \rangle \mathbf{i} + \langle 2, 1, \pm 1 | y | 3, 0, 0 \rangle \mathbf{j}.$$

- (h) Now show that these x and y matrix elements are almost identical, *i.e.*, show that

$$\pm \langle 2, 1, \pm 1 | x | 3, 0, 0 \rangle = i \langle 2, 1, \pm 1 | y | 3, 0, 0 \rangle .$$

Explain how you can use this to make your life simpler, *i.e.*, explain why you can just calculate one integral and still obtain all four matrix elements!!!

- (i) Do the x integral you wrote down in part g. You should find $\langle 2, 1, \pm 1 | x | 3, 0, 0 \rangle =$

$$\left[\sqrt{\frac{3}{8\pi}} \sqrt{\frac{1}{24}} a^{-\frac{3}{2}} \right] \left[\sqrt{\frac{1}{4\pi}} \frac{2}{\sqrt{27}} a^{-\frac{3}{2}} \right] \int_0^\infty \left[r \sin(\theta) \exp(\pm i\phi) \exp\left(\frac{-r}{2a}\right) \left(1 - \frac{2r}{3a} + \frac{2r^2}{27a^2} \right) \right] \\ \times \left[r \cos(\theta) \exp\left(\frac{-r}{3a}\right) \right] r^2 dr \sin\theta d\theta d\phi$$

so

$$\langle 2, 1, \pm 1 | x | 3, 0, 0 \rangle = \pm \left[-\frac{2^7 3^4}{5^6 \sqrt{3}} \right] a.$$

- (j) According to Fermi's Golden Rule Number 2, the electric dipole transition rates are proportional to the squares of the matrix elements. Calculate the squares of these matrix elements and show that the two of the three decay routes have identical transition rates and that the third route has twice the transition rate, *i.e.*, show that

$$\frac{1}{2} |\langle 2, 1, 0 | \mathbf{r} | 3, 0, 0 \rangle|^2 = |\langle 2, 1, 1 | \mathbf{r} | 3, 0, 0 \rangle|^2 = |\langle 2, 1, -1 | \mathbf{r} | 3, 0, 0 \rangle|^2 .$$

So, one half go by one decay route, and one quarter each go by the other two decay routes.

(k) Now the spontaneous emission rates via these three routes are given by

$$A = \frac{\omega^3 |\langle \mathbf{r} \rangle|^2}{3 \pi \epsilon_0 \hbar c^3},$$

so the the total decay rate is given by

$$R = 3 A = 3 \left(\frac{e^2}{3 \pi \epsilon_0 \hbar c^3} \right) \left(\frac{-5 E_1}{36 \hbar} \right)^3 \left(\frac{2^{15} 3^7}{5^{12}} \right) a^2 = 6.32 \times 10^6 \text{ seconds}^{-1},$$

and the lifetime of the $|3, 0, 0\rangle$ state is given by $\tau = (1/R) = 1.58 \times 10^{-7}$ seconds.

4.(a) For an electron transition between the $n = 3, l = 0, m = 0$ and ground states, given that it can but does not have to go to the ground state directly, there are nine possible transitions.

All nine possible transitions obey the $\Delta m = \pm 1$ or 0 selection rule.

The nine possible transitions are

$$|3, 0, 0\rangle \rightarrow |2, 1, 1\rangle$$

$$|3, 0, 0\rangle \rightarrow |2, 1, 0\rangle$$

$$|3, 0, 0\rangle \rightarrow |2, 1, -1\rangle$$

$$|3, 0, 0\rangle \rightarrow |2, 0, 0\rangle$$

$$|3, 0, 0\rangle \rightarrow |1, 0, 0\rangle$$

$$|2, 1, 1\rangle \rightarrow |1, 0, 0\rangle$$

$$|2, 1, 0\rangle \rightarrow |1, 0, 0\rangle$$

$$|2, 1, -1\rangle \rightarrow |1, 0, 0\rangle$$

$$|2, 0, 0\rangle \rightarrow |1, 0, 0\rangle$$

4.(b)

Six of these these transitions obey the $\Delta l = \pm 1$ selection rule.
 These six allowed transitions are

$$\begin{aligned}
 |3, 0, 0\rangle &\rightarrow |2, 1, 1\rangle \\
 |3, 0, 0\rangle &\rightarrow |2, 1, 0\rangle \\
 |3, 0, 0\rangle &\rightarrow |2, 1, -1\rangle \\
 \\
 |2, 1, 1\rangle &\rightarrow |1, 0, 0\rangle \\
 |2, 1, 0\rangle &\rightarrow |1, 0, 0\rangle \\
 |2, 1, -1\rangle &\rightarrow |1, 0, 0\rangle
 \end{aligned}$$

4.(c)

The six transitions listed in part b obey both dipole transition rules.

4.(d)

The three allowed transitions via an intermediate state are

$$\begin{aligned}
 |3, 0, 0\rangle &\rightarrow |2, 1, 1\rangle \rightarrow |1, 0, 0\rangle \\
 |3, 0, 0\rangle &\rightarrow |2, 1, 0\rangle \rightarrow |1, 0, 0\rangle \\
 |3, 0, 0\rangle &\rightarrow |2, 1, -1\rangle \rightarrow |1, 0, 0\rangle
 \end{aligned}$$

4.(e) The transition

$$\begin{aligned}
 \langle 2, 1, 0 | \vec{r} | 3, 0, 0 \rangle &= \langle \psi_{210} | \vec{r} | \psi_{300} \rangle \\
 &= \langle R_{21} Y_{10} | \vec{r} | R_{30} Y_{00} \rangle \\
 &= \int R_{21} Y_{10} \vec{r} R_{30} Y_{00} dV \\
 &= \int R_{21} R_{30} r^2 dr \int Y_{10} \vec{r} Y_{00} d\Omega
 \end{aligned}$$

The angular part of this equation is

$$\int \left(\frac{3}{4\pi}\right)^{1/2} \cos \theta \vec{r} \left(\frac{1}{4\pi}\right)^{1/2} d\Omega = \frac{\sqrt{3}}{4\pi} \int \vec{r} \cos \theta d\Omega.$$

Remember $\vec{z} = \vec{r} \cos \theta = z \hat{k}$ so generalizing back into Dirac notation,

$$\langle 2, 1, 0 | \vec{r} | 3, 0, 0 \rangle = \langle 2, 1, 0 | z | 3, 0, 0 \rangle \hat{k}.$$

4.(f) Evaluating the integral by inserting the appropriate radial and angular functions, we find that the matrix element we seek $\langle 2, 1, 0 | z | 3, 0, 0 \rangle$ is equal to the integral

$$I = \int_{-\infty}^{\infty} \left(\frac{1}{\sqrt{24}} a^{-3/2} \frac{r}{a} e^{-r/2a} \left(\frac{3}{4\pi} \right)^{1/2} \cos \theta \right)^* (z) \frac{2}{\sqrt{27}} a^{-3/2} \left(1 - \frac{2r}{3a} + \frac{2}{27} \frac{r^2}{a^2} \right) e^{-r/3a} \left(\frac{1}{4\pi} \right)^{1/2} dV.$$

Factoring out the constants and simplifying, we find:

$$\begin{aligned} I &= \frac{1}{\sqrt{24}} \frac{2}{\sqrt{27}} \frac{1}{a^4} \left(\frac{3}{4\pi} \right)^{1/2} \left(\frac{1}{4\pi} \right)^{1/2} \int_{-\infty}^{\infty} r e^{-r/2a} \cos \theta (r \cos \theta) \left(1 - \frac{2r}{3a} + \frac{2}{27} \frac{r^2}{a^2} \right) e^{-r/3a} dV \\ &= \frac{1}{12\pi\sqrt{6}a^4} \int_{-\infty}^{\infty} r^2 \cos^2 \theta \left(1 - \frac{2r}{3a} + \frac{2}{27} \frac{r^2}{a^2} \right) e^{-5r/6a} dV \end{aligned}$$

And by doing the angular integrals, we can reduce the problem to the radial integrals that we must do

$$\begin{aligned} I &= \frac{1}{12\pi\sqrt{6}a^4} \int_0^{\infty} r^4 e^{-5r/6a} \left(1 - \frac{2r}{3a} + \frac{2}{27} \frac{r^2}{a^2} \right) dr \int_0^{\pi} \cos^2 \theta \sin \theta d\theta \int_0^{2\pi} d\phi. \\ &= \frac{1}{12\pi\sqrt{6}a^4} \int_0^{\infty} r^4 e^{-5r/6a} \left(1 - \frac{2r}{3a} + \frac{2}{27} \frac{r^2}{a^2} \right) dr \int_0^{\pi} \cos^2 \theta \sin \theta d\theta (2\pi) \\ &= \frac{1}{6\sqrt{6}a^4} \int_0^{\infty} \left(r^4 e^{-5r/6a} - \frac{2}{3a} r^5 e^{-5r/6a} + \frac{2}{27a^2} r^6 e^{-5r/6a} \right) dr \left(\frac{\cos^3 \theta}{3} \Big|_0^{\pi} \right) \\ &= \frac{1}{6\sqrt{6}a^4} \int_0^{\infty} \left(r^4 e^{-5r/6a} - \frac{2}{3a} r^5 e^{-5r/6a} + \frac{2}{27a^2} r^6 e^{-5r/6a} \right) dr \left(\frac{-1-1}{3} \right) \\ &= -\frac{1}{9\sqrt{6}a^4} \left(\int_0^{\infty} r^4 e^{-5r/6a} dr - \frac{2}{3a} \int_0^{\infty} r^5 e^{-5r/6a} dr + \frac{2}{27a^2} \int_0^{\infty} r^6 e^{-5r/6a} dr \right). \end{aligned} \quad (1)$$

We can evaluate all three radial integrals using form 3.381.4 on page 317 of Gradshteyn and Ryzhik, which is

$$\int_0^{\infty} x^{\nu-1} e^{-\mu x} dx = \frac{1}{\mu^{\nu}} \Gamma(\nu), \quad \text{Re } \mu > 0, \quad \text{Re } \nu > 0.$$

For the first integral, $\nu = 5$ and $\mu = 5/6a$, so

$$\int_0^{\infty} r^4 e^{-5r/6a} dr = \frac{1}{(5/6a)^5} \Gamma(5) = \frac{6^5 a^5}{5^5} 4 \cdot 3 \cdot 2 = 24 \frac{6^5 a^5}{5^5}.$$

For the second integral, $\nu = 6$ and $\mu = 5/6a$, so

$$\frac{2}{3a} \int_0^{\infty} r^5 e^{-5r/6a} dr = \frac{1}{(5/6a)^6} \Gamma(6) = \frac{2}{3a} \frac{6^6 a^6}{5^6} 5 \cdot 4 \cdot 3 \cdot 2 = 80 \frac{6^6 a^5}{5^6}.$$

For the third integral, $\nu = 7$ and $\mu = 5/6a$, so

$$\frac{2}{27a^2} \int_0^\infty r^6 e^{-5r/6a} dr = \frac{1}{(5/6a)^7} \Gamma(7) = \frac{2}{27a^2} \frac{6^7 a^7}{5^7} 6 \cdot 5 \cdot 4 \cdot 3 \cdot 2 = \frac{160}{3} \frac{6^7 a^5}{5^7}.$$

Substituting these into equation (1),

$$\begin{aligned} \langle 2, 1, 0 | z | 3, 0, 0 \rangle &= -\frac{1}{9\sqrt{6}a^4} a^5 \left(24 \frac{6^5}{5^5} - 80 \frac{6^6}{5^6} + \frac{160}{3} \frac{6^7}{5^7} \right) \\ &= -\frac{a}{9\sqrt{6}} \frac{6^5}{5^6} \left(120 - 80 \cdot 6 + \frac{160 \cdot 6^2}{3 \cdot 5} \right) \\ &= -\frac{6^5 a}{5^6 3^2 \sqrt{6}} (120 - 480 + 384) \\ &= -\frac{6^5 a}{5^6 3^2 \sqrt{6}} (24) \\ &= -\frac{2^5 3^5 a}{5^6 3^2 \sqrt{6}} (2^3 \cdot 3) \end{aligned}$$

$$\Rightarrow \langle 2, 1, 0 | z | 3, 0, 0 \rangle = -\frac{2^8 3^4}{5^6 \sqrt{6}} a$$

4.(g) The integrals for $\langle 2, 1, \pm 1 | \vec{r} | 3, 0, 0 \rangle$ are easier. These integrals depend only on the x and y components of the \vec{r} operator. Here

$$\begin{aligned} \langle 2, 1, \pm 1 | \vec{r} | 3, 0, 0 \rangle &= \int R_{21}^* Y_{1,\pm 1}^*(\vec{r}) R_{30} Y_{00} dV \\ &= \int R_{21} R_{30} r^2 dr \int Y_{1,\pm 1}^*(\vec{r}) Y_{00} d\Omega. \end{aligned}$$

The angular integral is

$$\begin{aligned} \int Y_{1,\pm 1}^*(\vec{r}) Y_{00} d\Omega &= \int \left(\mp \left(\frac{3}{8\pi} \right)^{1/2} \right) \sin \theta e^{\mp i\phi}(\vec{r}) \left(\frac{1}{4\pi} \right)^{1/2} d\Omega \\ &= \mp \left(\frac{3}{8\pi} \right)^{1/2} \left(\frac{1}{4\pi} \right)^{1/2} \int \sin \theta e^{\mp i\phi}(\vec{r}) d\Omega \\ &= \mp \frac{1}{4\pi} \sqrt{\frac{3}{2}} \int (\vec{r}) \sin \theta (\cos \phi \mp i \sin \phi) d\Omega \\ &= \mp \frac{1}{4\pi} \sqrt{\frac{3}{2}} \int (\vec{r} \sin \theta \cos \phi \mp i(\vec{r} \sin \theta \sin \phi)) d\Omega. \end{aligned}$$

Realizing $\vec{r} \sin \theta \cos \phi = \vec{x} = x\hat{i}$ and $\vec{r} \sin \theta \sin \phi = \vec{y} = y\hat{j}$, we can write this

$$\int Y_{1,\pm 1}^*(\vec{r}) Y_{00} d\Omega = \mp \frac{1}{4\pi} \sqrt{\frac{3}{2}} \int (x\hat{i} \mp i(y\hat{j})) d\Omega,$$

i.e., we can look at directional or angular dependence as a function of \vec{x} and \vec{y} only. Generalizing back into Dirac notation, which is representation free so the constants are irrelevant,

$$\begin{aligned}\langle 2, 1, \pm 1 | \vec{r} | 3, 0, 0 \rangle &= \langle 2, 1, \pm 1 | x \hat{i} \mp i(y \hat{j}) | 3, 0, 0 \rangle \\ &= \langle 2, 1, \pm 1 | x | 3, 0, 0 \rangle \hat{i} \mp \langle 2, 1, \pm 1 | iy | 3, 0, 0 \rangle \hat{j}.\end{aligned}$$

The sign “ \mp ” between the two elements reflects only a phase convention, and we will choose without loss of generality the “ $+$ ” sign for our phase so

$$\langle 2, 1, \pm 1 | \vec{r} | 3, 0, 0 \rangle = \langle 2, 1, \pm 1 | x | 3, 0, 0 \rangle \hat{i} + \langle 2, 1, \pm 1 | iy | 3, 0, 0 \rangle \hat{j}.$$

4.(h) To show

$$\langle 2, 1, \pm 1 | x | 3, 0, 0 \rangle = i \langle 2, 1, \pm 1 | y | 3, 0, 0 \rangle$$

consider the commutator $[L_z, x] = i\hbar y$, and the eigenvalue equation $L_z |n, l, m\rangle = m\hbar |n, l, m\rangle$. In general

$$\begin{aligned}\langle n', l', m' | [L_z, x] | n, l, m \rangle &= \langle n', l', m' | i\hbar y | n, l, m \rangle \\ &= i\hbar \langle n', l', m' | y | n, l, m \rangle.\end{aligned}$$

This must be the same as $\langle n', l', m' | [L_z, x] | n, l, m \rangle$ when the commutator is evaluated explicitly, *i.e.*,

$$\begin{aligned}i\hbar \langle n', l', m' | y | n, l, m \rangle &= \langle n', l', m' | [L_z, x] | n, l, m \rangle \\ &= \langle n', l', m' | L_z x - x L_z | n, l, m \rangle\end{aligned}$$

where L_z can operate to the left or right. So

$$\begin{aligned}i\hbar \langle n', l', m' | y | n, l, m \rangle &= \langle n', l', m' | m' \hbar x - x m \hbar | n, l, m \rangle \\ &= \langle n', l', m' | (m' - m) \hbar x | n, l, m \rangle \\ &= (m' - m) \hbar \langle n', l', m' | x | n, l, m \rangle \\ \Rightarrow (m' - m) \langle n', l', m' | x | n, l, m \rangle &= i \langle n', l', m' | y | n, l, m \rangle.\end{aligned}$$

For the specific states of interest

$$\begin{aligned}(1 - 0) \langle 2, 1, 1 | x | 3, 0, 0 \rangle &= i \langle 2, 1, 1 | y | 3, 0, 0 \rangle \\ \Rightarrow \langle 2, 1, 1 | x | 3, 0, 0 \rangle &= i \langle 2, 1, 1 | y | 3, 0, 0 \rangle,\end{aligned}$$

and

$$\begin{aligned}(-1 - 0) \langle 2, 1, -1 | x | 3, 0, 0 \rangle &= i \langle 2, 1, -1 | y | 3, 0, 0 \rangle \\ \Rightarrow - \langle 2, 1, -1 | x | 3, 0, 0 \rangle &= i \langle 2, 1, -1 | y | 3, 0, 0 \rangle,\end{aligned}$$

so

$$\pm \langle 2, 1, \pm 1 | x | 3, 0, 0 \rangle = i \langle 2, 1, \pm 1 | y | 3, 0, 0 \rangle.$$

There are four matrix elements here. If we evaluate the two integrals in x though, we have the two integrals in y from the above relation. Also, because of the symmetry in ϕ , we can do both integrals in x at the same time, so in effect, we have only one integral to evaluate to get all four matrix elements.

4.(i) To evaluate the integrals in x , remember $x = r \sin \theta \cos \phi$, and

$$\pm \langle 2, 1, \pm 1 | x | 3, 0, 0 \rangle = \pm \langle 2, 1, \pm 1 | r \sin \theta \cos \phi | 3, 0, 0 \rangle \quad \text{so}$$

$$\begin{aligned} \pm \langle 2, 1, \pm 1 | x | 3, 0, 0 \rangle &= \int_{-\infty}^{\infty} R_{21}^* Y_{1,\pm 1}^* r \sin \theta \cos \phi R_{30} Y_{00} r^2 \Omega \\ &= \int_0^{\infty} R_{21} R_{30} r^3 dr \int Y_{1,\pm 1}^* \sin \theta \cos \phi Y_{00} d\Omega \\ &= \int_0^{\infty} \frac{1}{\sqrt{24}} a^{-3/2} \frac{r}{a} e^{-r/2a} \frac{2}{\sqrt{27}} a^{-3/2} \left(1 - \frac{2r}{3a} + \frac{2}{27} \frac{r^2}{a^2}\right) e^{-r/3a} r^3 dr \int \mp \sqrt{\frac{3}{8\pi}} \sin \theta e^{\mp i\phi} (\sin \theta \cos \phi) \sqrt{\frac{1}{4\pi}} d\Omega \\ &= \mp \frac{1}{\sqrt{24}} \frac{2}{\sqrt{27}} \frac{1}{a^4} \sqrt{\frac{3}{8\pi}} \sqrt{\frac{1}{4\pi}} \int_0^{\infty} r^4 e^{-5r/6a} \left(1 - \frac{2r}{3a} + \frac{2}{27} \frac{r^2}{a^2}\right) dr \int_0^{\pi} \sin^3 \theta d\theta \int_0^{2\pi} \cos \phi e^{\mp i\phi} d\phi, \end{aligned} \quad (1)$$

where the third factor of $\sin \theta$ is from $d\Omega = \sin \theta d\theta d\phi$. The constants are

$$\mp \frac{1}{\sqrt{24}} \frac{2}{\sqrt{27}} \frac{1}{a^4} \sqrt{\frac{3}{8\pi}} \sqrt{\frac{1}{4\pi}} = \mp \frac{1}{\sqrt{2^3 \cdot 3}} \frac{2}{\sqrt{3^3}} \frac{1}{a^4} \frac{1}{4\pi} \frac{\sqrt{3}}{\sqrt{2}} = \mp \frac{2\sqrt{3}}{\sqrt{2^4 \cdot 3^4}} \frac{1}{4\pi a^4} = \mp \frac{1}{24\pi a^4 \sqrt{3}}.$$

The azimuthal integral is

$$\begin{aligned} \int_0^{2\pi} \cos \phi e^{\mp i\phi} d\phi &= \int_0^{2\pi} \cos \phi (\cos \phi \mp i \sin \phi) d\phi = \int_0^{2\pi} \cos^2 \phi d\phi \mp i \int_0^{2\pi} \cos \phi \sin \phi d\phi \\ &= \left[\frac{1}{2} \phi + \frac{1}{4} \sin(2\phi) \right]_0^{2\pi} \mp i \left[\frac{1}{2} \sin^2 \phi \right]_0^{2\pi} = \left[\frac{1}{2} 2\pi - 0 + 0 - 0 \right] \mp i [0 - 0] = \pi. \end{aligned}$$

The polar integral is

$$\int_0^{\pi} \sin^3 \theta d\theta = -\frac{1}{3} \left[(\cos \theta)(\sin^2 \theta + 2) \right]_0^{\pi} = -\frac{1}{3} [(-1)(0+2) - (1)(0+2)] = -\frac{1}{3} [-2 - 2] = \frac{4}{3}.$$

The radial integral becomes three integrals

$$\int_0^{\infty} r^4 e^{-5r/6a} \left(1 - \frac{2r}{3a} + \frac{2}{27} \frac{r^2}{a^2}\right) dr = \int_0^{\infty} r^4 e^{-5r/6a} dr - \frac{2}{3a} \int_0^{\infty} r^5 e^{-5r/6a} dr + \frac{2}{27a^2} \int_0^{\infty} r^6 e^{-5r/6a} dr$$

and we have already evaluated these integrals Using the results of part (f),

$$\begin{aligned} \int_0^{\infty} r^4 e^{-5r/6a} dr &= 24 \frac{6^5 a^5}{5^5}, \\ \frac{2}{3a} \int_0^{\infty} r^5 e^{-5r/6a} dr &= 80 \frac{6^6 a^5}{5^6}, \\ \frac{2}{27a^2} \int_0^{\infty} r^6 e^{-5r/6a} dr &= \frac{160}{3} \frac{6^7 a^5}{5^7}. \end{aligned}$$

Compiling these six results, equation (1) becomes

$$\begin{aligned}
\pm \langle 2, 1, \pm 1 | x | 3, 0, 0 \rangle &= \mp \frac{1}{24\pi a^4 \sqrt{3}} \pi \frac{4}{3} \left(24 \frac{6^5 a^5}{5^5} - 80 \frac{6^6 a^5}{5^6} + \frac{160}{3} \frac{6^7 a^5}{5^7} \right) \\
&= \mp \frac{1}{18a^4 \sqrt{3}} \frac{6^5 a^5}{5^6} \left(24 \cdot 5 - 80 \cdot 6 + \frac{160}{3} \frac{6^2}{5} \right) \\
&= \mp \frac{a}{2 \cdot 3^2 \sqrt{3}} \frac{6^5}{5^6} (120 - 480 + 384) \\
&= \mp \frac{a}{2 \cdot 3^2 \sqrt{3}} \frac{2^5 \cdot 3^5}{5^6} \quad (24) \\
&= \mp \frac{2^5 \cdot 3^5 \cdot 2^3 \cdot 3}{2 \cdot 3^2 \cdot 5^6 \sqrt{3}} a
\end{aligned}$$

$$\Rightarrow \langle 2, 1, \pm 1 | x | 3, 0, 0 \rangle = \pm \left[-\frac{2^7 \cdot 3^4}{5^6 \sqrt{3}} \right] a,$$

and

$$\langle 2, 1, \pm 1 | y | 3, 0, 0 \rangle = \pm i \left[-\frac{2^7 \cdot 3^4}{5^6 \sqrt{3}} \right] a.$$

4.(j) According to Fermi's Golden Rule Number 2, the electric dipole transition rates are proportional to the squares of the matrix elements. We have all three matrix elements so we can calculate the relative rates of decays for the three paths. From part f, we have

$$|\langle 2, 1, 0 | \vec{r} | 3, 0, 0 \rangle|^2 = \left[-\frac{2^8 \cdot 3^4}{5^6 \sqrt{6}} a \right]^2 = \frac{2^{16} \cdot 3^8}{5^{12} \cdot 6} a^2 = \frac{2^{15} \cdot 3^7}{5^{12}} a^2,$$

and from parts g and i, we have

$$\langle 2, 1, \pm 1 | \vec{r} | 3, 0, 0 \rangle = \langle 2, 1, \pm 1 | x | 3, 0, 0 \rangle \pm i \langle 2, 1, \pm 1 | y | 3, 0, 0 \rangle,$$

so the total transition rate is the sum of the x and y induced rates, and is twice as large as the individual x and y matrix elements squared:

$$|\langle 2, 1, \pm 1 | \vec{r} | 3, 0, 0 \rangle|^2 = 2 \left[\mp \frac{2^7 \cdot 3^4}{5^6 \sqrt{3}} a \right]^2 = \frac{2^{15} \cdot 3^7}{5^{12}} a^2.$$

Consequently, we conclude that the three decay rates are equal:

$$|\langle 2, 1, 0 | \vec{r} | 3, 0, 0 \rangle|^2 = |\langle 2, 1, 1 | \vec{r} | 3, 0, 0 \rangle|^2 = |\langle 2, 1, -1 | \vec{r} | 3, 0, 0 \rangle|^2.$$

4.(k) The spontaneous emission rates are given by

$$A = \frac{\omega^3 |q \langle \psi_b | \vec{r} | \psi_a \rangle|^2}{3\pi\epsilon_0 \hbar c^3} \quad \text{where} \quad \omega = \frac{E_b - E_a}{\hbar}.$$

These are given by

$$\begin{aligned} A_{3,0,0 \rightarrow 2,1,0} &= \frac{[13.6/2^2 - 13.6/3^2]^3 \frac{1}{\hbar^3} e^2}{3\pi\epsilon_0 \hbar c^3} | \langle 3, 0, 0 | \vec{r} | 2, 1, 0 \rangle |^2 \\ &= \left(\frac{e^2}{4\pi\epsilon_0} \right) \frac{4}{3} \frac{1}{\hbar^4 c^3} \left[\frac{13.6}{4} - \frac{13.6}{9} \right]^3 \frac{2^{15} \cdot 3^7}{5^{12}} a^2 \\ &= (1.440 \text{ eV} \cdot \text{nm}) \frac{4 (2\pi)^4}{3 \hbar^4 c^3} [3.40 - 1.51]^3 (\text{eV})^3 0.294 a^2 \\ &= \frac{(1.440 \text{ eV} \cdot \text{nm})}{(hc)^3} \frac{64\pi^4}{3h} [1.89]^3 \text{ eV}^3 (0.294)(0.0529 \text{ nm})^2 \\ &= \frac{(1.440 \text{ eV} \cdot \text{nm})}{(1.240 \times 10^3 \text{ eV} \cdot \text{nm})^3} \frac{2078.06}{h} [6.75] (0.294)(0.00280) \text{ eV}^3 \text{ nm}^2 \\ &= \frac{(1.440 \text{ eV} \cdot \text{nm})}{1.907 \times 10^9 \text{ eV}^3 \cdot \text{nm}^3} \frac{11.547}{h} \text{ eV}^3 \text{ nm}^2 \\ &= \frac{8.72^{-9} \text{ eV}}{4.136 \times 10^{-15} \text{ eV} \cdot \text{s}} \\ &= 2.11 \times 10^6 \text{ s}^{-1} \end{aligned}$$

$$\Rightarrow \tau_{3,0,0 \rightarrow 2,1,0} = \frac{1}{A} = 4.75 \times 10^{-7} \text{ s}.$$

The spontaneous emission rates for $\langle 2, 1, 1 | \vec{r} | 3, 0, 0 \rangle$ and $\langle 2, 1, -1 | \vec{r} | 3, 0, 0 \rangle$ are calculated similarly, and since the matrix elements are identical in value, we find:

$$A_{3,0,0 \rightarrow 2,1,1} = A_{3,0,0 \rightarrow 2,1,-1} = A_{3,0,0 \rightarrow 2,1,0} = 2.11 \times 10^6 \text{ s}^{-1}.$$

So the rate via each path is the same:

$$\begin{aligned} \tau_{3,0,0 \rightarrow 2,1,1} &= \frac{1}{A} = 4.75 \times 10^{-7} \text{ s} \\ \tau_{3,0,0 \rightarrow 2,1,-1} &= \frac{1}{A} = 4.75 \times 10^{-7} \text{ s} \\ \tau_{3,0,0 \rightarrow 2,1,0} &= \frac{1}{A} = 4.75 \times 10^{-7} \text{ s}, \end{aligned}$$

and the total decay rate is set by

$$A_T = 3(2.11 \times 10^6 \text{ s}^{-1}) = 6.33 \times 10^6 \text{ s}^{-1},$$

which gives us the lifetime

$$\tau_T = \frac{1}{A_T} = 1.58 \times 10^{-7} \text{ s}.$$

Fermi's Summary

24- Emission and absorption of radiation.

(1) $\mathcal{H}_0 = e B z \cos \omega t$

B = amplitude,

at $t=0$ atom in state n . From (23-(10))

(2) $a_m(t) = -\frac{i}{\hbar} e B z_{mn} \int_0^t \cos \omega t e^{i \omega_{mn} t} dt$

$\omega_{mn} = \frac{E^{(m)} - E^{(n)}}{\hbar} > 0$

$\cos \omega t = \frac{e^{i \omega t} + e^{-i \omega t}}{2}$

$\frac{m}{\hbar \omega_{mn}}$
 $\frac{m}{\hbar \omega}$
 this term only important when

$\rightarrow \omega \approx \omega_{mn}$ then
 $a_m(t) \approx -\frac{i e B}{2 \hbar} z_{mn} \int_0^t e^{i(\omega_{mn} - \omega)t} dt =$
 $= + \frac{e B}{2 \hbar} z_{mn} \frac{e^{-i(\omega - \omega_{mn})t} - 1}{\omega - \omega_{mn}}$

(3) $|a_m(t)|^2 = \frac{e^2 B^2}{\hbar^2} |z_{mn}|^2 \frac{\sin^2 \frac{t}{2} (\omega - \omega_{mn})}{(\omega - \omega_{mn})^2}$
 Light intensity = $\frac{c B^2}{8 \pi}$

Comments on resonance

Absorption from continuum overlapping ω_{mn}

(4) $\frac{c B^2}{8 \pi} = \frac{dI}{d\omega} d\omega$ Substitute in (3), then $\int d\omega$
 use $\int \frac{\sin^2 \alpha x}{x^2} dx = \pi \alpha$

$|a_m|^2 = t \times \frac{4 \pi^2 e^2}{c \hbar^2} |z_{mn}|^2 \frac{dI}{d\omega}$

$\omega =$ ang. frequency
not solid angle!

(5) Rate of absorption = $\frac{4 \pi^2 e^2}{c \hbar^2} |z_{mn}|^2 \frac{dI}{d\omega}$

For isotropic radiation of volume energy density $u(\omega) d\omega$

(6) Rate of absorption = $\frac{4 \pi^2 e^2}{3 \hbar^2} |\vec{z}_{mn}|^2 u(\omega_{mn})$

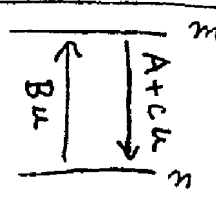
factor 1/3 from averaging over directions of polarization

Relationship between emission & absorption could be derived from quantum electrodynamics - However simpler to use Einstein's A & B method

Rate of $n \rightarrow m$ $B u(\omega) N(n) =$

From (6)

(7) $B = \frac{4\pi^2 e^2}{3\hbar^2} |\vec{x}_{mn}|^2$



This B is a coefficient. Has nothing to do with B of page 1

Rate of $m \rightarrow n$ $[A + C u(\omega)] N(m)$

This is number of atoms in state n or m

For thermal equilibrium

(8) $\frac{N(m)}{N(n)} = e^{-\frac{E(m) - E(n)}{kT}} = e^{-\frac{\hbar \omega_{mn}}{kT}}$ Boltzmann distribution

At equilibrium: Rate $n \rightarrow m$ = Rate $m \rightarrow n$

(9) $\frac{A}{B u(\omega)} + \frac{C}{B} = \frac{N_n}{N_m} = e^{\frac{\hbar \omega}{kT}}$

Planck's law

(10) $u = \frac{\hbar \omega^3 / \pi^2 c^3}{e^{\frac{\hbar \omega}{kT}} - 1}$

$\frac{\pi^2 c^3}{\hbar \omega^3} \frac{BA}{AB} (e^{\frac{\hbar \omega}{kT}} - 1) + \frac{C}{B} = e^{\frac{\hbar \omega}{kT}}$

Must hold at all T's Therefore:

$\frac{\pi^2 c^3}{\hbar \omega^3} \frac{BA}{AB} = 1$ $\frac{C}{B} = 1$

Einstein's relations

(11) $A = \frac{\hbar \omega^3}{\pi^2 c^3} B ; C = B$ then from (7)

(12) $\frac{1}{\tau} = A = \frac{4}{3} \frac{e^2 \omega^3}{\hbar c^3} |\vec{x}_{mn}|^2$ for spontaneous transitions

(12) generalized to many particles by change

$$(13) \quad e \vec{x} \rightarrow \sum e_i \vec{x}_i \quad (\text{sum to all particles})$$

$$(14) \quad \frac{1}{r} = \frac{4}{3} \frac{\omega^3}{\hbar c^3} \left| \sum e_i \langle m | \vec{x}_i | n \rangle \right|^2$$

Intensity of radiation proportional to square of matrix element of coordinates (for one electron) or of electric moment (13) for several charged particles.

Discuss - Limitations to validity of (12)

dimensions of atom $\ll \lambda$ of radiation
 Quadrupole radiation

Case of central forces - Selection rules (Subsect 7)

Spherical harmonics identities

$$\sqrt{\frac{8\pi}{3}} Y_{11} Y_{\ell, m-1} = \sqrt{\frac{(\ell+m)(\ell+1+m)}{(2\ell+1)(2\ell+3)}} Y_{\ell+1, m} - \sqrt{\frac{(\ell-m)(\ell+1-m)}{(2\ell+1)(2\ell-1)}} Y_{\ell-1, m}$$

$$(15) \quad \sqrt{\frac{4\pi}{3}} Y_{10} Y_{\ell, m} = \sqrt{\frac{(\ell+1)^2 - m^2}{(2\ell+1)(2\ell+3)}} Y_{\ell+1, m} + \sqrt{\frac{\ell^2 - m^2}{(2\ell+1)(2\ell-1)}} Y_{\ell-1, m}$$

$$\sqrt{\frac{8\pi}{3}} Y_{1,-1} Y_{\ell, m+1} = \sqrt{\frac{(\ell-m)(\ell+1+m)}{(2\ell+1)(2\ell+3)}} Y_{\ell+1, m} - \sqrt{\frac{(\ell+m)(\ell+1+m)}{(2\ell+1)(2\ell-1)}} Y_{\ell-1, m}$$

$$(16) \quad \left\{ \begin{array}{l} \sqrt{\frac{8\pi}{3}} Y_{11} = -\sin\vartheta e^{i\varphi} \\ \sqrt{\frac{4\pi}{3}} Y_{10} = \cos\vartheta \\ \sqrt{\frac{8\pi}{3}} Y_{1,-1} = \sin\vartheta e^{-i\varphi} \end{array} \right.$$

Follows: The matrix elements of the coordinates vanish unless

$$(17) \quad \ell' = \ell \pm 1 \quad \text{and} \quad m' = \begin{array}{l} m \pm 1 \\ \text{or } m \end{array}$$

Selection rules

Matrix elements

$$(18) \begin{cases} \langle n', l+1, m+1 | x+iy | n, l, m \rangle = -\gamma \sqrt{\frac{(l+m^2)(l+1+m)}{(2l+1)(2l+3)}} \\ \langle n', l+1, m+1 | x-iy | n, l, m \rangle = 0 \\ \langle n', l+1, m | z | n, l, m \rangle = \gamma \sqrt{\frac{(l+1)^2 - m^2}{(2l+1)(2l+3)}} \\ \langle n', l+1, m-1 | x+iy | n, l, m \rangle = 0 \\ \langle n', l+1, m-1 | x-iy | n, l, m \rangle = \gamma \sqrt{\frac{(l+1-m)(l+2-m)}{(2l+1)(2l+3)}} \end{cases}$$

$$(19) \quad \gamma = \int_0^{\infty} R_{nl}(r) R_{n', l+1}(r) r^3 dr$$

Derive

$$(20) \begin{cases} |\langle n', l+1, m+1 | \vec{x} | n, l, m \rangle|^2 + |\langle n', l+1, m | \vec{x} | n, l, m \rangle|^2 \\ + |\langle n', l+1, m-1 | \vec{x} | n, l, m \rangle|^2 = \frac{l+1}{2l+1} \gamma^2 \quad (\text{indep. of } m) \end{cases}$$

$$(21) \begin{cases} \text{Therefore: rate of transition} \\ (n, l, m) \rightarrow (n', l+1, \text{any } m') \\ = \frac{4}{3} \frac{e^2 \omega^3}{\hbar c^3} \frac{l+1}{2l+1} \gamma^2 \end{cases} \quad \text{Comments on independence of } m$$

Similarly

$$(22) \begin{cases} \text{Rate}(n, l, m \rightarrow n', l-1, \text{any } m) = \\ = \frac{4}{3} \frac{e^2 \omega^3}{\hbar c^3} \frac{l}{2l-1} \left\{ \int_0^{\infty} R_{nl}(r) R_{n', l-1}(r) r^3 dr \right\}^2 \end{cases}$$

Example - Life time of $2p$ state of hydrogen

$$R_{1s}(r) = \frac{2}{a^{3/2}} e^{-r/a}; \quad R_{2p}(r) = \frac{1}{\sqrt{24}a^3} \frac{r}{a} e^{-r/2a}$$

$$Y = \int R_{1s} R_{2p} r^3 dr = \frac{192\sqrt{2}}{243} a$$

$$\begin{aligned} \text{Rate}(2p \rightarrow 1s) &= \frac{294912}{177147} \frac{e^2 \omega^3 a^2}{hc^3} & \omega &= \frac{3}{4} \frac{me^4}{2\hbar^3} \\ &= \frac{1152}{6561} \left(\frac{e^2}{hc} \right)^3 \left(\frac{me^4}{2\hbar^3} \right) & a &= \frac{\hbar^2}{me^2} \\ &= 1.41 \times 10^9 \text{ sec}^{-1} & \frac{e^2}{hc} &= \frac{1}{137} \end{aligned}$$

$\frac{R_{\text{Ryd}}}{\hbar} = 2.067 \times 10^{16} \text{ sec}^{-1}$

Topics for discussion

Permitted & forbidden lines

Metastable states

Generalization of selection rules

Irradiation by a linear oscillator

Sum rule & effective number of electrons

Polarization of emitted light

Golden Rule Number 1

Light and Atoms:

Scattering

Diffraction anomalous fine structure: Unifying x-ray diffraction and x-ray absorption with DAFS

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Abstract

This chapter describes a developing x-ray spectroscopic, structural, and crystallographic method called the diffraction anomalous fine structure technique (DAFS), which measures the elastic Bragg reflection intensities versus photon energy. This new method combines the long-range order and crystallographic sensitivities of x-ray diffraction with the spectroscopic and short-range order sensitivities of x-ray absorption techniques.

In the extended fine structure region, DAFS provides the same short-range structural information as EXAFS: the bond lengths, coordination numbers, neighbor types, and bond disorders for the atoms surrounding the resonantly scattering atoms. In the near-edge region, DAFS provides the same structural and spectroscopic sensitivities as XANES: the valence, empty orbital and bonding information for the resonant atoms.

Because DAFS combines the capabilities of diffraction, EXAFS and XANES into a single technique, it has two enhanced sensitivities compared to the separate techniques: (1) Wavevector selectivity. DAFS can provide EXAFS- and XANES-like information for the specific subset of atoms selected by the diffraction condition. (2) Site selectivity. DAFS can provide site-specific absorption-like spectroscopic and structural information for the inequivalent sites of a single atomic species within the unit cell.

We present the theory, experimental methods, and analysis techniques that we have developed, and we show that they work very precisely for Cu metal. We also show that DAFS can yield its enhanced sensitivities while maintaining a precision comparable to that of the best EXAFS and XANES measurements. Wavevector selectivity is demonstrated with a study of a buried 400Å thick $\text{In}_{0.2}\text{Ga}_{0.8}\text{As}$ layer which is wavevector separated from its GaAs substrate and cap. Site selectivity is demonstrated with a study of the two inequivalent Cu sites in a 2400Å thick $\text{YBa}_2\text{Cu}_3\text{O}_{6.6}$ superconductor film.

1. INTRODUCTION

The presence of oscillatory fine structure in the x-ray absorption spectra of atoms in solids has been known for over 70 years [1], and the analogous fine structure in x-ray diffraction has been known for almost 40 years [2]. It was not until intense synchrotron radiation sources became available, however, that the extended x-ray absorption fine

structure technique (EXAFS) [3] became a routine spectroscopic method. In the last few years, with the development of modern multiple scattering MS-XAFS theory and analysis techniques, EXAFS has realized its potential as an accurate probe of distances and structure [4]. Recently, again because of synchrotron radiation sources, the diffraction anomalous fine structure technique (DAFS) has started to be used as a combined spectroscopic, structural, and crystallographic method [5–11]. Because the diffraction and absorption fine structures are closely related by unitarity and causality, the same sophisticated MS-XAFS techniques can be applied to DAFS measurements. This chapter describes the theoretical and experimental considerations behind DAFS, explains how DAFS measurements can be analyzed using unitarity and causality to relate and to isolate the real and imaginary components of the scattering amplitude, and illustrates how generalized MS-DAFS theory can be used to analyze the isolated diffraction fine structure.

The common physical origin of DAFS and XAFS is illustrated schematically in Fig. 1. In both DAFS and XAFS, the incoming photon promotes an electron from a compact

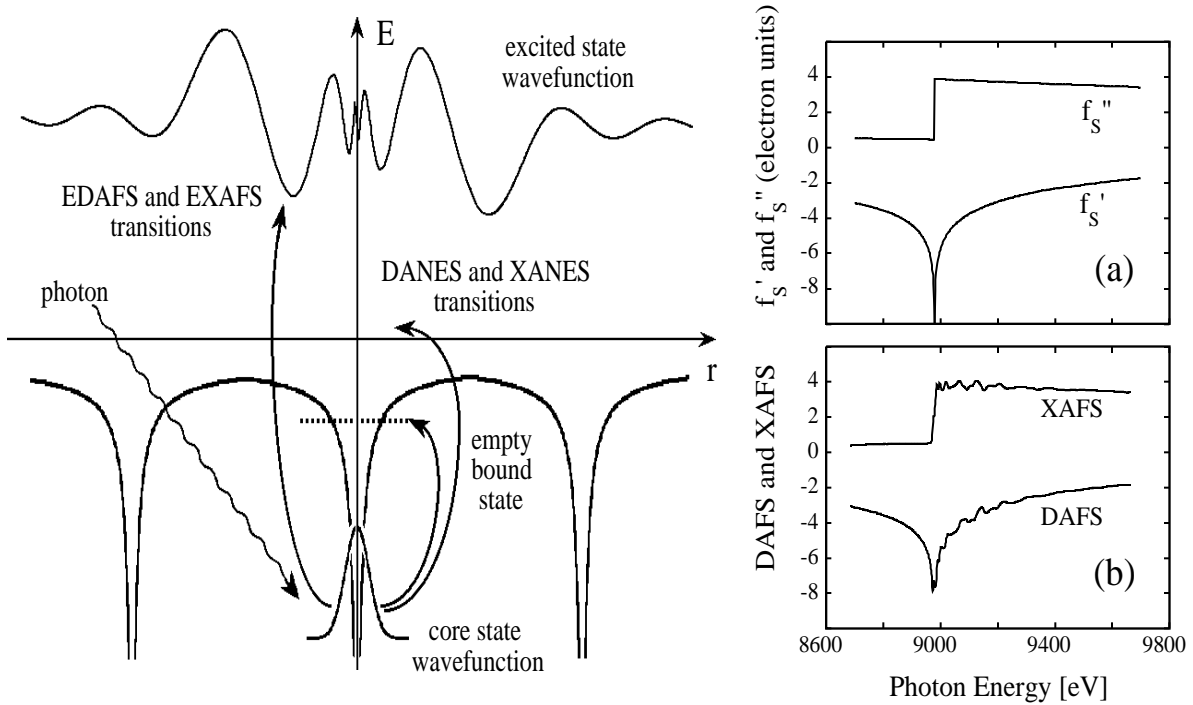


Figure 1. The one-electron picture for the origin of the DAFS and XAFS fine structure. The excited state wavefunction is shown for a 200 eV photoelectron in a fully screened Cu atom without neighbors. When neighbors are present, the wavefunction is changed, and these changes versus photon energy produce the oscillatory DAFS and XAFS signals. (a) The calculated Cromer-Lieberman real and imaginary scattering amplitudes for Cu have a smooth cusp in f'_s and a step in f''_s . Throughout this chapter, the steps are shown in their conventional positive form [12]. (b) The measured DAFS and XAFS signals both have extended oscillations versus the photon energy. These extended oscillations provide structural and spectroscopic information about the atoms and their neighbors.

core state to an empty continuum state, or to an empty bound state. When the electron is promoted to the continuum states at least 30 eV above the edge, the absorption and diffraction oscillatory fine structure signals are called EXAFS and EDAFS, respectively [3]. When the electron is promoted to an empty bound state, or to the continuum states below about 30 eV, the fine structure signals are called XANES and DANES [3]. The intensity of the DAFS and XAFS signals for each photon energy depends on the matrix elements between the ground state wavefunction (the core state) and the excited state wavefunction. For the EDAFS and EXAFS signals, the intensities depend on how well the excited state wavefunctions fit into the “effective boxes” produced by the central atom and the neighbors. For a simple box, these interference effects would vary as $\sin(2KR_j + \Phi_j)$, where the photoelectron wavenumber $K = (2m(E - E_0)/\hbar^2)^{\frac{1}{2}}$ depends on the difference between the photon energy, E , and the electron binding energy, E_0 . Note that the interference effects depend on the size of the box, which is set by the bond length, R_j , between the central atom and the neighboring atom. Thus in this simple case, the oscillatory fine structure would consist of a sum over all the neighbors, labeled by j , of $\sin(2KR_j + \Phi_j)$ terms. Because the walls of the “real boxes” are formed by the screened excited central atom and by the surrounding atoms, there are photoelectron wavenumber dependent phase shifts, $\Phi_j(K) = \phi_j(K) + 2\delta_c(K)$, that slightly complicate the analysis. Fortunately, the recent theoretical MS-XAFS advances have made it possible to calculate the EDAFS and EXAFS signals precisely, and the full power of these techniques can now be obtained routinely [4].

The physical origin of the causal relationship between the real and imaginary components of the forward scattering amplitude, and the connection between the forward dispersion relations and the analyticity of the scattering amplitude, are discussed very clearly by Toll [13]. Toll uses a proof by contradiction (see Fig. 2): Assume that a system could absorb some frequency components without disturbing any of the other frequency components, and consider the incoming Gaussian packet shown in Fig. 2a, which is composed of many different frequency components which extend over all time. Its central frequency components are shown in Fig. 2b. If the hypothetical system could absorb just these central components, with no change in the remaining components, then the output would be the original packet minus the absorbed components shown in Fig. 2c. This, however, would clearly violate causality because there would be an output before the incoming packet reaches the absorber. Therefore, the system cannot absorb some frequency components without phase shifting the remaining components to maintain zero output before the input arrives. *Absorption and dispersion are intimately connected.* Figure 2d shows the hypothetical output if the central frequency components are phase shifted by the imaginary component of the system’s non-forward scattering amplitude, instead of being absorbed. Again this would clearly violate causality. *At a fixed momentum transfer, the real and the imaginary components of the scattering amplitude are intimately connected.* For each incoming and outgoing direction, the complex scattering amplitude is an analytic function of the energy. Consequently, the real and imaginary components of the scattering amplitude are related by Cauchy’s theorem: they are a Kramers-Kronig or Hilbert transform pair.

The argument given above explains why the real and imaginary components of the scattering amplitude in any fixed direction are so closely related. To establish the con-

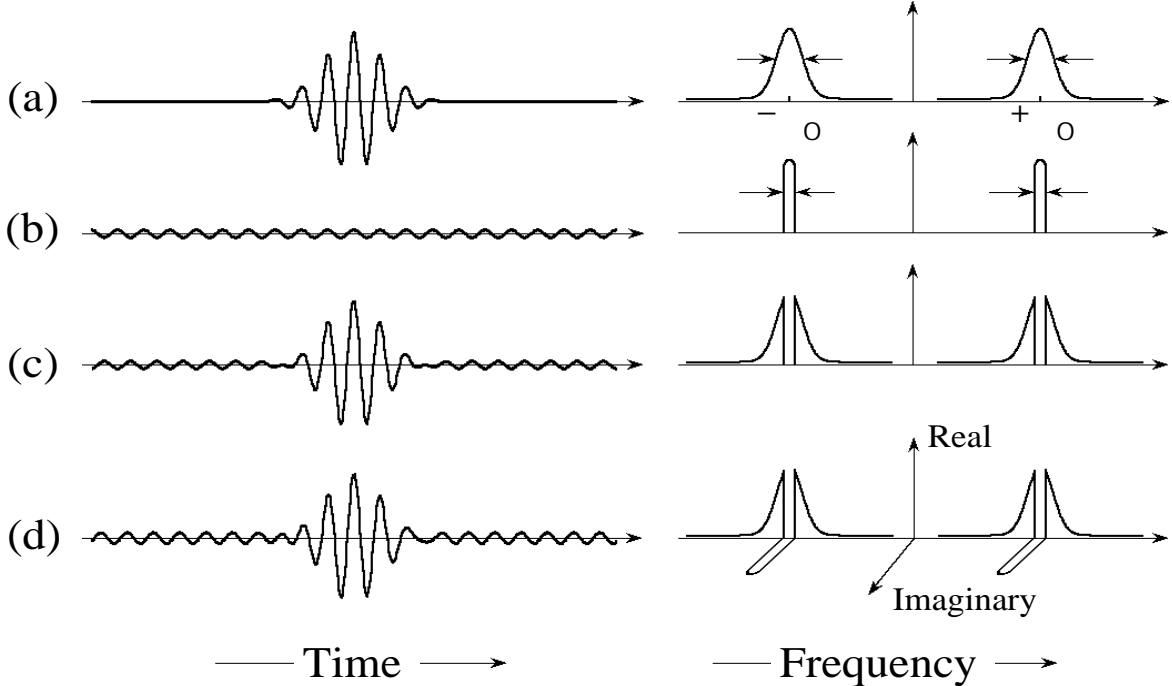


Figure 2. The acausal behavior that would be produced if a system could selectively absorb, or could selectively phase shift, some of the frequency components of a Gaussian wave packet without affecting any of the other frequency components. Both the time and frequency domain signals are shown for: (a) The incident Gaussian packet with $\Delta\omega/\omega_0 = 0.1$. (b) The central frequency components with $\delta\omega/\omega_0 = 5 \times 10^{-3}$, which are to be selectively absorbed or phase shifted. For visual clarity, $\delta\omega$ is shown larger than its actual size in the frequency domain; all of the time domain signals are shown without distortion. (c) The acausal behavior that would be produced by absorbing only the central frequency components. (d) The acausal behavior that would be produced by phase shifting only the central frequency components.

nection between DAFS and XAFS, however, we need a relationship between the forward and non-forward amplitudes. The necessary connection comes from unitarity: To conserve probability, the incoming packet must be either transmitted, absorbed, scattered with a phase shift, or scattered without a phase shift. The optical theorem (a special case of unitarity) tells us that the sum of all the outgoing and absorbed waves must equal the incoming wave. For each photon energy, the optical theorem connects the angular integral of the elastic scattering (DAFS) over all directions to the absorption (XAFS). In general, this is the only connection. In the special case of pure dipole scattering, the scattering amplitude has the same energy dependence in all directions. Consequently, for pure dipole scattering the energy dependence of the imaginary component of the scattering amplitude is identical to that of the absorption, and the energy dependence of the real component is given by the Kramers-Kronig transform of the absorption. Because x-ray scattering is often predominantly dipolar, DAFS and XAFS can usually be related by angle independent Kramers-Kronig transforms.

2. DAFS THEORY

This section describes the resonant and non-resonant atomic scattering amplitudes, and shows how the atomic components combine to produce the observed smooth and oscillatory DAFS and XAFS signals from a crystal.

2.1. Form of the Thomson and anomalous amplitudes

In non-relativistic quantum mechanics, neglecting the magnetic scattering terms, the total atomic scattering amplitude, $f = f_0 + \Delta f$, for photons with energy $E = \hbar\omega$ and with incident and scattered momenta \mathbf{k}_1 and \mathbf{k}_2 , is the sum of the non-resonant Thomson scattering amplitude, f_0 , and the ‘‘anomalous’’ scattering amplitude, Δf (see Fig. 3).

The Thomson and anomalous scattering amplitudes are given, in terms of the classical single electron scattering amplitude, $r_0 = e^2/mc^2$, by [12, 14–16]

$$f_0(\mathbf{k}_2 - \mathbf{k}_1) = f_0(\mathbf{Q}) = -r_0 \hat{\mathbf{e}}_2^* \cdot \hat{\mathbf{e}}_1 \sum_j \langle j | e^{-i(\mathbf{k}_2 - \mathbf{k}_1) \cdot \mathbf{r}} | j \rangle, \quad (1)$$

$$\begin{aligned} \Delta f(\mathbf{k}_1, \mathbf{k}_2, E) &= f'(\mathbf{k}_1, \mathbf{k}_2, E) + i f''(\mathbf{k}_1, \mathbf{k}_2, E) \\ &= \frac{r_0}{m} \sum_j \sum_n \frac{\langle j | \hat{\mathbf{e}}_2^* \cdot \mathbf{p} e^{-i\mathbf{k}_2 \cdot \mathbf{r}} | n \rangle \langle n | \hat{\mathbf{e}}_1 \cdot \mathbf{p} e^{+i\mathbf{k}_1 \cdot \mathbf{r}} | j \rangle}{E_n - E_j - \hbar\omega + (\Delta_n - \frac{1}{2}i\Gamma_n)} \\ &\quad + \frac{\langle j | \hat{\mathbf{e}}_1 \cdot \mathbf{p} e^{+i\mathbf{k}_1 \cdot \mathbf{r}} | n \rangle \langle n | \hat{\mathbf{e}}_2^* \cdot \mathbf{p} e^{-i\mathbf{k}_2 \cdot \mathbf{r}} | j \rangle}{E_n - E_j + \hbar\omega}. \end{aligned} \quad (2)$$

The self-energy corrections that produce the Lamb-shift $\Delta_n(E_n + \hbar\omega)$ and the linewidth $\Gamma_n(E_n + \hbar\omega)$ of the resonant term are shown explicitly [15].

The Thomson amplitude is a scalar which depends on the photon momentum transfer, $\hbar\mathbf{Q} = \hbar(\mathbf{k}_2 - \mathbf{k}_1)$, and on the photon polarization factors, $\hat{\mathbf{e}}_2^* \cdot \hat{\mathbf{e}}_1$, but is independent of the photon energy. The Thomson amplitude is proportional to the Fourier transform of the atom’s electronic charge distribution. In contrast, the anomalous amplitude depends separately on the incident and scattered wavevectors, \mathbf{k}_1 and \mathbf{k}_2 , and also depends on the photon energy, E . Thus, in general, Δf is a tensor which depends on the matrix elements between the ground state and the virtual intermediate states, and is not proportional to the Fourier transform of the total or subshell charge density [17]. It has been established experimentally, however, that the \mathbf{k}_1 and \mathbf{k}_2 dependencies of anomalous scattering are often small, and the full photon energy- and momenta-dependent $\Delta f(\mathbf{k}_1, \mathbf{k}_2, E)$ is conventionally [14] approximated by its momenta-independent forward scattering limit, denoted $\Delta f(E) = f'(E) + i f''(E)$. Consequently, the total atomic scattering amplitude, f , depends on the photon energy, E , via its f' and f'' terms, and on the wavevector transfer, \mathbf{Q} , via its f_0 term.

2.2. Separation of the smooth and oscillatory DAFS terms

For an atom in a solid, the total atomic scattering amplitude can be subdivided into smooth and oscillating fine structure components,

$$f(\mathbf{Q}, E) = [f_0(\mathbf{Q}) + f'_s(E) + i f''_s(E)] + [f''_s(E) \tilde{\chi}(E)]. \quad (3)$$

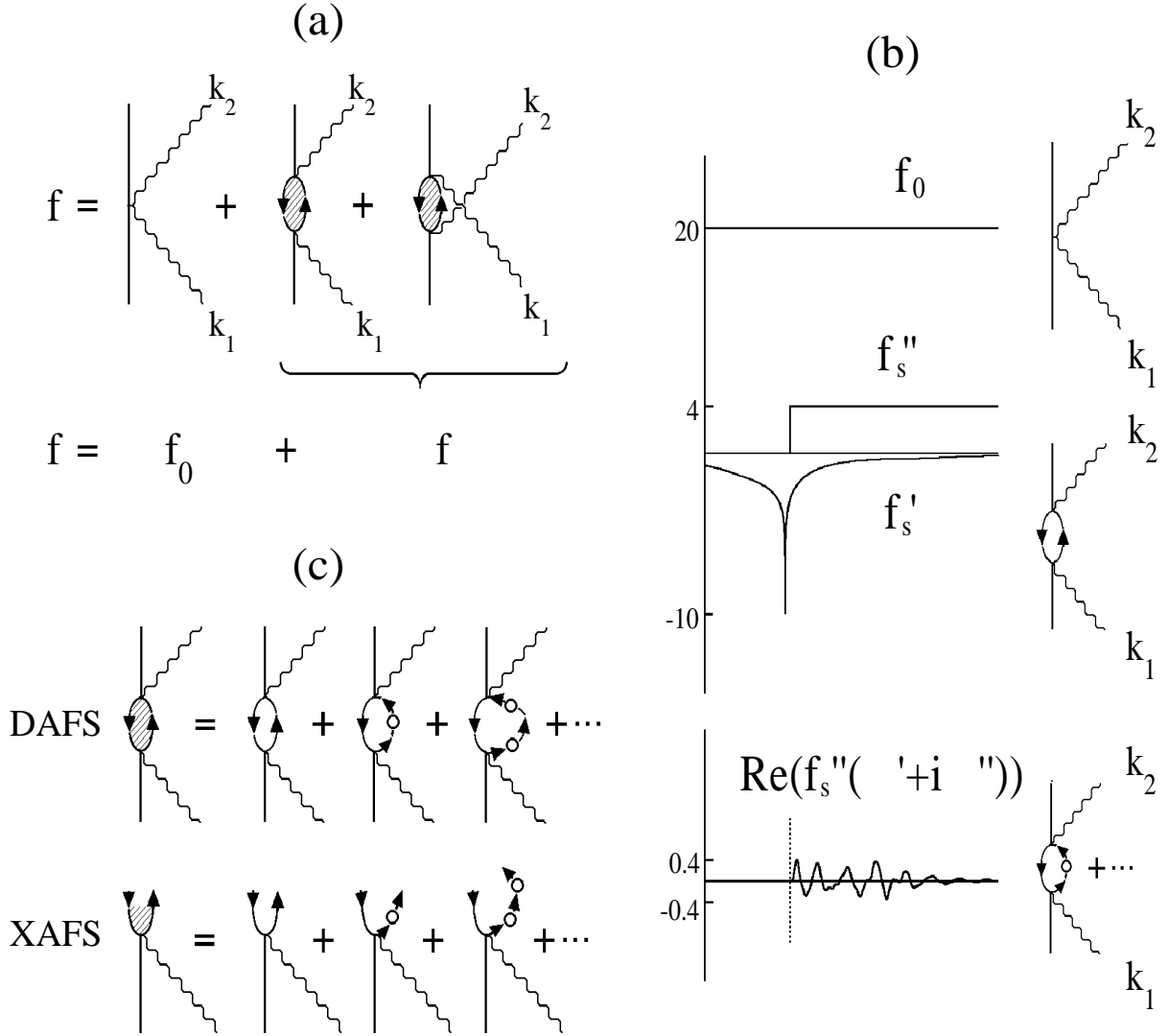


Figure 3. (a) The total nonrelativistic photon-atom scattering amplitude, f , is the sum of three contributions: the non-resonant Thomson amplitude, f_0 , and the resonant and antiresonant amplitudes that together are called the “anomalous” amplitude, Δf , which can be divided into smooth and oscillatory components: $\Delta f = [f_s' + if_s''] + [f_s''(\chi' + i\chi'')]$. (b) The relative sizes of the contributions due to f_0 , f_s' , f_s'' and $f_s''(\chi' + i\chi'')$ are shown for Cu in electron units [12]. (c) The DAFS and XAFS signals are generated by the quantum mechanical interference of the photoelectrons moving through the atoms. In XAFS there is a real photoelectron in the final state, and the interference can be calculated as a sum over photoelectron reflections from the neighbors. In DAFS there is a virtual photoelectron in the transient intermediate state, and the interference can be calculated as a sum over virtual photoelectron reflections from the neighbors. To calculate the DAFS and XAFS signals, we must sum over all possible photoelectron paths. The sum over paths without reflections from the neighbors produces the smooth $f_s' + if_s''$ component. The sum over paths with reflections produces the oscillatory $f_s''(\chi' + i\chi'')$ component.

**Back to
Golden Rule
Number 2**

Nuclear Physics

Fermi's Theory of Beta Decay

Fermi Theory of Beta Decay

In 1930, Wolfgang Pauli postulated the existence of the [neutrino](#) to explain the continuous [distribution of energy](#) of the electrons emitted in [beta decay](#). Only with the emission of a third particle could momentum and energy be [conserved](#). By 1934, Enrico Fermi had developed a theory of beta decay to include the neutrino, presumed to be massless as well as chargeless.

Treating the beta decay as a transition that depended upon the strength of coupling between the initial and final states, Fermi developed a relationship which is now referred to as [Fermi's Golden Rule](#):

$$\lambda_{if} = \frac{2\pi}{\hbar} |M_{if}|^2 \rho_f$$

Fermi's Golden Rule

Transition probability Matrix element for the interaction Density of final states

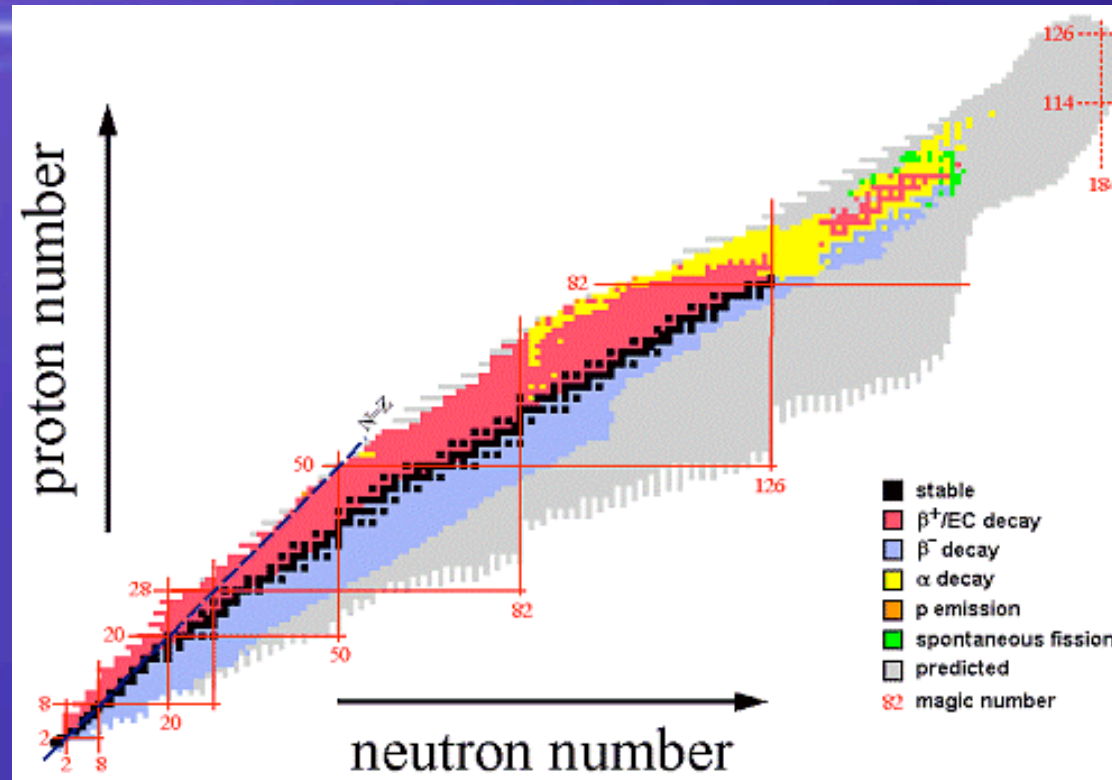
Straightforward in concept, Fermi's Golden Rule says that the transition rate is proportional to the strength of the coupling between the initial and final states factored by the density of final states available to the system. But the nature of the interaction which led to beta decay was unknown in Fermi's time (the [weak interaction](#)). It took some 20 years of work (Krane) to work out a detailed model which fit the observations. The nature of that model in terms of the distribution of electron momentum p is summarized in the relationship below.

The Fermi Selection Rule for Beta Decay

(`fer·me si`lek·shen `rül)

**There is no change in the total
angular momentum or the parity
of the nucleus**

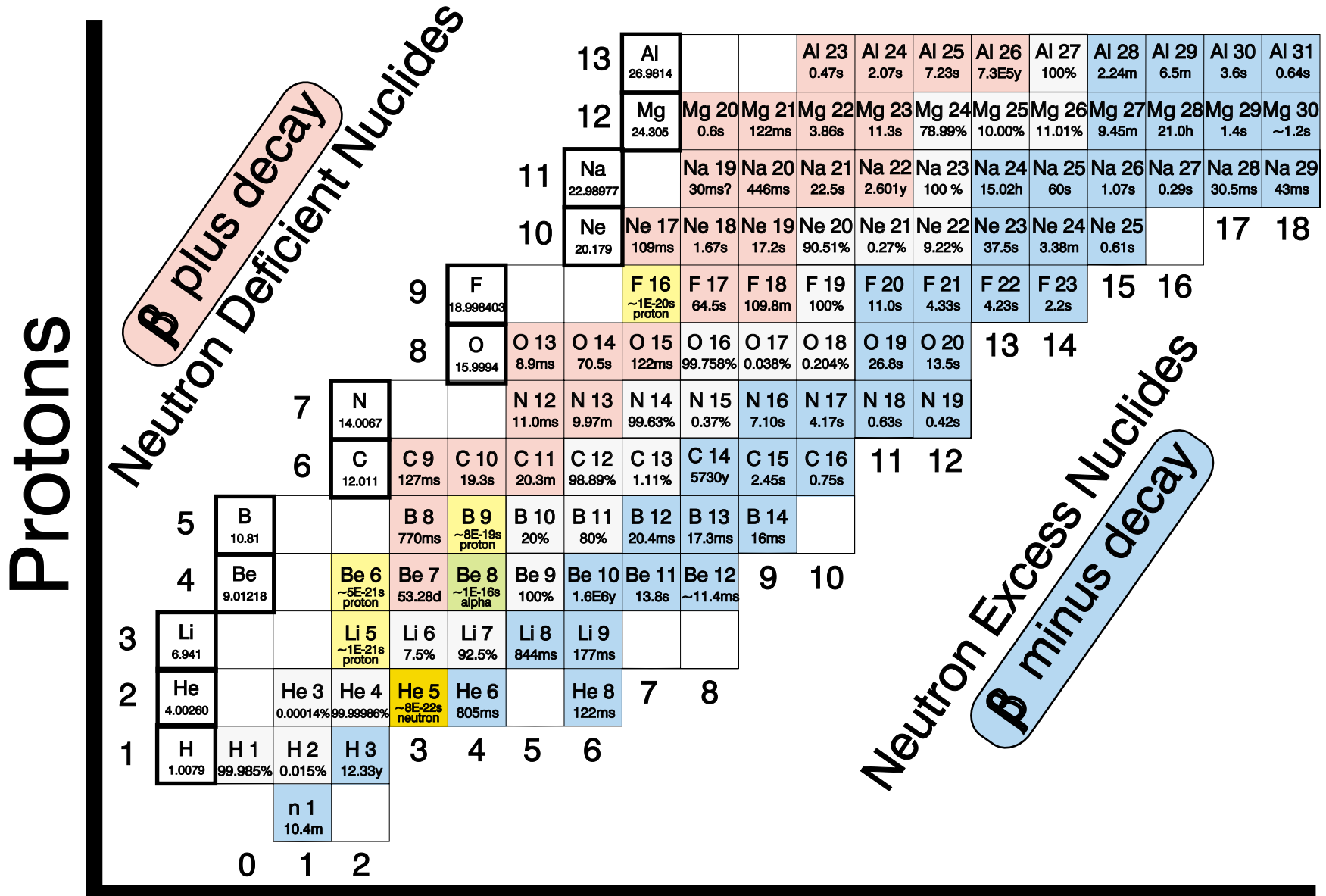
Requirements - I



1.) $m(A,Z) > m(A,Z+2)$

2.) Single beta decay must be forbidden ($m(A,Z) < m(A,Z+1)$)
or at least strongly suppressed (large change in angular momentum)

CHART OF THE NUCLIDES

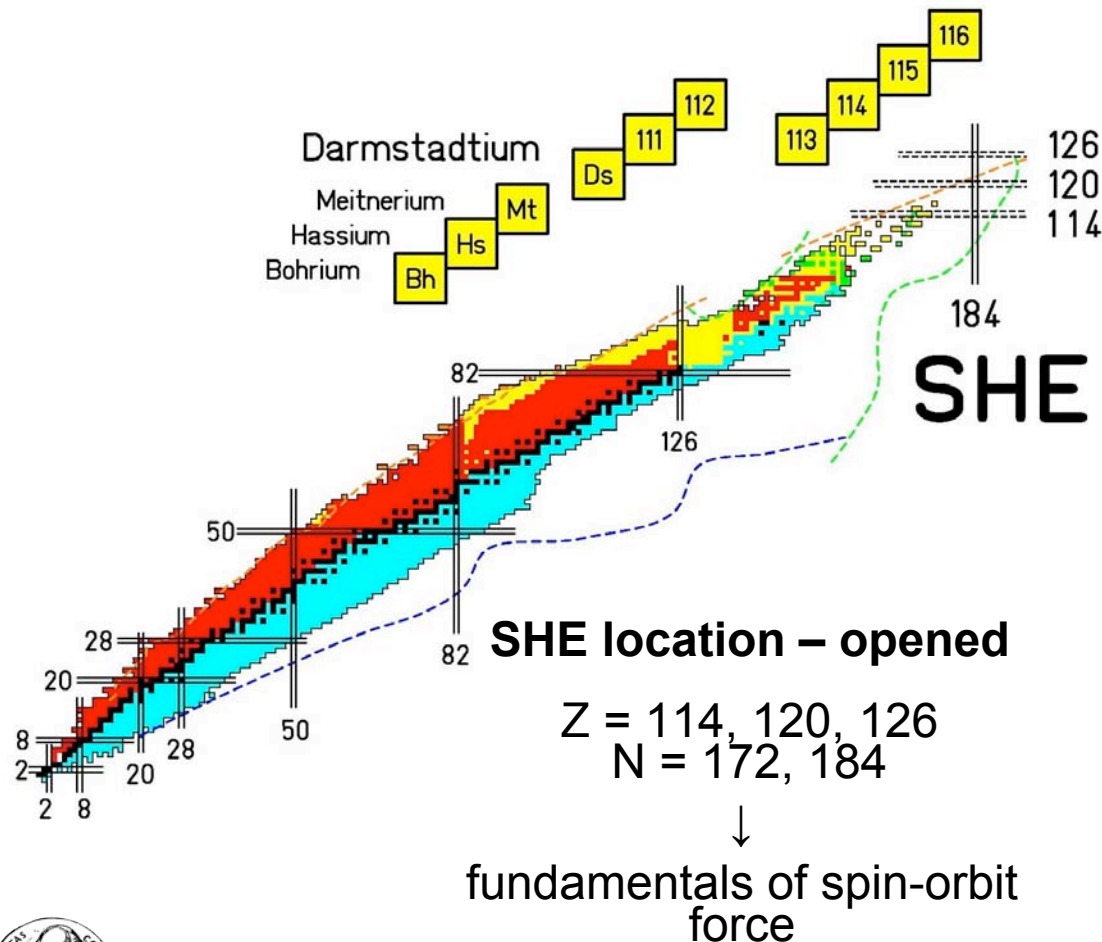


Neutrons

Physical Motivation

Predictions of the island of SHE

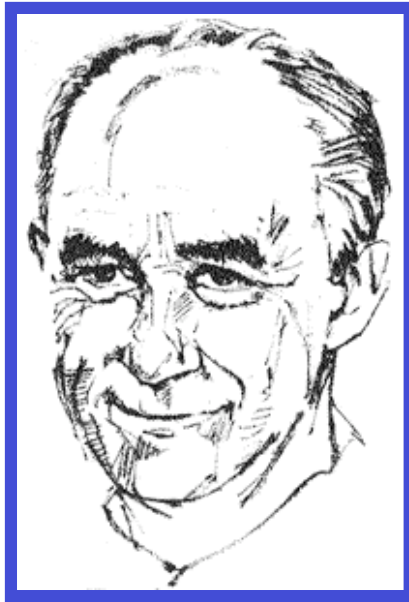
- nuclei beyond Fm exist only due to shell effects



- predictions of highly stabilized SHE ($T_{\text{theo}} \sim \text{min } -y$)
- failure to synthesize SHE by reactions of the type $\text{Pb} + \text{Pb}$ ($\text{U} + \text{U}$)

- 1) Production of SHE via “hot” and “cold” fusion
- 2) Systematic study of nuclear structure of transfermium isotopes





Enrico Fermi Centennial Symposium

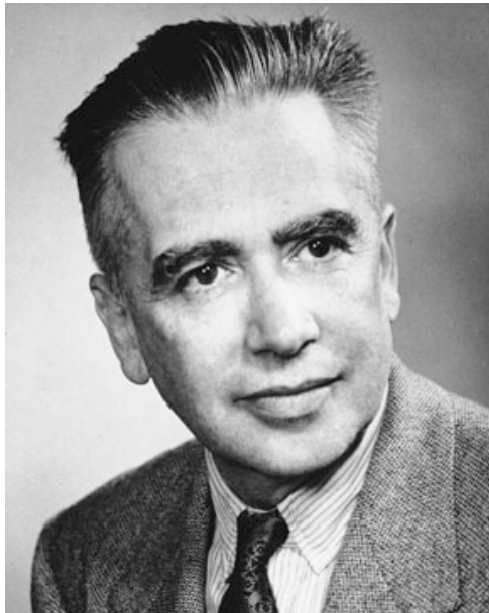
September 28, 2001

Fermi National Accelerator Laboratory

Weak Interactions

Stuart Freedman

University of California at Berkeley



Emilio Segre
Physics 115

Quantum Mechanics

E. Fermi Physics 341
Winter 1954

1-1

1- Optics - Mechanics analogy:

Dictionary	
Mass point	Wave packet
Trajectory	Ray
Velocity (V)	Group velocity (V)
No simple analog	Phase velocity (v)
Potential function of position U(x)	Refractive index (or v) function of position
(1) Energy (W) $W=W(v)$	Frequency (dispersive medium) $\nu(\nu, x)$

First: Trajectory = Ray
 ↓ ↓
 from Maupertuis from Fermat

$$(2) \int \sqrt{W-U} ds = \text{min}; \quad \int \frac{ds}{v} = \text{min} \quad (3)$$

Proof of Maupertuis:

$$\delta \int \sqrt{W-U} ds = \int \left(\sqrt{W-U} \delta ds - \frac{\delta U}{2\sqrt{W-U}} ds \right) = 0$$

$$\text{use } \delta ds = \int \frac{dx}{ds} \delta dx, \quad \delta U = \int \frac{\partial U}{\partial x} \delta x$$

and part. integr. Find minimum equations

$$\frac{d}{ds} \left(\sqrt{W-U} \frac{dx}{ds} \right) = - \frac{1}{2\sqrt{W-U}} \frac{\partial U}{\partial x}$$

$$\text{use } v = \sqrt{\frac{2}{m}} \sqrt{W-U}, \quad dt = \frac{ds}{v} = \sqrt{\frac{m}{2}} \frac{ds}{\sqrt{W-U}}$$

$$\rightarrow m \frac{d^2 x}{dt^2} = - \frac{\partial U}{\partial x} \quad \text{Therefore; (2) is true}$$

Proof of Fermat because of eq. of motion

$$\int \frac{ds}{v} = \text{min} \rightarrow \int \frac{ds}{\lambda} = \text{min} \rightarrow \int \frac{ds}{\lambda} = \text{min} \rightarrow \text{No of waves} = \text{min}$$

means no of waves stationary; hence positive interference.

E. Fermi's publications on the Weak Interaction

E. Fermi, "Tentative Theory of Beta Rays"
Letter Submitted to Nature (1933)

ANNO IV - VOL. II - N. 12

QUINDICINALE

31 DICEMBRE 1933 - XII

LA RICERCA SCIENTIFICA

ED IL PROGRESSO TECNICO NELL'ECONOMIA NAZIONALE

Tentativo di una teoria dell'emissione dei raggi "beta"

Note del prof. ENRICO FERMI

Riassunto: Teoria della emissione dei raggi β delle sostanze radioattive, fondata sull'ipotesi che gli elettroni emessi dai nuclei non esistano prima della disintegrazione ma vengano formati, insieme ad un neutrino, in modo analogo alla formazione di un quanto di luce che accompagna un salto quantico di un atomo. Confronto della teoria con l'esperienza.

Published in Nuovo Cimento and Zeitschrift fur Physik



Pauli's "Neutrino"

Dear Radioactive Ladies and Gentlemen:

Zurich, December 4, 1930

I beg you to receive graciously the bearer of this letter who will report to you in detail how I have hit on a desperate way to escape from the problems of the "wrong" statistics of the N and Li6 nuclei and of the continuous beta spectrum in order to save the "even-odd" rule of statistics and the law of conservation of energy. Namely the possibility that electrically neutral particles, which I would like to call neutrons might exist inside nuclei; these would have spin $1/2$, would obey the exclusion principle, and would in addition differ from photons through the fact that they would not travel at the speed of light. The mass of the neutron ought to be about the same order of magnitude as the electron mass, and in any case could not be greater than 0.01 proton masses. The continuous beta spectrum would then become understandable by assuming that in beta decay a neutron is always emitted along with the electron, in such a way that the sum of the energies of the neutron and electron is a constant. Now, the question is, what forces act on the neutron? The most likely model for the neutron seems to me, on wave mechanical grounds, to be the assumption that the motionless neutron is a magnetic dipole with a certain magnetic moment μ (the bearer of this letter can supply details). The experiments demand that the ionizing power of such a neutron cannot exceed that of a gamma ray, and therefore μ probably cannot be greater than e (10^{-13} cm). [e is the charge of the electron].

At the moment I do not dare to publish anything about this idea, so I first turn trustingly to you, dear radioactive friends, with the question: how could such a neutron be experimentally identified if it possessed about the same penetrating power as a gamma ray or perhaps 10 times greater penetrating power?

I admit that my way out may look rather improbable at first since if the neutron existed it would have been seen long ago. But nothing ventured, nothing gained. The gravity of the situation with the continuous beta spectrum was illuminated by a remark by my distinguished predecessor in office, Mr. DeBye, who recently said to me in Brussels, "Oh, that's a problem like the new taxes; one had best not think about it at all." So one ought to discuss seriously any way that may lead to salvation. Well, dear radioactive friends, weigh it and pass sentence! Unfortunately, I cannot appear personally in Tubingen, for I cannot get away from Zurich on account of a ball, which is held here on the night of December 6-7

With best regards to you and to Mr. Baek,

Your most obedient servant,
W. Pauli


Fermi's notes on QM

23-2

Important special case, at $t=0$ system in state n . Then $a_n(0)=1$, all other a 's are zero.

$$(10) \quad a_s(t) = -\frac{i}{\hbar} \int_0^t V_{sn}(t) e^{\frac{i}{\hbar}(E_s^{(1)} - E_n^{(0)})t} dt$$

Matrix element $V_{sn}(t)$ causes transitions $n \rightarrow s$.
Transitions from n to a continuum of states

(11)  Assume V_{sn} indep. of time, then

$$a_s(t) = -V_{sn} \frac{e^{\frac{i}{\hbar}(E_s^{(1)} - E_n^{(0)})t} - 1}{E_s^{(1)} - E_n^{(0)}}$$

$$|a_s(t)|^2 = 4 |V_{sn}|^2 \frac{\sin^2 \frac{\omega t}{2\hbar} (E_s^{(1)} - E_n^{(0)})}{(E_s^{(1)} - E_n^{(0)})^2}$$

Prob of transition to one state s

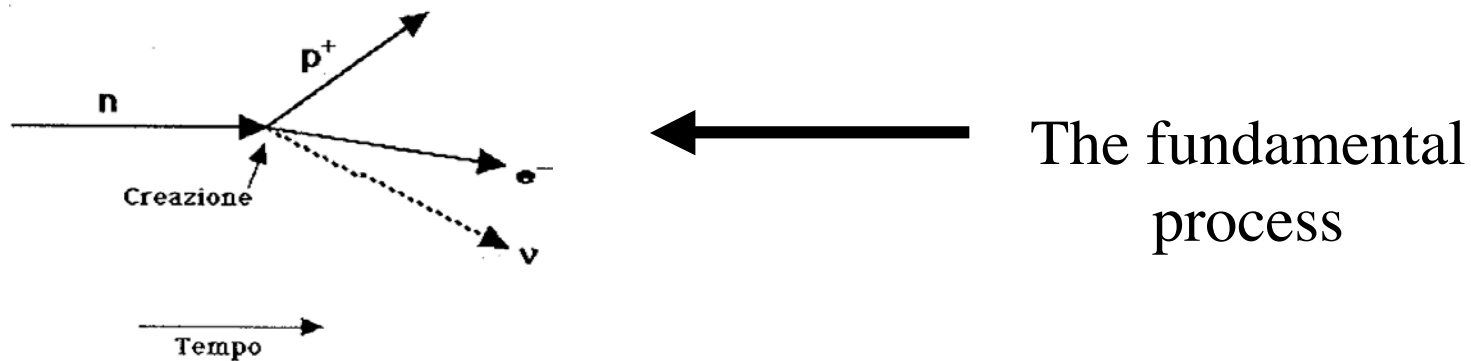
$$(12) \quad \begin{cases} P(t) = \sum_s |a_s(t)|^2 = 4 |V_{sn}|^2 \sum \frac{\sin^2 \frac{\omega t}{2\hbar} (E_s^{(1)} - E_n^{(0)})}{(E_s^{(1)} - E_n^{(0)})^2} = \\ = 4 |V_{sn}|^2 \rho(E_n) \int \frac{\sin^2 \frac{\omega t}{2\hbar} (E^s - E_n^{(0)}) d(E^s - E_n^{(0)})}{(E^s - E_n^{(0)})^2} \\ = t \frac{2\pi}{\hbar} |V_{sn}|^2 \rho(E_n) \underbrace{\frac{\pi t}{2\hbar}}_{\int \frac{\sin^2 x}{x^2} dx = \pi} \end{cases}$$

(13) $\rho(E_n)$ = no of states s , close to E_n per unit energy interval.

$$\text{Rate of transition} = \frac{2\pi}{\hbar} |V_{sn}|^2 \rho(E_n)$$

Discuss: distribution of final states as function of t & relation with uncertainty principle

**Fermi's
"Golden Rule #2"**



- In analogy with the theory of radiation Fermi applied the creation and destruction operators of Dirac-Jordan-Klein-Wigner and Dirac's relativistic theory for spin 1/2 particles
- Of the possibilities in Dirac invariant interactions (S, V, A, T, P) Fermi chose a vector interaction for the nucleon current and the lepton current.

$$H(x) = g [p^+(x) \gamma^0 \gamma^\mu n(x)] [e^+(x) \gamma_0 \gamma_\mu \nu(x)]$$

Fermi's Lectures on Nuclear Physics

CHAPTER IV BETA DECAY

A. Introduction

β decay is the process in which an electron or a positron is emitted by a nucleus. The term is extended to include absorption of electrons.

(The most remarkable feature of β decay phenomena is the apparent failure of energy conservation.) In other nuclear processes, such as α decay, energy is clearly conserved. For example, if nucleus A decays to nucleus B, producing an α , the energy equation is $E_A = E_B + E_\alpha$. If the nuclei are in excited states before and after, the energy equation may be different: $E_A = E_B + E_\alpha$, but always energy is conserved. In β emission, such an energy equation involving only the observed particles cannot be written. The reason is that the energies of β 's from a single type of process have a continuous distribution of values. Empirically, the relative number of β 's of a given energy, $N(E)$, as a function of energy is a curve like FIG. IV.1. No β is emitted having energy greater than some value E_{β}^{\max} .

A conceivable explanation that retains the energy conservation law is that the states of the final nucleus are very closely spaced, and the various β energies correspond to various final states. But we must account for the extra energy of the final excited state. The only conceivable mode of decay to the ground state is by gamma emission.

Since for some cases of β emission there is no gamma radiation at all, and in any case no gamma radiation with a nearly continuous energy spectrum, the hypothesis of many final states of the nucleus must be discarded.

There is no alternative to admitting that the final and initial states of the nucleus are definite, but that the β may have any energy below E_{β}^{\max} .

Experimentally, to within about 20 kev., $E_{\beta}^{\max} = E_A - E_B$, showing that although energy may disappear, none is ever gained. The law of energy conservation might be forsaken, and replaced by: $E_{\text{initial}} \geq E_{\text{final}}$, a law that energy either is conserved or disappears, but never increases. Such a law would forbid perpetual motion machines of the first kind and accord with β decay phenomena.

The most favored explanation of this apparent non-conservation of energy is the neutrino hypothesis first suggested by Pauli. It postulates that an additional particle, the neutrino, (or perhaps more than one) is produced in β decay and carries away the missing energy. To accord with experiment, the neutrino, denoted by ν , must be made very difficult to detect. This is done by postulating that it is electrically neutral, (conservation of charge also imposes this), and of very small mass. Under the neutrino hypothesis, the energy balance equation is: $E_A - E_B = E_e + E_{\nu}$.

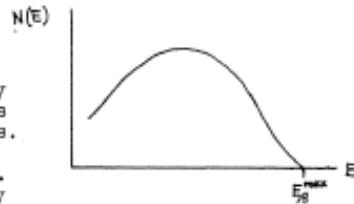


FIG. IV.1

$$\rho(E) \propto pE(E-E_0)^2 dE$$



field of large gradient has not been observed,

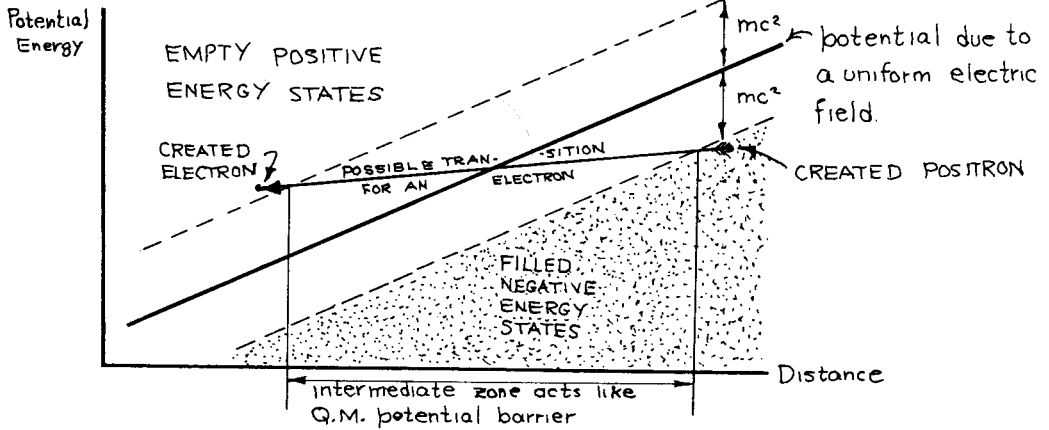


FIG. IV. 7

(b) Statistical arguments favor the proton-neutron theory of nuclear constitution. A nucleus having an odd number of elementary particles has Fermi statistics; a nucleus having an even number has Bose-Einstein statistics. The different hypotheses for the composition of nuclei lead to different numbers of particles. For the nucleus $Z(A)$,

Electrons-in-nucleus	Neutron hypothesis
A protons	Z protons
A-Z electrons	A-Z neutrons
2A-Z elem. particles	A elem. particles

For example, the ${}^7\text{N}^{14}$ nucleus has 14 particles under the neutron hypothesis, but 21 under the electron-in-nucleus hypothesis. Experiments in molecular spectroscopy* show that ${}^7\text{N}^{14}$ has Bose-Einstein statistics, therefore an even number of particles, confirming the neutron-in-nucleus hypothesis.

(c) The spin of the nucleus, whether integral or half-odd, depends on the number of elementary particles, and can be determined experimentally. The evidence again favors the neutron hypothesis.

Since the electron does not exist in the nucleus, it must be formed at the moment of its emission just as a photon is formed at the moment of its emission from an atom. The neutrino is created at the moment of emission, also. These particles are created into states represented by the wave-functions Ψ_β and Ψ_ν . Assume these are functions for plane waves with momenta \underline{p}_β and \underline{p}_ν , respectively,

$$\Psi_\beta = N_\beta e^{i \underline{p}_\beta \cdot \underline{x} \hbar^{-1}}, \quad \Psi_\nu = N_\nu e^{i \underline{p}_\nu \cdot \underline{x} \hbar^{-1}} \tag{IV.1}$$

where N is a normalization factor. Ψ_α is actually more complicated than given here because it is affected by the nuclear charge Z. The plane wave Ψ_β is a good approximation if the energy of the electron is much larger than Zx (Rydberg). For a low energy electron, say 200 Kev, near a nucleus of high Z, Ψ_β is strongly perturbed.

The probability of emission will be assumed to depend on the

* See Chapter I, sec. D.

expectation value for the electron and the neutrino to be at the nucleus, i.e., on the factor $|\Psi_\beta(0)|^2 |\Psi_\nu(0)|^2$. It also depends on other factors, whose nature is uncertain.

One factor is the square modulus of a matrix element \mathcal{M} taken between the initial and final states of the nucleus. This matrix element is analogous to the matrix element in the theory of emission of photons. In photon emission the matrix element is definitely known and has the form (for dipole radiation)

$$\int \Psi_{final}^* (\text{electric moment}) \Psi_{initial} d\tau$$

\mathcal{M} , in β theory, is not known. There are several possible forms. For the case $N \rightarrow P$, the simplest is

$$\mathcal{M} = \int \Psi_P^* \Psi_N d\tau \quad \text{IV.2}$$

assuming just one nucleon participates. Ψ_N represents the initial state of the nucleon, Ψ_P the final, i.e., proton, state of the nucleon. According to another form of the theory, \mathcal{M} is a vector having x component

$$\mathcal{M}_x = \int \Psi_P^* \sigma_x \Psi_N d\tau \quad \text{IV.3}$$

where σ_x is the x component of a (relativistic) spin operator. Then

$$|\mathcal{M}|^2 = |\mathcal{M}_x|^2 + |\mathcal{M}_y|^2 + |\mathcal{M}_z|^2 \quad \text{IV.4}$$

The choice of \mathcal{M} determines the selection rules, discussed in section H.

The expression for the probability of emission includes also a constant factor g^2 which represents the strength of the coupling giving rise to emission, and is a universal constant. Experimentally,

$$g = 10^{-48} \text{ to } 10^{-49} \text{ g cm}^5 \text{ sec}^{-2} \quad \text{IV.5}$$

Altogether, the probability of emission per unit time is*

$$\frac{2\pi}{\hbar} (|\Psi_\beta(0)| |\Psi_\nu(0)| |\mathcal{M}| g)^2 \frac{dn}{dE} \quad \text{IV.6}$$

where dn/dE = energy density of final states, and 0 refers to the location of the nucleus. The Ψ functions are normalized in a volume Ω so that $\int_\Omega \Psi^* \Psi d\tau = 1$. Therefore $N = 1/\sqrt{\Omega}$

$$\text{and } \Psi_\beta = \frac{1}{\sqrt{\Omega}} e^{ik_\beta \cdot \underline{r}} \quad \Psi_\nu = \frac{1}{\sqrt{\Omega}} e^{ik_\nu \cdot \underline{r}} \quad \text{IV.8}$$

It has meaning to say the nucleus is at $\underline{r} = 0$ only if Ψ changes little over the dimension of the nucleus. The rapidity of variation of Ψ is measured by $\lambda = \hbar/p \approx 10^{-11}$ cm, for a usual value of p . But the nucleus is about 10^{-12} cm in diameter. Therefore it is permissible to say that the nucleus is at $\underline{r} = 0$.

* This is analogous to the usual Q.M. formula for transition probability per unit time. This formula, "Golden Rule No. 2", is

$$\text{prob. per second} = \frac{2\pi}{\hbar} |\mathcal{H}_{21}|^2 \frac{dn}{dE}, \text{ where } \mathcal{H}_{21} = \int \Psi_2^* H' \Psi_1 d\tau.$$

Ψ_1 and Ψ_2 are the wave functions of the initial and final states, resp. This is derived, for example, in Schiff, Q.M., p. 193. It is discussed in more detail in Ch. VIII, sec. B.

For $\underline{r} = 0$

$$\Psi_{\beta}(0) = \frac{1}{\sqrt{\Omega}} \quad \Psi_{\nu}(0) = \frac{1}{\sqrt{\Omega}}$$

IV.9

The number of plane wave states having magnitude of momentum between p and $p + dp$, with the particle anywhere in Ω , is*

$$\frac{p^2 dp \Omega}{2\pi^2 \hbar^3} \quad \text{IV.10}$$

Therefore $dn = \frac{p_{\beta}^2 dp_{\beta}}{2\pi^2 \hbar^3} \times \frac{p_{\nu}^2 dp_{\nu}}{2\pi^2 \hbar^3} \times \Omega^2 = \Omega^2 \frac{p_{\beta}^2 p_{\nu}^2}{4\pi^4 \hbar^6} dp_{\beta} dp_{\nu}$

$dp_{\beta} dp_{\nu} = J dp_{\beta} dE$ where J is the Jacobian. Using the relation $E = cp_{\nu} + E_{\beta}$, J is found to be $1/c$.* (Mass of ν assumed zero for this derivation.)

Thus $\frac{dn}{dE} = \Omega^2 \frac{p_{\beta}^2 p_{\nu}^2}{4\pi^4 \hbar^6 c} dp_{\beta}$

Using this to express IV.6, the probability of emission per unit time, $P(p_{\nu}, p_{\beta}) dp_{\beta}$, is

$$P(p_{\nu}, p_{\beta}) dp_{\beta} = \frac{2\pi}{\hbar} \left(\frac{1}{\Omega} |M|^2 g \right)^2 \frac{\Omega^2 p_{\beta}^2 p_{\nu}^2 dp_{\beta}}{4\pi^4 \hbar^6 c} \quad \text{IV.14}$$

Using the relation $p_{\nu} c = E_{\nu} = E_{\beta}^{\max} - E_{\beta}$ to eliminate p_{ν} , and writing p for p_{β} from now on,

$$P(p) dp = \frac{g^2 |M|^2}{2\pi^3 \hbar^7 c^3} (E_{\beta}^{\max} - E_{\beta})^2 p^2 dp \quad \text{IV.15}$$

Using the equation $E_{\beta}^{\max} = \sqrt{m^2 c^4 + c^2 p_{\max}^2}$ to define p_{\max} , IV.16 we get:

$$P(p) dp = \frac{g^2 |M|^2}{2\pi^3 \hbar^7 c^3} \left(\sqrt{m^2 c^4 + c^2 p_{\max}^2} - \sqrt{m^2 c^4 + p^2 c^2} \right)^2 p^2 dp \quad \text{IV.17}$$

E. Rate of Decay

The lifetime τ is found by integrating over all possible p .

* For simplicity, assume Ω is a cubical box of side L . $\Omega = L^3$. That the particle is confined to the box means that the potential rises to ∞ at the sides. Schrödinger's equation within the box is

$$-\nabla^2 \mu = \frac{2mE}{\hbar^2} \mu = (p_x^2 + p_y^2 + p_z^2) \hbar^{-2}$$

Solutions satisfying the boundary condition $u = 0$ at $x, y, z = 0$, and $u = 0$ at $x, y, z = L$ are $\mu = \sin \frac{p_x}{\hbar} x \sin \frac{p_y}{\hbar} y \sin \frac{p_z}{\hbar} z$

where p_x/\hbar is restricted to the values $n_x \pi/L$, etc. The number of states, n , representing momentum less than p equals the number of combinations of p_x, p_y, p_z such that $p_x^2 + p_y^2 + p_z^2 < p^2$, or, using the condition on the p 's, $n_x^2 + n_y^2 + n_z^2 < p^2 L^2 / \pi^2 \hbar^2$. $n_x, n_y, n_z > 0$ since - values give no new independent solutions. The number of sets of n_x, n_y, n_z satisfying the condition above equals 1/8 the number of points of a cubical lattice enclosed by a sphere of radius $\sqrt{\frac{p^2 L^2}{\pi^2 \hbar^2}}$. The 1/8 comes from restricting $n_x, n_y, n_z > 0$.

Then the number of states, $n' = \frac{1}{8} \frac{4\pi}{3} \left(\frac{pL}{\pi\hbar} \right)^3$. IV.18

The number of states having momentum between p and $p+dp$ is

$$\frac{dn'}{dp} dp = \Omega p^2 dp / 2\pi^2 \hbar^3$$

* $J = \begin{vmatrix} \frac{\partial p_{\beta}}{\partial p_{\beta}} & \frac{\partial p_{\beta}}{\partial E} \\ \frac{\partial p_{\nu}}{\partial p_{\beta}} & \frac{\partial p_{\nu}}{\partial E} \end{vmatrix} = \begin{vmatrix} 1 & \frac{\partial p_{\beta}}{\partial E} \\ 0 & \frac{1}{c} \end{vmatrix} = \frac{1}{c}$

hundertmal kleiner sind als die der α -
 laubten Überlegen.

7. Die Masse des Neutrinos. Durch die Ueber-
 gangswahrscheinlichkeit (32) bestimmte
 ist die Form der kontinuierlichen β -Spektrum
 bestimmt. Wir wollen zuerst diskutieren,
 wie diese Form von der Ruhmasse μ des
 Neutrinos abhängt, um von einem
 Vergleich mit den empirischen Kurven
 diese Konstante zu bestimmen. Die
 Abhänge μ ist in dem Faktor p_0^2/v_0
 enthalten. Die Abhängigkeit der Form
 der Energieverteilungskurve von μ
 ist am ausgeprägtesten in der
 Nähe des Endpunkts der Verteilungskurve
 bei E_0 die Grenzenergie der β -Strahlen,
 so sieht man ohne Schwierigkeit dass
 die Verteilungskurve der β -Strahl Energie
 für Energien E in der Nähe von E_0 , propor-
 zional ist durch zu

$$\frac{p_0^2}{v_0} = \frac{1}{c^3} (\mu c^2 + E_0 - E) \sqrt{(E_0 - E)^2 + 2\mu c^2 (E_0 - E)}$$

$$(36) \quad \frac{p_0^2}{v_0} = \frac{1}{c^3} (\mu c^2 + E_0 - E) \cdot \sqrt{(E_0 - E)^2 + 2\mu c^2 (E_0 - E)}$$

$$(36) \quad \frac{p_0^2}{v_0} = \frac{1}{c^3} (\mu c^2 + E_0 - E) \sqrt{(E_0 - E)^2 + 2\mu c^2 (E_0 - E)}$$

Nella fig. 1 la fine della curva di distribuzione è rappresentata per $\mu = 0$,
 e per un valore piccolo e uno grande di μ . La maggiore somiglianza con le

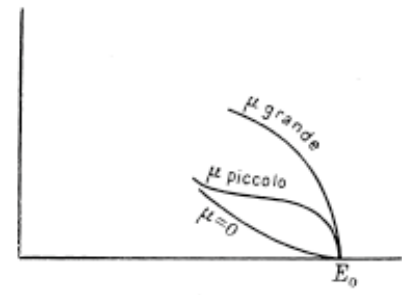


Fig. 1.

curve sperimentali si ha per la curva teorica corrispondente a $\mu = 0$. Arriviamo così a concludere che la massa del neutrino è uguale a zero o, in ogni caso, piccola in confronto della massa dell'elettrone⁽⁹⁾. Nei calcoli che seguono porremo per semplicità $\mu = 0$.

Fermi's paper on beta decay:

- Established a predictive realization of Pauli's proposal
- Established the connection between quantum field theory and particles.
- Predicted the statistical shape of the beta spectrum and the consequences of finite neutrino mass.
- Anticipated the most likely experimental distortions to beta spectrum.
- Discussed the dominant electromagnetic corrections to the beta decay spectrum.
- Established a theory that remains the (essentially) correct description of beta decay.

Fermi's theory remains the "correct" description of beta decay except:

- As pointed out by Gamow and Teller in 1936 another component of the Hamiltonian is required to account for decays like ${}^6\text{He}$
- Neutrons and protons are not elementary particles and there are forbidden contributions (induced terms) due to their structure

Dear Enrico,

October 4, 1952

We thought that you might be interested in the latest version of our experiment to detect the free neutrino, hence this letter. As you recall, we planned to use a nuclear explosion for the source because of the background difficulties. Only last week it occurred to us that background problems could be reduced to the point where a Hanford pile would suffice by counting only delayed coincidences between the positron pulse and neutron capture pulse. You will remember that the reaction we plan to use is $p + \nu \rightarrow n + \beta^+$. Boron loading a liquid scintillator makes it possible to adjust the mean time T between these two events and we are considering $T \sim 10 \mu\text{sec}$. Our detector is a 10 cubic foot fluor filled cylinder surrounded by about 90 5819's operating as two large tubes of 45 5819's each. These two banks of ganged tubes isotropically distributed about the curved cylindrical wall are in coincidence to cut tube noise. The inner wall of the chamber will be coated with a diffuse reflector and in all we expect the system to be energy sensitive, and not particularly sensitive to the position of the event in the fluor. This energy sensitivity will be used to discriminate further against background. Cosmic ray anti-coincidence will be used in addition to mercury of low background lead for shielding against natural radioactivity. We plan to immerse the entire detector in a large borax water solution for further necessary reduction of pile background below that provided by the Hanford shield.

Fortunately, the fast reactor here at Los Alamos provides the same leakage flux as Hanford so that we can check our gear before going to Hanford. Further, if we allow enough fast neutrons from the fast reactor to leak into our detector we can simulate double pulses because of the proton recoil pulse followed by the neutron capture which occurs in this case. We expect a counting rate at Hanford in our detector about six feet from the pile face of $\sim 1/\text{min}$ with a background somewhat lower than this.

As you can imagine, we are quite excited about the whole business, have canceled preparations for use of a bomb, and we are working like mad to carry out the ideas sketched above. Because of the enormous simplification in the experiment. We have already made rapid progress with the electronic gear and associated equipment and expect that in the next few months we shall be at Hanford reaching for the slippery particle.

We would of course appreciate any comments you might care to make.

Sincerely,

Fred Reines, Clyde Cowan

Dear Fred,

October 8, 1952

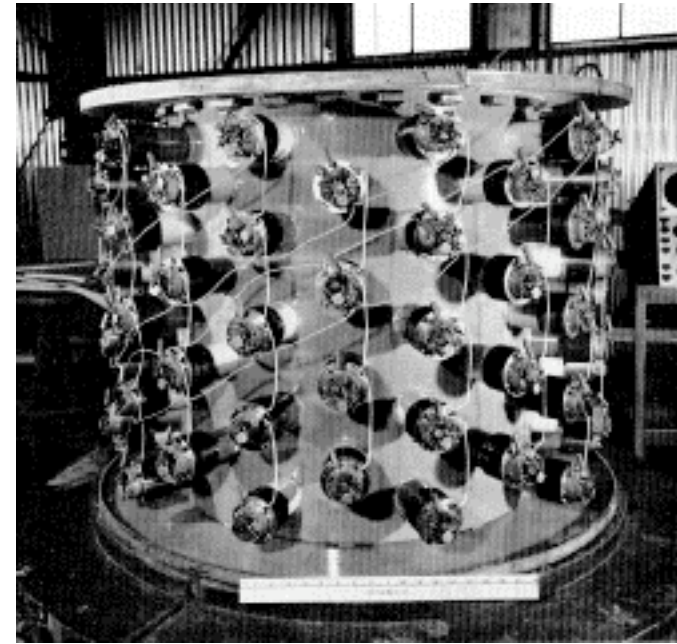
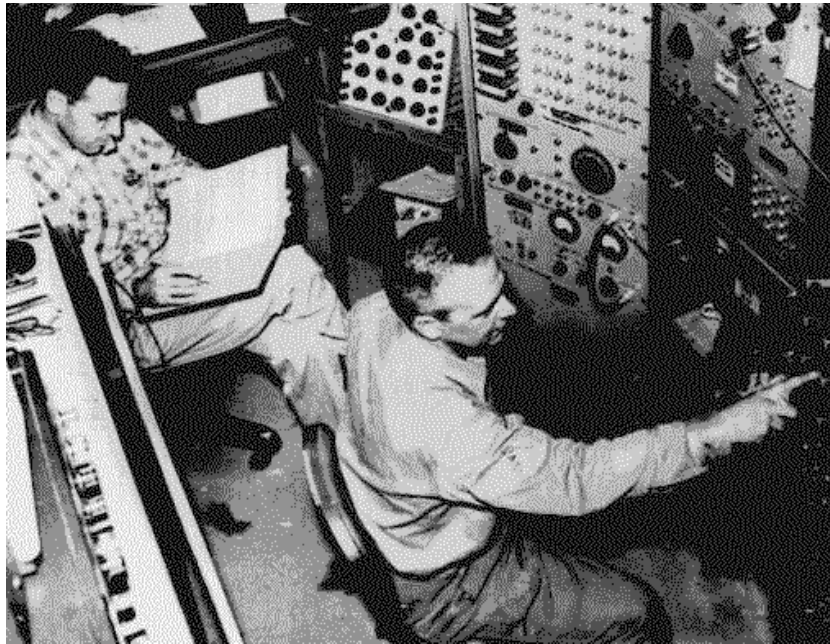
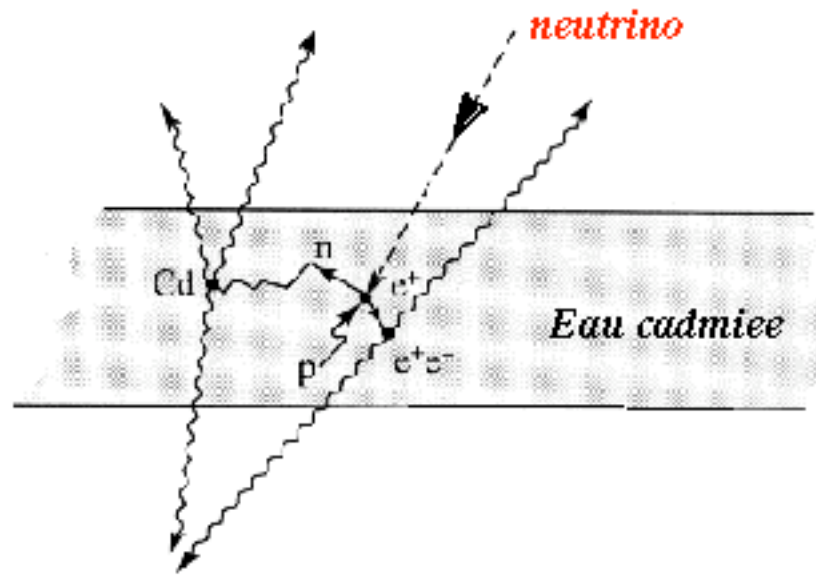
Thank you for your letter of October 4th by Clyde Cowan and yourself. I was very much interested in your new plan for the detection of the neutrino. Certainly your new method should be much simpler to carry out and have the great advantage that the measurement can be repeated any number of times. I shall be very interested seeing how your 10 cubic foot scintillation counter is going to work, but I do not know of any reason why it should not.

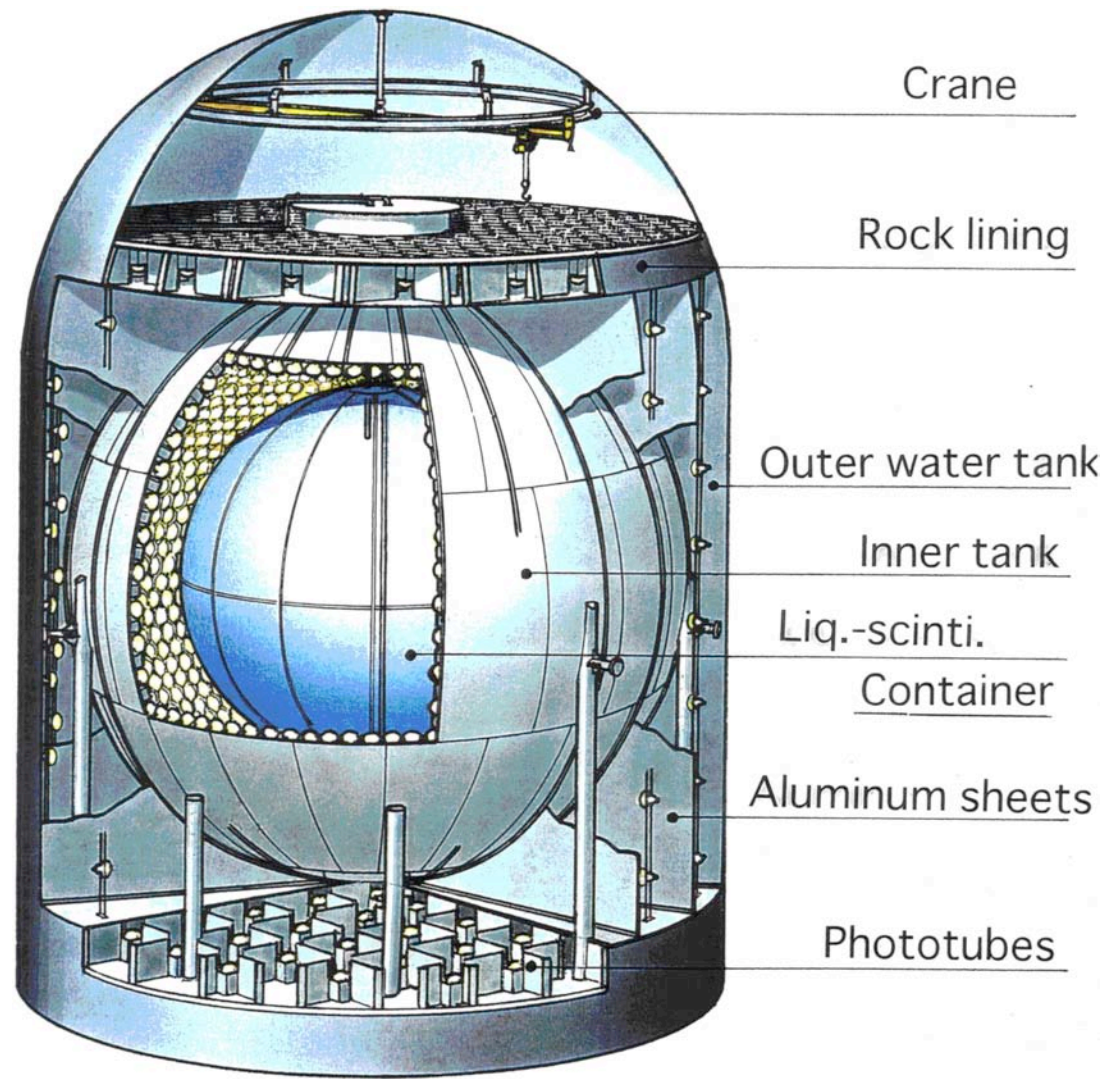
Good Luck.

Sincerely yours,

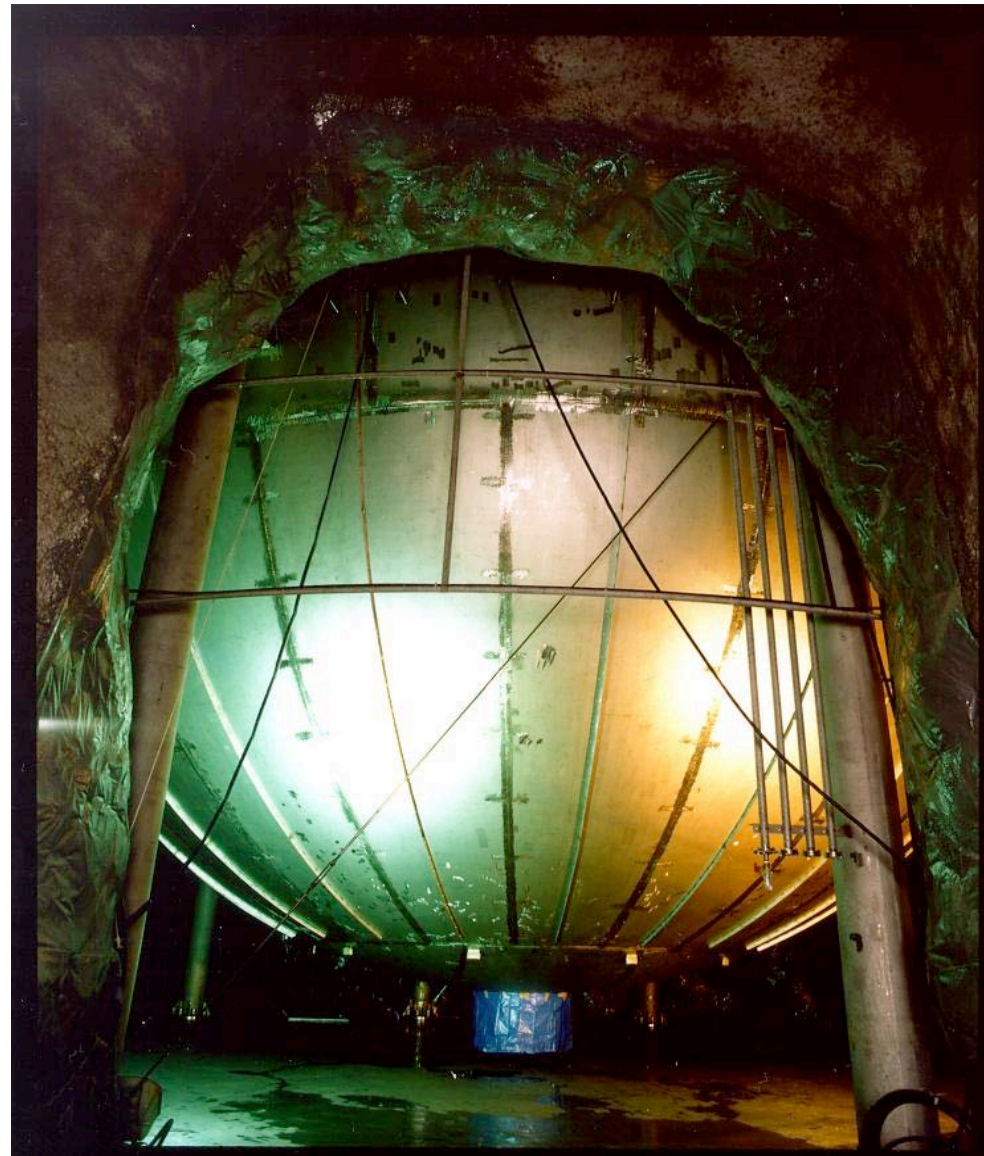
Enrico Fermi

Direct Detection of the Neutrino

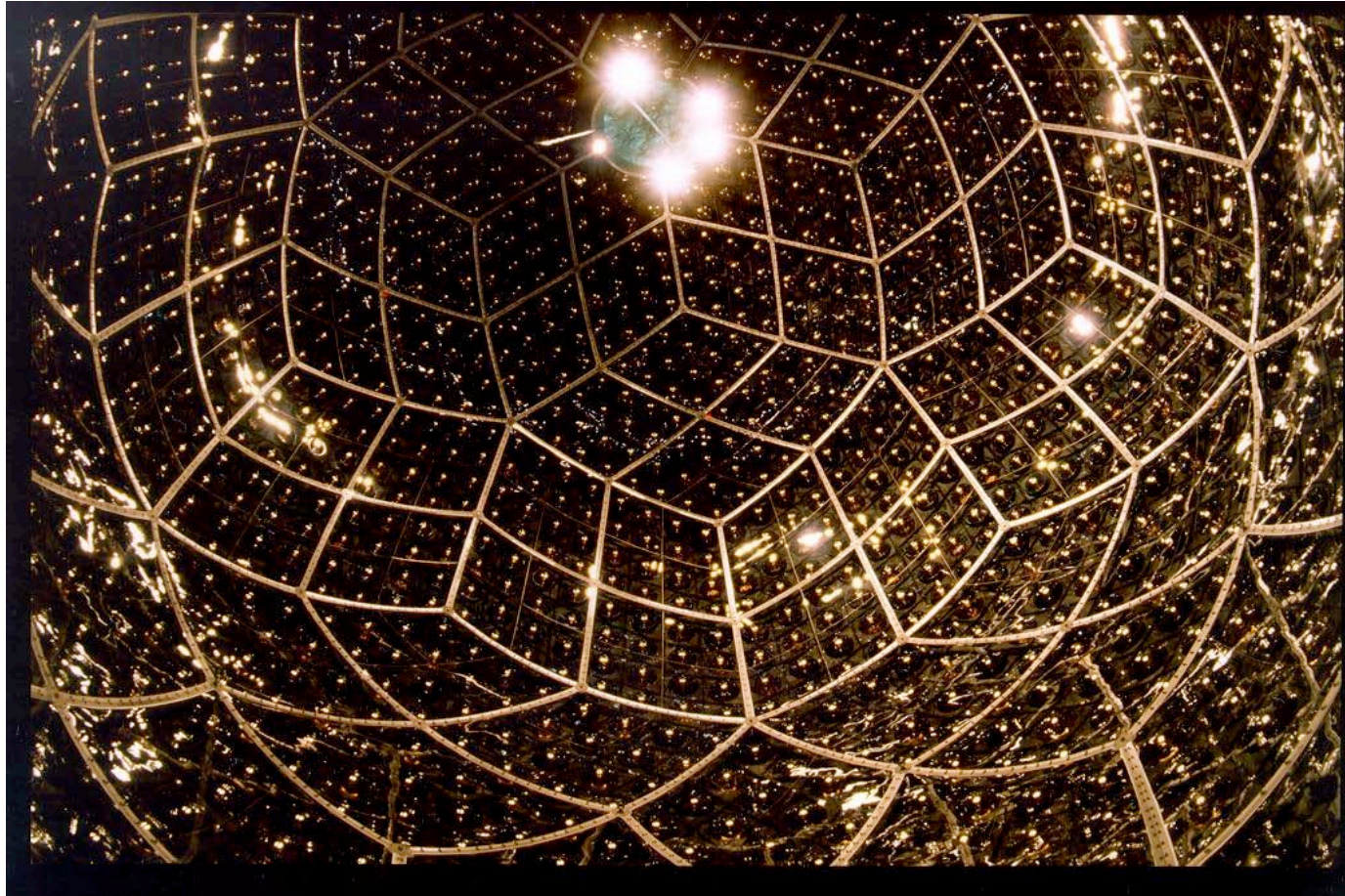




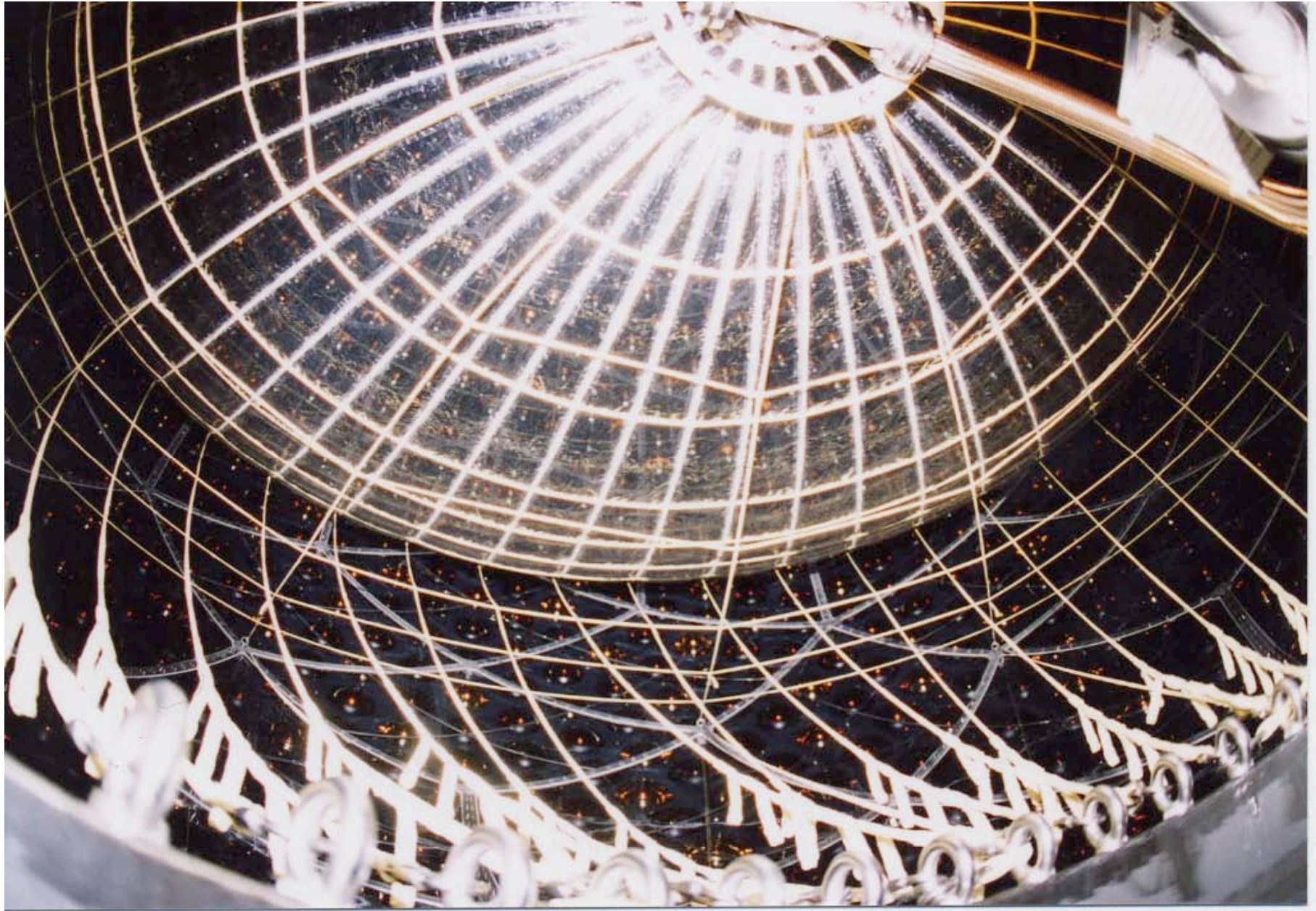
Cutaway view of the KamLAND detector



Exterior view of KamLAND sphere



Interior of KamLAND sphere October 2000



KamLAND Detector Ready for Fill May 2001



“I shall be very interested seeing how your 40,624 cubic foot scintillaton counter is going to work, but I do not know of any reason why it should not.”

The Neutrino: From Poltergeist to Particle

Nobel Lecture, December 8, 1995

Frederick Reines

The Second World War had a great influence on the lives and careers of very many of us for whom those were formative years. I was involved during, and then subsequent to, the war in the testing of nuclear bombs, and several of us wondered whether this man-made star could be used to advance our knowledge of physics. For one thing this unusual object certainly had lots of fissions in it, and hence, was a very intense neutrino source. I mulled this over somewhat but took no action.

Then in 1951, following the tests at Eniwetok Atoll in the Pacific, I decided I really would like to do some fundamental physics. Accordingly, I approached my boss, Los Alamos Theoretical Division Leader, J. Carson Mark, and asked him for a leave in residence so that I could ponder. He agreed, and I moved to a stark empty office, staring at a blank pad for several months searching for a meaningful question worthy of a life's work. It was a very difficult time. The months passed and all I could dredge up out of the subconscious was the possible utility of a bomb for the direct detection of neutrinos. After all, such a device produced an extraordinarily intense pulse of neutrinos and thus the signals produced by neutrinos might be distinguishable from background. Some handwaving and rough calculations led me to conclude that the bomb was the best source. All that was needed was a detector measuring a cubic meter or so. I thought, well, I must check this with a real expert.

It happened during the summer of 1951 that Enrico Fermi was at Los Alamos, and so I went down the hall, knocked timidly on the door and said, "I'd like to talk to you a few minutes about the possibility of neutrino detection." He was very pleasant, and said, "Well, tell me what's on your mind?" I said, "First off as to the source, I think that the bomb is best." After a moment's thought he said, "Yes, the bomb is the best source." So far, so good! Then I said, "But one needs a detector which is so big. I don't know how to make such a detector." He thought about it some and said he didn't either. Coming from the Master that was very crushing. I put it on the back burner until a chance conversation with Clyde Cowan. We were on our way to Princeton to talk with Lyman Spitzer about controlled fusion when the airplane was grounded in Kansas City because of engine trouble. At loose ends we wandered around the place, and started to discuss what to do that's interesting in physics. "Let's do a real challenging problem," I said. He said, "Let's work on positronium." I said, "No, positronium is a very good thing but Martin Deutsch has that sewed-up. So let's not work on positronium." Then I said, "Clyde let's work on the neutrino." His immediate

response was, “GREAT IDEA.” He knew as little about the neutrino as I did but he was a good experimentalist with a sense of derring do. So we shook hands and got off to working on neutrinos.

Need for Direct Detection

Before continuing with this narrative it is perhaps appropriate to recall the evidence for the existence of the neutrino at the time Clyde and I started on our quest. The neutrino of Wolfgang Pauli[1] was postulated in order to account for an apparent loss of energy-momentum in the process of nuclear beta decay. In his famous 1930 letter to the Tübingen congress, he stated: “I admit that my expedient may seem rather improbable from the first, because if **neutrons*** existed they would have been discovered long since.

***When the neutron was discovered by Chadwick, Fermi renamed Pauli’s particle the “neutrino”.**

Nevertheless, nothing ventured nothing gained... We should therefore be seriously discussing every path to salvation.”

All the evidence up to 1951 was obtained “at the scene of the crime” so to speak since the neutrino once produced was not observed to interact further. No less an authority than Niels Bohr pointed out in 1930[2] that no evidence “either empirical or theoretical” existed that supported the conservation of energy in this case. He was, in fact, willing to entertain the possibility that energy conservation must be abandoned in the nuclear realm. However attractive the neutrino was as an explanation for beta decay, the proof of its existence had to be derived from an observation at a location other than that at which the decay process occurred - the neutrino had to be observed in its free state to interact with matter at a remote point.

It must be recognized, however, that, independently of the observation of a free neutrino interaction with matter, the theory was so attractive in its explanation of beta decay that belief in the neutrino as a “real” entity was general. Despite this widespread belief, the free neutrino’s apparent undetectability led it to be described as “elusive, a poltergeist.”

So why did we want to detect the free neutrino? Because everybody said, you couldn’t do it. Not very sensible, but we were attracted by the challenge. After all, we had a bomb which constituted an excellent intense neutrino source. So, maybe we had an edge on others. Well, once again being brash, but nevertheless having a certain respect for certain authorities, I commented in this vein to Fermi, who agreed. A formal way to make some of these comments is to say that, if you demonstrate the existence of the neutrino in the free state, i.e. by an observation at a remote location, you extend the range of

applicability of these fundamental conservation laws to the nuclear realm. On the other hand, if you didn't see this particle in the predicted range then you have a very real problem.

As Bohr is reputed to have said, "A deep question is one where either a yes or no answer is interesting." So I guess this question of the existence of the "free" neutrino might be construed to be deep. Alright, what about the problem of detection? We fumbled around a great deal before we got to it. Finally, we chose to look for the reaction $T_e + p + n + e'$. If the free neutrino exists, this inverse beta decay reaction has to be there, as Hans Bethe and Rudolf Peierls recognized, and as I'm sure did Fermi, but they had no occasion to write it down in the early days. Further, it was not known at the time whether V_1 and V_2 were different. We chose to consider this reaction because if you believe in what we today call "crossing symmetry" and use the measured value of the neutron half life then you know what the cross section has to be - a nice clean result. (In fact, as we learned some years later from Lee and Yang, the cross section is a factor of two greater because of parity nonconservation and the handedness of the neutrino.) Well, we set about to assess the problem of neutrino detection. How big a detector is required? How many counts do we expect? What features of the interaction do we use for signals? Bethe and Peierls in 1934 [3], almost immediately after the Fermi paper on beta decay[4], estimated that if you are in the few MeV range the cross section with which you have to deal would be $\sim 10^{-44}$ cm². To appreciate how minuscule this interaction is we note that the mean free path is ~ 1000 light years of liquid hydrogen. Pauli put his concern succinctly during a visit to Caltech when he remarked: "I have done a terrible thing. I have postulated a particle that cannot be detected." No wonder that Bethe and Peierls concluded in 1934 "there is no practically possible way of observing the neutrino." I confronted Bethe with this pronouncement some 20 years later and with his characteristic good humor he said, "Well, you shouldn't believe everything you read in the papers."

Reflecting on the trail that took us from bomb to reactor, it is evident that it was our persistence which led us from a virtually impossible experiment to one that showed considerable promise. The stage had been set for the detection of neutrinos by the discovery of fission and organic scintillators - the most important barrier was the generally held belief that the neutrino was undetectable.

Absorption Test

The only known particles, other than those produced by the fission process, were discriminated against by means of a gamma-ray and neutron shield. When a bulk shield measured to attenuate gamma rays and

neutrons by at least an order of magnitude was added, the signal was observed to remain constant; that is the reactor-associated signal was 1.74 ± 0.12 /hour with, and 1.69 ± 0.17 /hour without the shield.

Telegram to Pauli

The tests were completed and we were convinced. It was a glorious feeling to have participated so intimately in learning a new thing, and in June of 1956 we thought it was time to tell the man who had started it all when, as a young fellow, he wrote his famous letter in which he postulated the neutrino, saying something to the effect that he couldn't come to a meeting and tell them about it in person because he had to go out to a dance! The message was forwarded to him at CERN, where he interrupted the meeting he was attending to read the telegram to the conferees and then made some impromptu remarks regarding the discovery. That message reads, "We are happy to inform you that we have definitely detected neutrinos from fission fragments by observing inverse beta decay of protons. Observed cross section agrees well with expected six times ten to minus forty four square centimeters." We learned later that Pauli and some friends consumed a case of champagne in celebration! Many years later (~ 1986) C.P. Enz, a student of Pauli's, sent us a copy of a night letter Pauli wrote us in 1956, but which never arrived. It says, "Thanks for the message. Everything comes to him who knows how to wait. Pauli"

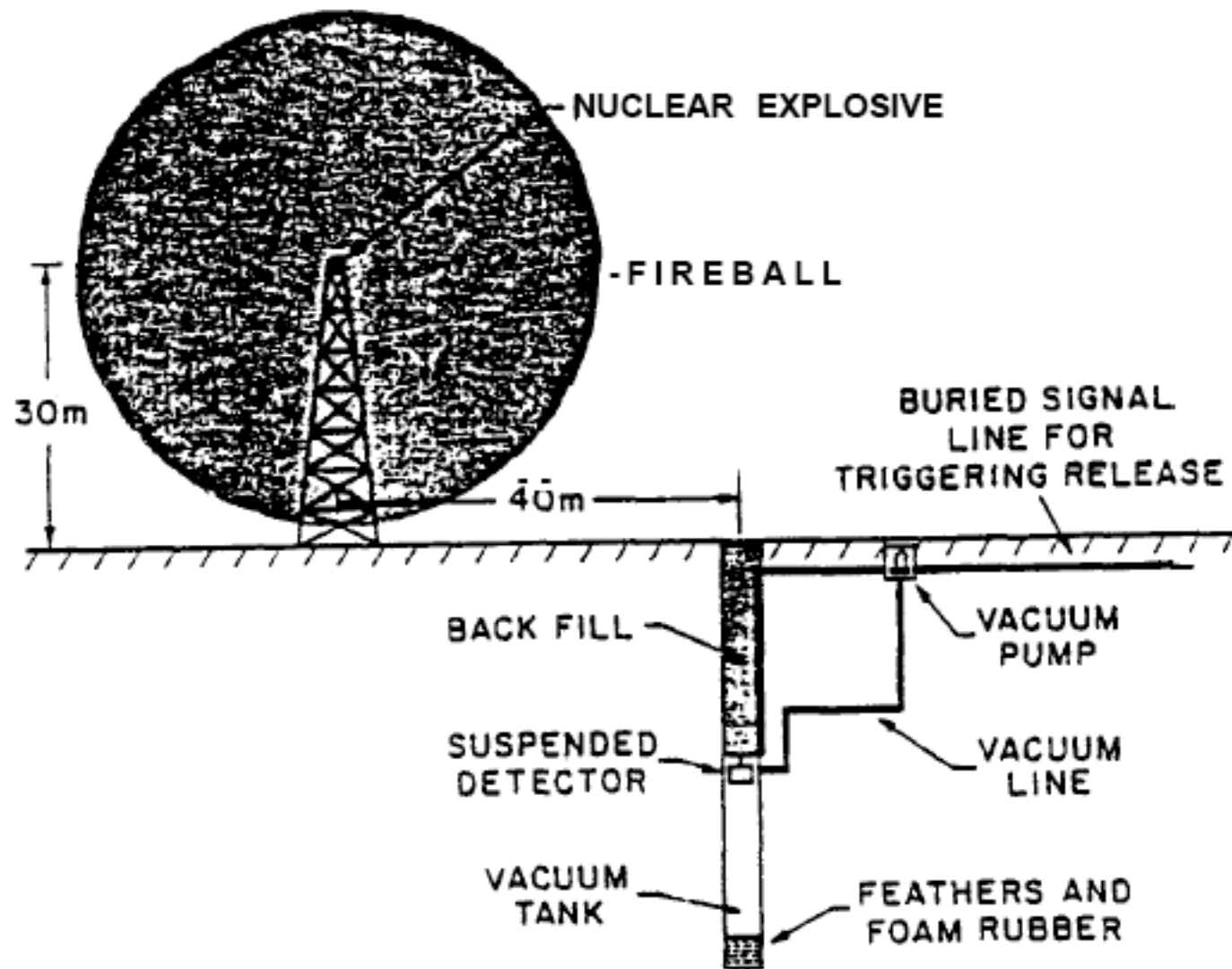


Figure 1. Sketch of the originally proposed experimental setup to detect the neutrino using a nuclear bomb. This experiment was approved by the authorities at Los Alamos but was superseded by the approach which used a fission reactor.

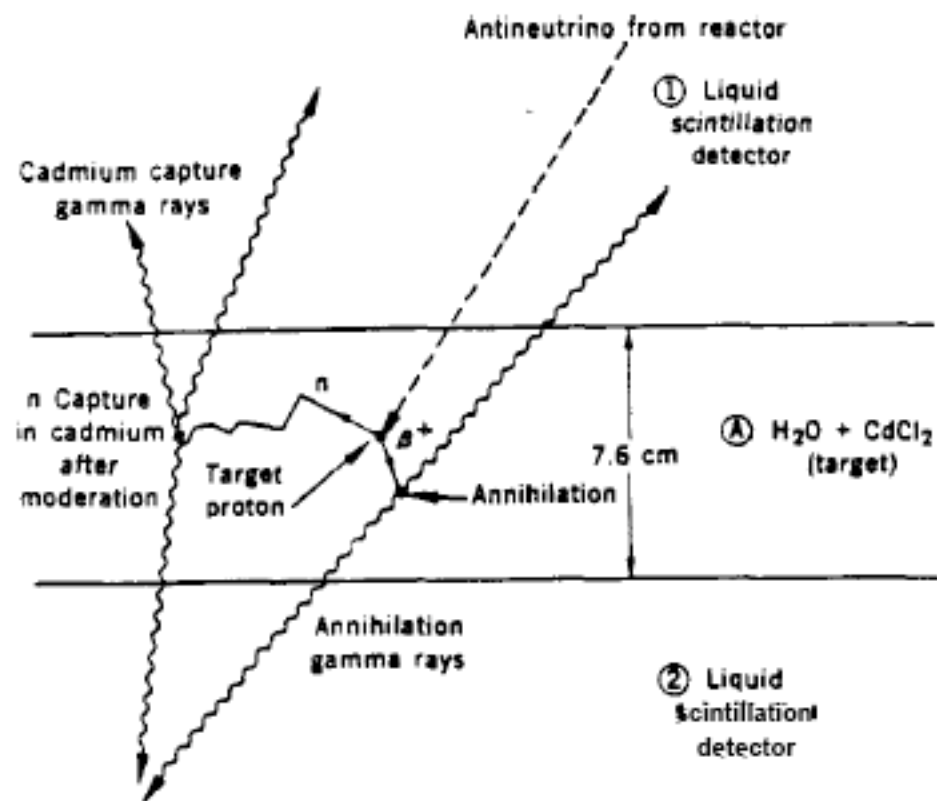


Figure 4. Schematic of the detection scheme used in the Savannah River experiment. An antineutrino from the reactor interacts with a proton in the target, creating a positron and a neutron. The positron annihilates on an electron in the target and creates two gamma rays which are detected by the liquid scintillators. The neutron slows down (in about 10 microseconds) and is captured by a cadmium nucleus in the target; the resulting gamma rays are detected in the liquid scintillators.

Neutrino Detection

Neutrinos are elusive. A low energy neutrino has some chance of passing through 1000 light-years of lead without interacting!

Cosmic Gall

-John Updike-

Neutrinos, they are very small.
They have no charge and have no mass
And do not interact at all.
The earth is just a silly ball
To them, through which they simply pass,
Like dustmaids through a drafty hall
Or photons through a sheet of glass.
They snub the most exquisite gas,
Ignore the most substantial wall,
Cold-shoulder steel and sounding brass,
Insult the stallion in his stall,
And scorning barriers of class,
Infiltrate you and me! Like tall
And painless guillotines, they fall
Down through our heads into the grass.
At night, they enter at Nepal
And pierce the lover and his lass
From underneath the bed-you call
It wonderful; I call it crass.

The New Yorker Magazine, Inc. , 1960

YOU are now being invaded by about 10^{14} neutrinos each second!

Particle Physics

Weak Decays

WEAK INTERACTION (1)

Presentation based on "*Introduction to Elementary Particles*"
by David Griffiths

Let's start with...



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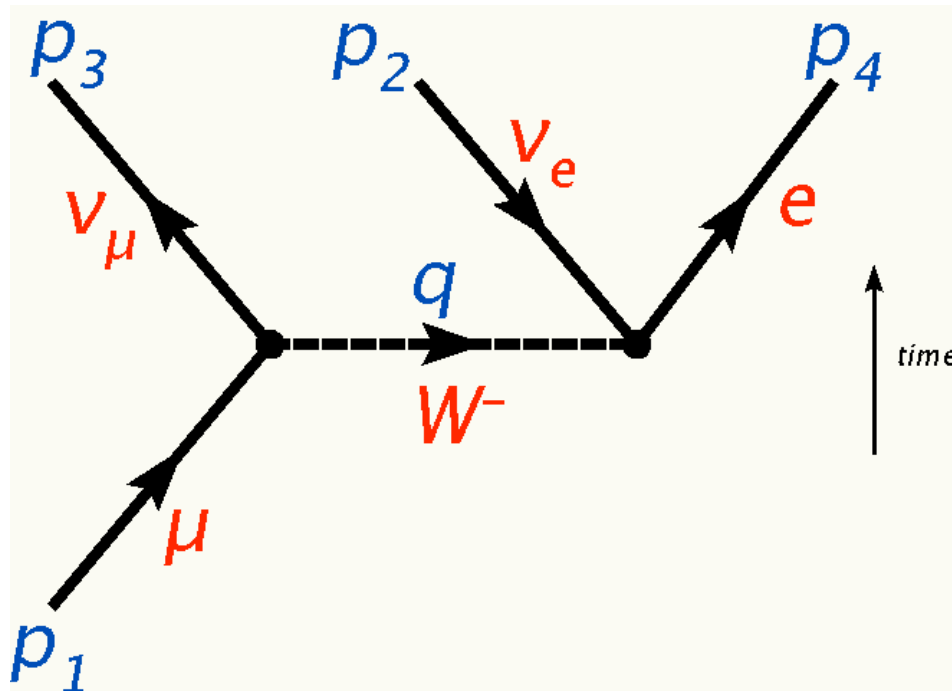
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DECAY OF THE MUON



$$\mu \rightarrow e + \nu_\mu + \bar{\nu}_e$$

The amplitude :

$$\mathcal{M} = \frac{g_W^2}{8(M_W c)^2} [\bar{u}(3)\gamma^\mu (1 - \gamma^5) u(1)] [\bar{u}(4)\gamma_\mu (1 - \gamma^5) v(2)]$$

As before :

$$\langle |\mathcal{M}|^2 \rangle = 2 \left(\frac{g_W}{M_W c} \right)^4 (p_1 \cdot p_2) (p_3 \cdot p_4)$$

DECAY OF THE MUON

In the muon rest frame : $\mathbf{p}_1 = (m_\mu c, \vec{0})$

$$\mathbf{p}_1 \cdot \mathbf{p}_2 = m_\mu E_2$$

$$\mathbf{p}_1 = \mathbf{p}_2 + \mathbf{p}_3 + \mathbf{p}_4$$

$$(\mathbf{p}_3 + \mathbf{p}_4)^2 = \mathbf{p}_3^2 + \mathbf{p}_4^2 + 2\mathbf{p}_3 \cdot \mathbf{p}_4 = m_e^2 c^2 + 2\mathbf{p}_3 \cdot \mathbf{p}_4$$

$$(\mathbf{p}_3 + \mathbf{p}_4)^2 = (\mathbf{p}_1 - \mathbf{p}_2)^2 = \mathbf{p}_1^2 + \mathbf{p}_2^2 - 2\mathbf{p}_1 \cdot \mathbf{p}_2 = m_\mu^2 c^2 - 2\mathbf{p}_1 \cdot \mathbf{p}_2$$

$$\mathbf{p}_3 \cdot \mathbf{p}_4 = \frac{(m_\mu^2 - m_e^2) c^2}{2} - m_\mu E_2$$

Let : $m_e = 0$

Plug in :

$$\langle |\mathcal{M}|^2 \rangle = 2 \left(\frac{g_W}{M_W c} \right)^4 (\mathbf{p}_1 \cdot \mathbf{p}_2) (\mathbf{p}_3 \cdot \mathbf{p}_4)$$

DECAY OF THE MUON

$$\langle |\mathcal{M}|^2 \rangle = \left(\frac{g_W}{M_W c} \right)^4 m_\mu^2 E_2 (m_\mu c^2 - 2E_2)$$

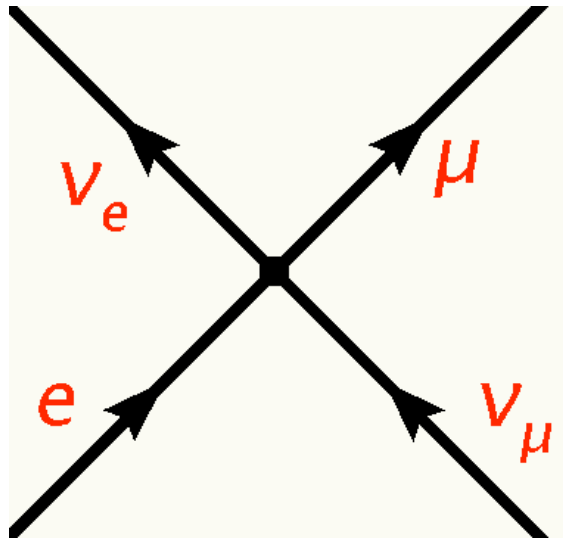
The decay rate given by **Golden Rule*** :

$$d\Gamma = \frac{\langle |\mathcal{M}|^2 \rangle}{2\hbar m_\mu} \left(\frac{c d^3 \vec{p}_2}{(2\pi)^3 2E_2} \right) \left(\frac{c d^3 \vec{p}_3}{(2\pi)^3 2E_3} \right) \left(\frac{c d^3 \vec{p}_4}{(2\pi)^3 2E_4} \right) \times \\ \times (2\pi)^4 \delta^4 (p_1 - p_2 - p_3 - p_4)$$

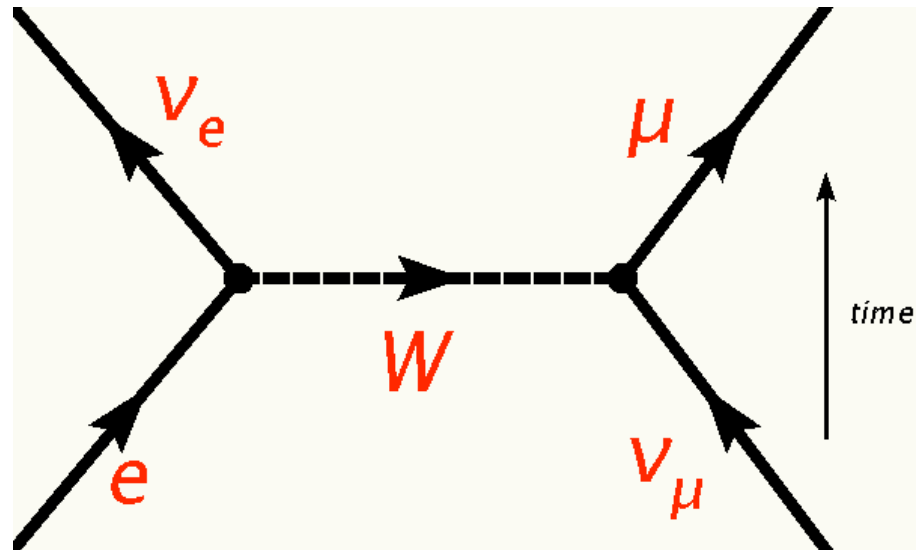
where : $E_2 = |\vec{p}_2| c$, $E_3 = |\vec{p}_3| c$, $E_4 = |\vec{p}_4| c$

* a lot of work, since this is a *three body decay*

DECAY OF THE MUON



In **Fermi's** original theory of beta decay there was no **W**; the interaction was a direct four-particle coupling.



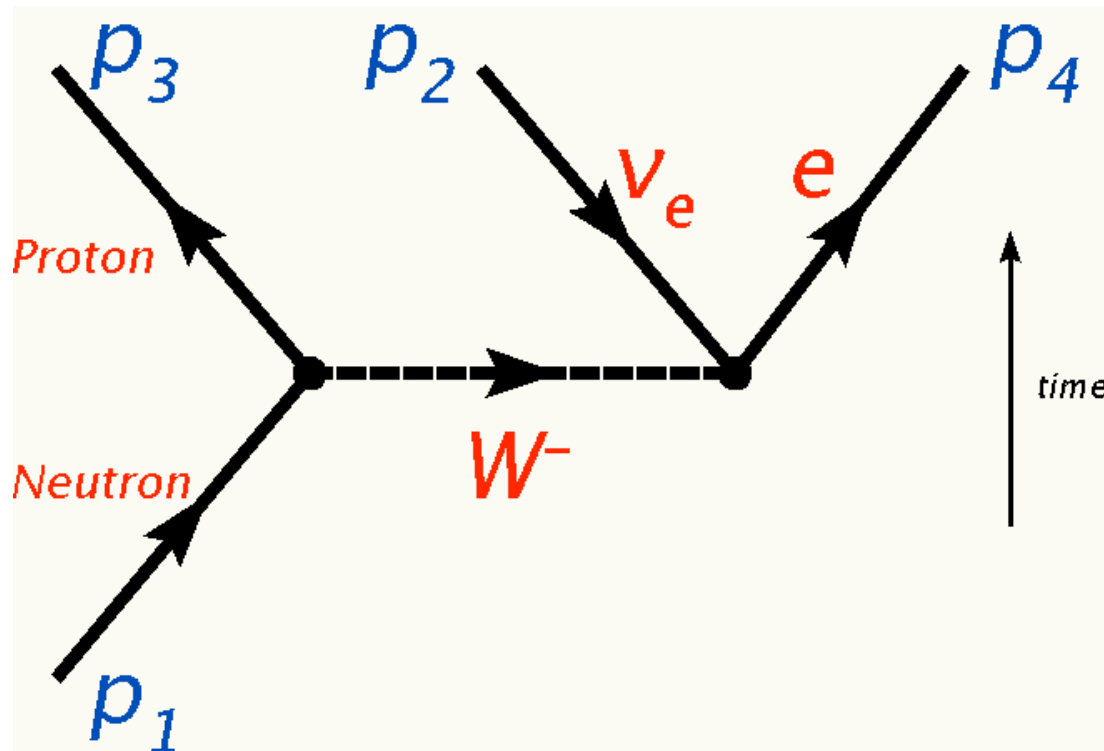
Using the observed muon lifetime and mass :

$$\frac{G_F}{(\hbar c)^3} = \frac{\sqrt{2}}{8} \left(\frac{g_W}{M_W c^2} \right)^2 = 1.166 \times 10^{-5} (\text{GeV}^2)^{-1} \quad \text{and : } g_W = 0.66$$

“Weak fine structure constant” : $\alpha_W = \frac{g_W^2}{4\pi} = \frac{1}{29}$

Larger than electromagnetic fine structure constant

DECAY OF THE NEUTRON



$$\langle |\mathcal{M}|^2 \rangle = 2 \left(\frac{g_W}{M_W c} \right)^4 (p_1 \cdot p_2)(p_3 \cdot p_4)$$

(the same as in previous case)

DECAY OF THE NEUTRON

In the rest frame of the neutron :

$$\langle |\mathcal{M}|^2 \rangle = \left(\frac{g_W}{M_W c} \right)^4 m_n E_2 \left[(m_n^2 - m_p^2 - m_e^2) c^2 - 2m_n E_2 \right]$$

We can't ignore the mass of the electron.

As before :

$$d\Gamma = \frac{\langle |\mathcal{M}|^2 \rangle}{2\hbar m_n} \left(\frac{c d^3 \vec{p}_2}{(2\pi)^3 2E_2} \right) \left(\frac{c d^3 \vec{p}_3}{(2\pi)^3 2E_3} \right) \left(\frac{c d^3 \vec{p}_4}{(2\pi)^3 2E_4} \right) \times \\ \times (2\pi)^4 \delta^4 (\mathbf{p}_1 - \mathbf{p}_2 - \mathbf{p}_3 - \mathbf{p}_4)$$

where :

$$E_2 = c |\vec{p}_2|, \quad E_3 = c \sqrt{|\vec{p}_3|^2 + m_p^2 c^2}, \quad E_4 = c \sqrt{|\vec{p}_4|^2 + m_e^2 c^2}$$

DECAY OF THE NEUTRON

The \vec{p}_2 integral yields :

$$d\Gamma = \frac{2 \langle |\mathcal{M}|^2 \rangle c^3}{(4\pi)^5 \hbar m_n} \frac{(d^3 \vec{p}_2)(d^3 \vec{p}_4)}{E_2 E_3 E_4} \delta \left(m_n c - \frac{E_2}{c} - \frac{E_3}{c} - \frac{E_4}{c} \right)$$

$$\text{and : } E_3 = c \sqrt{|\vec{p}_2 + \vec{p}_4|^2 + m_p^2 c^2}$$

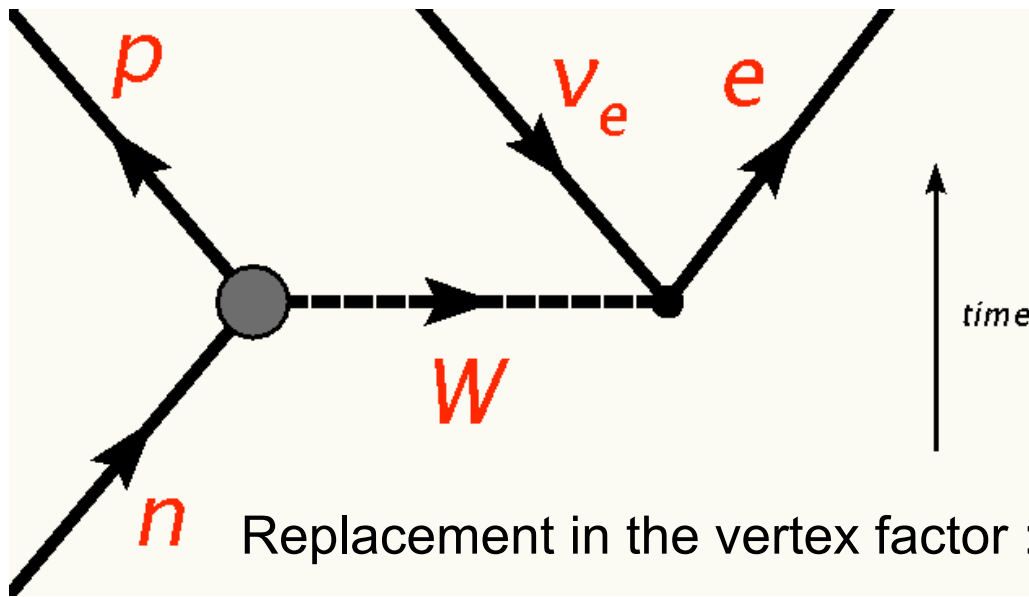
$$d^3 \vec{p}_2 = |\vec{p}_2|^2 d|\vec{p}_2| \sin \theta d\theta d\varphi = \frac{E_2^2}{c^3} dE_2 \sin \theta d\theta d\varphi$$

Setting the z-axis along \vec{p}_4 (which is *fixed*, for the purposes of the \vec{p}_2 integral), we have :

$$E_3 = c \sqrt{|\vec{p}_2|^2 + |\vec{p}_4|^2 + 2|\vec{p}_2||\vec{p}_4| \cos \theta + m_p^2 c^2} \equiv cx$$

$$\text{and : } \frac{E_2 \sin \theta d\theta}{E_3} = - \frac{dx}{|\vec{p}_4|}$$

DECAY OF THE NEUTRON



But the proton and neutron are not point particles.

Replacement in the vertex factor: $(1 - \gamma^5) \rightarrow (c_V - c_A \gamma^5)$

$$c_V = 1.000 \pm 0.003, \quad c_A = 1.26 \pm 0.02$$

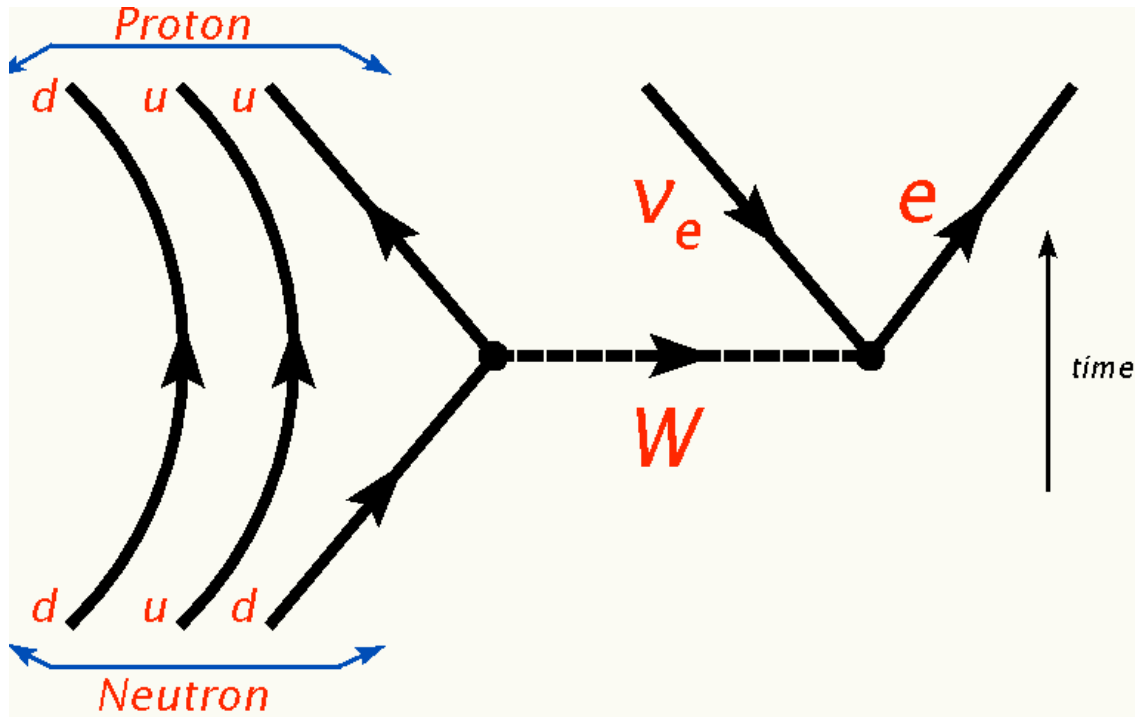
c_V is the correction to the **vector** "weak charge"

c_A is the correction to the **axial vector** "weak charge"

$$\Gamma \rightarrow \Gamma \times \frac{1}{4} (c_V^2 + 3c_A^2) = \Gamma \times 1.44$$

$$\tau \rightarrow \frac{\tau}{1.44} = \frac{1316 \text{ s}}{1.44} = 914 \text{ s}$$

DECAY OF THE NEUTRON

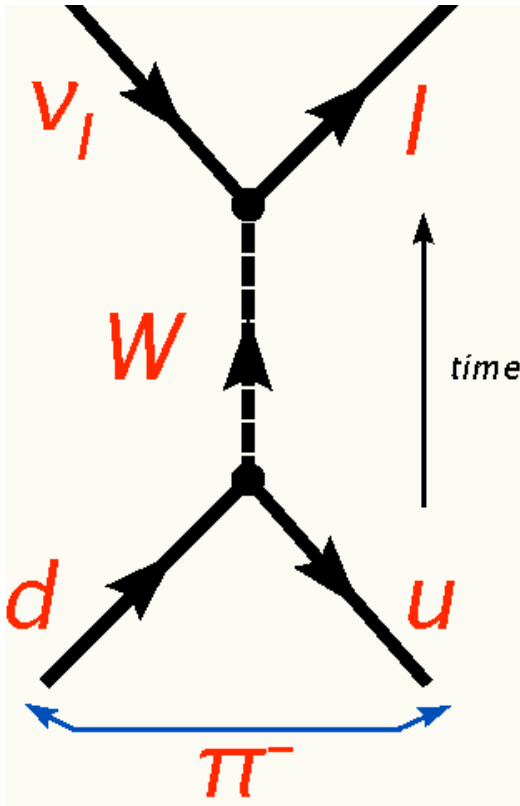


Another correction, the quark vertex carries a factor of $\cos \theta_C$

$\theta_C = 13.1^\circ$ is the **Cabibbo** angle.

Lifetime :
$$\tau \rightarrow \frac{\left(\frac{\tau}{1.44} \right)}{\cos^2 \theta_C} = 963 \text{ s}$$

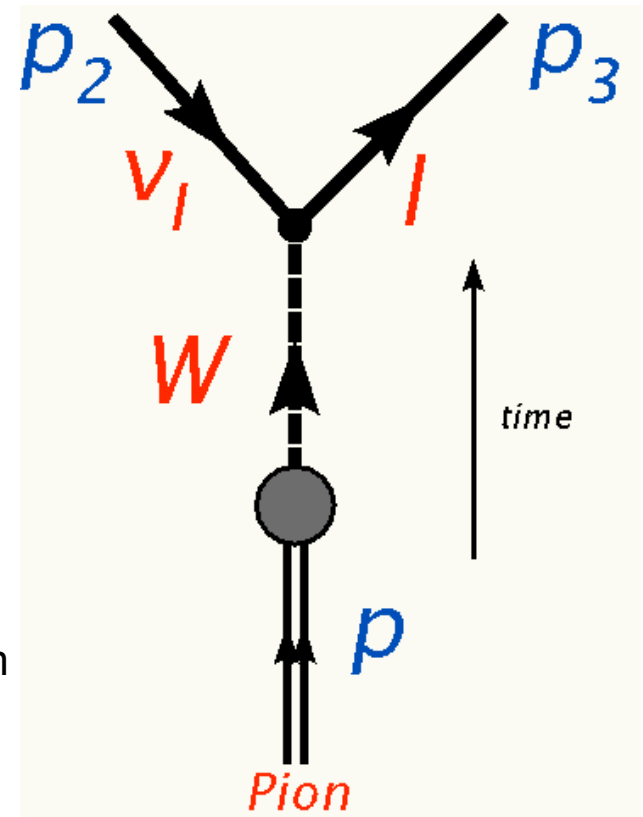
DECAY OF THE PION



$$\pi^- \rightarrow l^- + \bar{\nu}_l$$

The decay of the pion is really a scattering event in which the incident quarks happen to be bound together.

We do not know how the W couples to the pion. Use the "form factor".



$$\mathcal{M} = \frac{g_w^2}{8(M_w c)^2} \left[\bar{u}(3) \gamma_\mu (1 - \gamma^5) v(2) \right] F^\mu$$

$$F^\mu = f_\pi p^\mu \quad \text{"form factor"}$$

DECAY OF THE PION

$$\begin{aligned} \langle |\mathcal{M}|^2 \rangle &= \left[\frac{f_\pi}{8} \left(\frac{g_w}{M_w c} \right)^2 \right]^2 p_\mu p_\nu \text{Tr} \left[\gamma^\mu (1 - \gamma^5) \not{p}_2 \gamma^\nu (1 - \gamma^5) (\not{p}_3 + m_l c) \right] = \\ &= \frac{1}{8} \left[f_\pi \left(\frac{g_w}{M_w c} \right)^2 \right]^2 \left[2(p \cdot p_2)(p \cdot p_3) - p^2 (p_2 \cdot p_3) \right] \end{aligned}$$

$$p = p_2 + p_3, \quad p \cdot p_2 = p_2 \cdot p_3, \quad p \cdot p_3 = m_l^2 c^2 + p_2 \cdot p_3$$

$$p^2 = p_2^2 + p_3^2 + 2p_2 \cdot p_3, \quad 2p_2 \cdot p_3 = (m_\pi^2 - m_l^2) c^2$$

$$\langle |\mathcal{M}|^2 \rangle = \left(\frac{g_w}{2M_w} \right)^4 f_\pi^2 m_l^2 (m_\pi^2 - m_l^2)$$

DECAY OF THE PION

$$\Gamma = \frac{|\vec{p}_2|}{8\pi\hbar m_\pi^2 c} \langle |\mathcal{M}|^2 \rangle \quad |\vec{p}_2| = \frac{c}{2m_\pi} (m_\pi^2 - m_l^2)$$

The decay rate :

$$\Gamma = \frac{f_\pi^2}{\pi\hbar m_\pi^3} \left(\frac{g_w}{4M_w} \right)^4 m_l^2 (m_\pi^2 - m_l^2)^2$$

The following ratio could be computed without knowing the decay constant :

$$\frac{\Gamma(\pi^- \rightarrow e^- + \bar{\nu}_e)}{\Gamma(\pi^- \rightarrow \mu^- + \bar{\nu}_\mu)} = \frac{m_e^2 (m_\pi^2 - m_e^2)^2}{m_\mu^2 (m_\pi^2 - m_\mu^2)^2} = 1.28 \times 10^{-4}$$

Experimental value : $(1.23 \pm 0.02) \times 10^{-4}$

Relativistic Version

$$d\sigma \propto \prod_i \left(\frac{d^3 p_i}{E} \right) \delta \left(\sum_i p_i \right) |M|^2$$

“Fermi’s Golden Rule”

$$M = \frac{4\pi\alpha}{q^2} J_\mu^e(q) J^{\mu,p}(q)$$

“Amplitude”

$$J_\mu^e(q) = \bar{u}(k') \gamma_\mu u(k)$$

Electron (easy)

$$J^{\mu,p}(q) = \bar{u}(p') \left[F_1(q^2) \gamma^\mu + i \frac{q^\nu \sigma_{\mu\nu} \kappa}{2M} F_2(q^2) \right] u(p')$$

Proton (hard & extended!)

$$\frac{d\sigma}{d\Omega} = \frac{\alpha^2 \cos^2(\theta/2)}{4E^2 \sin^4(\theta/2)} \frac{E'}{E} \left[\left(F_1^2 + \frac{\kappa^2 Q^2}{4M^2} F_2^2 \right) + \frac{Q^2}{2M^2} (F_1 + \kappa F_2)^2 \tan^2(\theta/2) \right]$$

“Rosenbluth Formula”

$$Q^2 = -q^2$$

V-A: Universal Theory of Weak Interaction

The story of the discovery of the Chiral V-A interaction in the classic weak processes of beta decay, muon capture by nuclei, and muon decay has been told many times. Sudarshan was a student working under the supervision of Robert Marshak. Marshak suggested in early 1956 that he should study weak interactions. Sudarshan studied every paper on weak interactions beginning with Sargent, Fermi, Yukawa, Gamow and Teller, Konopinski, Wu, and a multitude of others. He had also read the paper by Tiomno and Wheeler on the possibility of a Universal Fermi Interaction. Fermi had postulated a scalar, formed out of four Fermi fields, for the form of the weak interactions, in analogy with electromagnetic interactions. Soon it was found that the form of the interaction had to be generalized to include spin-dependent interactions as pointed out by Gamow and Teller. However, when special relativity had to be taken into account, the most general form for the interaction Lagrangian turned out to be

$$\mathcal{L}_i = \sum_{i=1}^5 g_i \{ \bar{\psi}_1 \mathcal{O}^i \psi_2 \} \{ \bar{\psi}_3 \mathcal{O}_i \psi_4 \} \quad (1)$$

where the operator $\mathcal{O}_i = (\mathbf{1}, \gamma_\mu, \sigma_{\mu\nu}, i\gamma_5\gamma_\mu, \text{ or } \gamma_5)$, and ψ_i are the four spinor fields involved in the decay. These covariant forms were called scalar (S), vector (V), tensor (T), axial vector (A), and pseudoscalar (P), respectively. In the non-relativistic limit, S and V reduce to the Fermi interaction, while T and A reduce to Gamow-Teller.

The consensus at that time, based on many experiments, was that the beta decay weak interaction was scalar and tensor. After the discovery of parity violation in 1956, papers on this subject appeared in torrents. Having studied all of them, by the end of 1956, Sudarshan was convinced that if there was a Universal Fermi Interaction it had to include the axial vector interaction since the charged pion decay may be viewed as if it were beta decay of a “nucleus with zero atomic weight”. He then systematically studied all the work up to that time, both theoretical and experimental, with this criterion in mind.

By December 1956 - January 1957, Sudarshan had discovered that the results of angular correlation experiments on “classical” (non parity violating) beta decays were internally inconsistent! The electron-neutrino angular correlation in the neutron and in the Ne¹⁹ decays were indicative of S, T or V, A. But the available data on He⁶ showed it to be tensor T. On this basis, the preferred combination was S, T. But the Ar³⁵ decay, which is dominantly

of the Fermi type, showed that it is V. Not all these could be true at the same time. In muon decay, since the neutrino and antineutrino were taken to be massless and chiral, the only interaction was vector or axial vector, or a combination of both [in the charge retention order $(\mu e)(\nu\nu)$].

At the time of the Rochester conference in spring 1957, Sudarshan had essentially all the arguments in place for Chiral V-A interaction, but there were four experiments which stood in the way. He wanted to present it at the Rochester High Energy Conference, but it was ruled out since he was still only a graduate student! Marshak himself was very preoccupied with the nucleon-nucleon strong interactions. He had chosen to present a phenomenological nucleon-nucleon potential at the conference. P.T. Matthews, a visiting professor at Rochester, was entrusted with reporting the V-A theory in a few lines, but he forgot to do so. There was much inconclusive discussion between experts about the form of the weak interactions which Sudarshan could have resolved had he been given a few minutes to present his theory.

Marshak was going to be at the RAND Corporation in Los Angeles and offered Sudarshan and Bryan (another student of his) one-month summer salary if they could be in Los Angeles. As an alien, Sudarshan could not enter RAND, so it was arranged that they meet outside off and on. At that time Gell-Mann was also a consultant to RAND. Marshak told him briefly about their work on weak interactions and Gell-Mann was appreciative of it. So, ten days later Marshak had arranged lunch at a nearby restaurant. The lunch group included Marshak, Gell-Mann, Bryan, Leona Marshall, Felix Boehm, A.H. Wapstra, Berthold Stech, and Sudarshan. Sudarshan was asked to give a presentation which he did in full detail. (This was the only time he was invited to give a talk on V-A!) He made the observation that the data was internally inconsistent. He also singled out the experiments which were most likely to be mistaken. He suggested that the weak decay interaction was of the universal form V-A with maximal parity violation, in which every field was multiplied by the chiral projection operator. Incidentally, if this is so, both the charge exchange and the charge retention ordering give the same unique interaction. As presented, Sudarshan's work was a critical examination of all the existing data on all weak interactions, and it showed that the only possibility was Chiral V-A. Gell-Mann was enthusiastic about Sudarshan and Marshak's discovery.

Marshak asked Sudarshan to write up the work, which he did, and gave it to Marshak

that weekend. Marshak decided to present this fundamental discovery at the Padua-Venice conference on Mesons and Newly Discovered Particles in September 1957 [1], rather than to have it published immediately (which probably cost him and Sudarshan a Nobel prize). Later, Marshak decided that a sequel to the presentation at the Padua-Venice conference (which, incidentally, was published two years later) should be published in the Physical Review [2].

In the meantime, Feynman and Gell-Mann published a paper in the Physical Review *asserting* the V-A structure of the weak interactions, merely thanking Sudarshan for “important discussions”. Their paper, which most people quote in precedence over the Sudarshan-Marshak paper, does not contain any analysis of the data, including those of the experiments that Sudarshan and Marshak had singled out to be most likely in error. These experiments were eventually redone and gave the results predicted by Sudarshan and Marshak.

Many fables and some actual accounts about this have been presented by various people. Notably, Feynman made a public statement in 1963 [3]: “The V-A theory that was discovered by Sudarshan and Marshak, publicized by Feynman and Gell-Mann —”. Marshak has also spoken and written about this history ([4–8]).

Weak interaction theory (V-A) could be extended to the leptonic decays of baryons and mesons. The question arises as to the isotopic spin transformation properties of these. The simplest is to assume that the interaction current in leptonic decays transforms as $I=\frac{1}{2}$. This leads to sum rules [9]. The non-leptonic decays of hyperons have also been studied and shown to involve near-maximal parity violation and consequent baryon polarization [10, 11].

In quantum electrodynamics the conservation of the electric current led to the Ward-Takahashi identities. This was generalized to cases where the divergence of the interaction current does not vanish but is a multiple of the pion field, resulting in generalized Ward-Takahashi identities [12].

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