AN INTRODUCTION TO QUANTUM ELECTRODYNAMICS *

by

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Preface

These lectures were given as part of a seminar course in Theoretical Chemistry in April, 1965. They were designed to make quantum electrodynamics appear as much like the familiar presentations of the non-relativistic quantum mechanics of particles, as possible. For this reason the techniques are very much "pre-war" - there are no propagators, no Feynman diagrams and no temporal or longitudinal photons. Also there are almost no positrons.

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FIRST LECTURE

[1.] An important point to keep firmly in mind during these lectures is that in quantum electrodynamics, Maxwell's equations do not play a role similar to that of Schrödinger's equation. Rather they are analogous to Newton's equations. $\underline{\mathcal{E}}$ and $\underline{B}$ are not similar to ψ, rather they are similar to $\underline{x}$ and $\underline{p}$; they are the dynamical variables which characterize the electromagnetic field. Just as $\underline{x}$ and $\underline{p}$ become operators in quantum mechanics, so do $\underline{\mathcal{E}}$ and $\underline{B}$. Just as Newton's equations of motion remain valid as operator equations in quantum mechanics, so do Maxwell's equations.

[2.] In any field theory we have an infinite number of dynamical variables - the value at a given time, of the field quantities at each point in space. In order not to obscure the basic ideas with the complications of a vector field in three space dimensions, let us consider the simplest sort of a field - that which describes the small vibrations of a string. What we will show is that the string can be regarded as a collection of harmonic oscillators. To "quantize the string" we will then simply quantize the oscillators.

[3.] Let us denote the displacement of the string from equilibrium by $\phi(x,t)$. Then ϕ satisfies the one-dimensional wave equation

(we assume for simplicity that the string has a uniform mass per unit length ρ and is under a uniform tension T)

$$\frac{1}{c^2}\,\frac{\partial^2\phi}{\partial t^2} = \frac{\partial^2\phi}{\partial x^2} \qquad (1)$$

where c , the velocity of waves on the string, is given by

$$\frac{1}{c^2} = \frac{\rho}{T} \qquad (2)$$

Note that we have no dispersion, in exact analogy with the propagation of electromagnetic waves in free space.

[4.] Associated with the motion of the string is an energy H given by

$$H = \int dx \left[\frac{1}{2}\,\rho\left(\frac{\partial\phi}{\partial t}\right)^2 + \frac{1}{2}\,T\left(\frac{\partial\phi}{\partial x}\right)^2\right] \qquad (3)$$

the first term in the integrand clearly being the kinetic energy per unit length and the second term the potential energy.

[5.] The motion of the string also produces momentum which propagates along the string. To infer a formula for it, let us write eqn. (3) as

$$H = \int h\,dx \quad .$$

Then we have (what we want to do is derive an analogue of Poynting's theorem in electromagnetism)

$$\frac{\partial h}{\partial t} = \rho \frac{\partial \phi}{\partial t} \frac{\partial^2 \phi}{\partial t^2} + T \frac{\partial \phi}{\partial x} \frac{\partial^2 \phi}{\partial t \partial x}$$

which, using (1) and (2) becomes

$$\frac{\partial h}{\partial t} = T \frac{\partial \phi}{\partial t} \frac{\partial^2 \phi}{\partial x^2} + T \frac{\partial \phi}{\partial x} \frac{\partial^2 \phi}{\partial t \partial x}$$

or

$$\frac{\partial h}{\partial t} = \frac{\partial}{\partial x}\left(T \frac{\partial \phi}{\partial t} \frac{\partial \phi}{\partial x}\right)$$

which is just the desired analogue of Poynting's theorem with the quantity

$$- T \frac{\partial \phi}{\partial t} \frac{\partial \phi}{\partial x}$$

playing the role of Poynting's vector and giving the energy flux. We now argue by analogy that, just as in electromagnetic theory where the Poynting vector divided by c^2 also yields the momentum density, so here. Thus we infer that the "wave momentum" is

$$\mathcal{P} = - \int \frac{T}{c^2} \frac{\partial \phi}{\partial t} \frac{\partial \phi}{\partial x} \, dx \qquad (4)$$

[6.] The general motion of a string can be quite complex and depends on the initial conditions. However, there are certain especially simple forms of oscillation - the normal modes of oscillation - wherein all parts of the string move in a simple harmonic fashion with the same frequency. It is trivial to verify that a superposition of plane waves, one going to the right, the other to the left

$$\beta_k \, e^{i(kx-\omega_k t)} + \beta_k^* \, e^{-i(kx-\omega_k t)} \qquad (5)$$

with β_k constant and

$$\left(\frac{\omega_k}{k}\right)^2 = c^2 \qquad (6)$$

is a (real) normal mode of oscillation. That is (i) clearly all parts of the string are oscillating with frequency ω_k, and (ii) this expression is a solution of eqn. (1) under the conditions indicated.

[7.] A remark on notation: In what follows ω_k will always be taken to be a positive number whereas k may have either sign. This clearly involves no loss of generality.

[8.] So far we have not mentioned how long our string is nor have we discussed boundary conditions. To have an analogue to electromagnetic waves in space it would appear that we should deal with a

string of infinite length. However, it proves convenient to consider a finite length L and then go to the limit $L = \infty$. As to boundary conditions, the simplest ones to employ are the so-called <u>periodic boundary conditions</u> which require, if we assume our string to stretch from $-L/2$ to $L/2$ that

$$\phi(-\frac{L}{2}, t) = \phi(\frac{L}{2}, t) \quad .$$

Applied to (5) this implies that

$$kL = 2\nu\pi \quad , \quad \nu = 0, \pm 1, \pm 2, \ldots \tag{7}$$

which, in turn, insures the orthogonality of the normal modes:

$$\int_{-L/2}^{L/2} dx \; e^{i(k-k')x} = L \, \delta_{k,k'} \quad . \tag{8}$$

Other choices of boundary conditions, for example, that the string be fixed at the two ends, i.e.

$$\phi(-L/2,t) = \phi(\frac{L}{2},t) = 0$$

imply restrictions on k <u>and</u> β_k and are more cumbersome to deal with. In any case one can argue that in the limit $L \to \infty$, which is the case of real interest to us, the exact nature of the

boundary conditions should be unimportant.

[9.] The general motion of the string can be written as

$$\phi(x,t) = \sum_k \left(\beta_k \, e^{i(kx - \omega_k t)} + \beta_k^* \, e^{-i(kx - \omega_k t)} \right)$$

where the β_k and β_k^* may be determined from $\phi(x,0)$ and $\left(\frac{\partial \phi}{\partial t}\right)_{x,0}$ via Fourier's theorem (recall eqn. (7) and (8)).

[10.] Let us now introduce the dynamical variables (i.e. they are time dependent) $b_k = \beta_k \, e^{-i\omega_k t}$ and write

$$\phi(x,t) = \sum_k \left(b_k \, e^{ikx} + b_k^* \, e^{-ikx} \right) \quad .$$

Then we see that the infinite and trivial set of differential equations

$$\frac{db_k}{dt} = -i \, \omega_k b_k \quad , \quad \frac{db_k^*}{dt} = i \, \omega_k b_k^* \qquad (9)$$

are exactly equivalent to eqn. (1) - the normal coordinates b_k give a dynamical description equivalent to that provided by the field. Further from our point of view, the introduction of the b_k as dynamical variables rather than the field will be especially helpful because:

(a) they form a discrete (though infinite) set, more like x and p and

(b) because their equations of motion, the ordinary differential equations (9), begin to seem more like Newton's equations which we know how to quantize, than the partial differential equation (1).

[11.] However, in classical mechanics one is not used to dealing with complex dynamical variables and the relation of (9) to a Newtonian equation is certainly not clear. Evidently, however, (9) is describing a simple harmonic oscillation and indeed, in the quantum mechanical treatment of the harmonic oscillator, it has proved convenient to introduce complex variables. Namely, let us define (we are discussing an harmonic oscillator now)

$$b \equiv (m\omega x + ip)$$

Then from the definition of momentum

$$m \frac{dx}{dt} = p$$

and Newton's equation

$$\frac{dp}{dt} = -m\omega^2 x$$

one readily finds that

$$\frac{db}{dt} = -i\omega b \quad , \qquad \frac{db^*}{dt} = i\omega b^* \tag{10}$$

just of the form (9). Thus we have shown that we can describe the string by a set of dynamical variables which formally behave like a set of harmonic oscillators.

[12.] So far all this has been classical. To prepare for the introduction of quantum mechanics it is convenient to redefine our dynamical variables a bit. For the field we will write

$$b_k = \sqrt{\frac{\hbar}{2\rho\omega_k L}}\; a_k$$

and for our harmonic oscillator we write

$$b = \sqrt{2m\hbar\omega}\; a \quad .$$

a_k and a, of course, still satisfy equations of the form (9) and (10) respectively.

Further, for the harmonic oscillator, we see immediately that the energy expressed in terms of the a and a^* becomes

$$H = \frac{p^2}{2m} + \frac{1}{2} m\omega^2 x^2 = \frac{\hbar}{2}\omega(a^*a + aa^*)$$

where, in preparation for the introduction of quantum mechanics, we have been careful about the order of factors.

We will now show that thanks to our choice of constants in the definition of a_k, the energy and momentum of the string take the form

$$H = \sum_k \frac{\hbar}{2} \omega_k (a_k^* a_k + a_k a_k^*) \tag{11}$$

$$\mathcal{P} = \sum_k \frac{1}{2} \hbar k \, (a_k^* a_k + a_k a_k^*) \tag{12}$$

The calculation involves simply substituting

$$\phi = \sum_k \sqrt{\frac{\hbar}{2\rho\omega_k L}} \, (a_k e^{ikx} + a_k^* e^{-ikx}) \tag{13}$$

and

$$\frac{\partial \phi}{\partial t} = \sum_k \sqrt{\frac{\hbar}{2\rho\omega_k L}} \, (-i\omega_k)(a_k e^{ikx} - a_k^* e^{-ikx}) \tag{14}$$

into (3) and (4) and carrying out the integrations using (8). Let us illustrate by calculating H. It is convenient to rewrite (13) and (14) by changing the variable of summation in the a^* terms from k to $-k$. Then we may write

$$\phi = \sum_k q_k e^{ikx} \quad , \quad \frac{\partial \phi}{\partial t} = \sum_k p_k e^{ikx}$$

where

$$q_k = \sqrt{\frac{\hbar}{2\rho\omega_k L}}\,(a_k + a_{-k}^*) \quad \text{and} \quad p_k = \sqrt{\frac{\hbar}{2\rho\omega_k L}}\,(-i\omega_k)(a_k - a_{-k}^*).$$

Then since

$$\frac{\partial\phi}{\partial x} = \sum_k ikq_k e^{ikx}$$

(3) becomes, using (8)

$$H = \sum_k L\left(\frac{1}{2}\rho p_k p_{-k} + \frac{1}{2} T k^2 q_k q_{-k}\right).$$

Reinserting the definitions of p_k and q_k and $Tk^2 = \omega_k^2\rho$ (using (2) and (6), this becomes

$$H = \frac{1}{4}\sum_k \hbar\omega_k \left[\begin{array}{l} -(a_k - a_k^*)(a_{-k} - a_k^*) \\ \\ +(a_k + a_{-k}^*)(a_{-k} + a_k^*) \end{array}\right]$$

$$= \frac{1}{2}\sum_k \hbar\omega_k (a_k a_k^* + a_{-k}^* a_{-k})$$

which is exactly eqn. (11) when one notes that $\sum_k \hbar\omega_k a_{-k}^* a_{-k} = \sum_k \hbar\omega_k a_k^* a_k$. The calculation of ρ is similar.

Note that, as must be the case, H and ρ are <u>independent of time</u>, all time dependent terms like $a_k^* a_{-k}^*$ or $a_k a_{-k}$ having cancelled out.

[13] We are now ready to introduce quantum mechanics. Consider again the harmonic oscillator. The standard rule

$$[x, p] = i\hbar \tag{15}$$

immediately implies

$$[a, a^*] = 1$$

with a^* now identified as the Hermitian conjugate of a. "Newton's" equations of motion,

$$\frac{da}{dt} = -i\omega a \quad , \quad \frac{da^*}{dt} = i\omega a^*$$

as an operator equation then follows from the standard quantum mechanical formula for a time derivative:

$$\frac{dF}{dt} = \frac{i}{\hbar}[H,F]$$

with F replaced successively by a and a^*.

This suggests that for the string we similarly introduce the commutation relations:

$$[a_k, a_{k'}^*] = \delta_{kk'} \tag{16}$$

$$[a_k, a_{k'}] = 0 \quad , \quad [a_k^*, a_{k'}^*] = 0 \tag{17}$$

where we have assumed that dynamical variables associated with <u>different</u> normal coordinates <u>commute</u>, much as one assumes that variables referring to different particles commute.

These assumptions are then (partially) justified by noting that the "field equations"

$$\frac{da_k}{dt} = -i\omega_k a_k \quad , \quad \frac{da_k^*}{dt} = i\,\omega_k a_k^*$$

then follow directly as <u>operator equations</u> from

$$\frac{da_k}{dt} = \frac{i}{\hbar}\,[H,\, a_k] \qquad , \text{ etc.}$$

[14.] What are the eigenvalues, E and P of H and $\mathcal{P}$? For the harmonic oscillator we see that since $aa^* = a^*a+1$ we can write

$$H = \hbar\omega\,(a^*a + \frac{1}{2}\,)$$

and since the eigenvalues are well known to be $E_n = \hbar\omega\,(n + \frac{1}{2}\,)$, we infer that the eigenvalues of a^*a are the integers - <u>a^*a is the number operator</u>. Then, by analogy, the energy and momentum eigenvalues for the string are

$$E\,\{N_k\} = \sum_k \hbar\omega_k (N_k + \frac{1}{2}\,)\;;\quad N_k = 0,1,2\,\text{--} \qquad (18)$$

$$P\{N_k\} = \sum_k \hbar k \left(N_k + \frac{1}{2}\right) \qquad (19)$$

i.e. we have quanta! - but that's about all. That is, it should be emphasized that the upshot of all this discussion has been rather trivial: Each normal mode of the "free" string is characterized by its wave number k. In each mode we can have an arbitrary number of quanta (Bose-Einstein statistics) each having energy $\hbar\omega_k$ and momentum $\hbar k$.

[15.] The ground state or "vacuum" is that state with all $N_k = 0$. For this state $E = \sum_k \frac{\hbar\omega_k}{2}$ is infinite. On the other hand, from symmetry, (we have as many positive k's as negative) the momentum of this state, $P = \sum_k \frac{1}{2}\hbar k = 0$ and the $\sum_k \hbar k\frac{1}{2}$ term may be omitted from (19).

The presence of the infinite "zero point energy" in (18) is a bit disturbing. One may argue it away by saying that anyway only energy differences are important. Alternatively one may say that classically we could anyway have replaced $a_k^* a_k + a_k a_k^*$ by $2a_k^* a_k$. However, what cannot be talked away is the non-trivial character of the ground state - that there are quantities such as $a_k a_k^*$ which have non-zero expectation values in the vacuum (applied to the harmonic oscillator, the non-trivial character is revealed as the finite extension of both the coordinate and momentum wave functions - the particle doesn't just sit at the bottom of the well).

This is a true and observable quantum mechanical effect. The vacuum, so to speak, has properties!

[16.] As we have mentioned, our results to this point are essentially trivial. Things become interesting when one introduces <u>interactions</u> (perturbations). In dealing with interactions we will need <u>matrix elements of our dynamical variables</u> between the energy eigenstates of the free field. Happily these are quite simple for harmonic oscillators and all calculations may be done <u>without explicitly introducing wave functions for the field</u>. (such wave functions would be <u>infinite products</u> of harmonic oscillator wave functions, one for each mode, which are functions of $x_k \sim a_k + a_k^*$).

Let us first deal with the harmonic oscillator, the generalization to the string being immediate. Consider the nth excited eigenstate ψ_n. For this state $a^* a \psi_n = n \psi_n$. Consider now the state $a\psi_n$. If we let $a^* a$ act on this state we have

$$a^* a \, a \psi_n = [a^* a, a] \psi_n + a a^* a \psi_n$$

$$= - a \psi_n + an \psi_n$$

$$= (n-1) \, a \psi_n$$

whence we infer that $a \psi_n$ is proportional to ψ_{n-1}. More detailed discussion shows that in fact

$$a\psi_n = \sqrt{n}\,\psi_{n-1} \qquad (20)$$

In a similar way one shows that

$$a^*\psi_n = \sqrt{n+1}\,\psi_{n+1} \qquad (21)$$

For the harmonic oscillator then a is a lowering operator, and a^* is a raising operator. In field theory, by analogy, a_k is best described as a destruction operator and a_k^* as a creation operator. Applied to a state with N_k quanta in mode k, and arbitrary numbers of quanta in other modes, a_k produces $\sqrt{N_k}$ times the state with one less quantum in the kth mode, the number of quanta in other modes remaining unchanged. The a_k^* produces $\sqrt{N_k + 1}$ times the state with one more quantum in mode k, the number of quanta in other modes again remaining the same. Applied to the vacuum any a_k yields zero.

[17.] There is another approach to the quantization of the string, the so-called canonical method, which is very elegant, but which unfortunately doesn't work in a simple way for the electromagnetic field. It is most directly derived by considering the string as the limit of a large number of particles joined by a weightless string. One quantizes the particles and then passes to the limit. The $\phi(x,t)$ would then be the position of the particle at while $\frac{\partial\phi}{\partial t}$ would be its velocity.

We will not carry through the details of this procedure, but we mention it because this picture then leads us to expect that $[\phi(x,t),\phi(x',t)] = 0$ for all x and x', while $\left[\phi(x,t), \left(\frac{\partial\phi}{\partial t}\right)_{x',t}\right]=0$ for $x \neq x'$, but not for $x = x'$ just corresponding to (15) and to the fact (see also [13.]) that dynamical variables associated with different particles commute.

Direct calculation then shows, using (13) and (14), (16) and (17) that, as we expect

$$[\phi(x,t),\ \phi(x',t)] = 0$$

$$\left[\phi(x,t),\ \pi\left(\frac{\partial\phi}{\partial t}\right)_{x',t}\right] = ih\,\delta(x-x')$$

where we have used

$$\frac{1}{L}\sum_{k} e^{ik(x-x')} = \delta(x-x') \quad .$$

[18.] Given the Hamiltonian $\frac{\hbar\omega}{2}(a^*a+aa^*)$ and the requirement that

$$\frac{da}{dt} = \frac{i}{\hbar}[H,a]$$

should yield

$$\frac{da}{dt} = -i\omega a$$

and similarly for a^*, another possible quantum rule is

$$a^*a + aa^* = 1 \quad , \quad aa = a^*a^* = 0$$

which one can show yields Fermi-Dirac statistics.

For the string we might thus use

$$a_k^* a_{k'} + a_{k'} a_k^* = \delta_{kk'}$$

$$a_k a_{k'} + a_{k'} a_k = 0$$

$$a_k^* a_{k'}^* + a_{k'}^* a_k^* = 0 \quad .$$

However, when applied to ϕ this yields, for $x = x'$

$$\phi(x,t)\,\phi(x,t) + \phi(x,t)\,\phi(x,t) = 0$$

that is, $\phi^2 = 0$, which implies that $\phi \equiv 0$ since ϕ is a Hermitian operator. Since $\phi \equiv 0$ means "no theory" we conclude that we cannot consistently quantize the string according to Fermi-Dirac Statistics.

[19.] In the commutation relations we have written down thus far, all operators have been evaluated at the same time. Since, for the string, we know in detail how the operators depend on time we could also (though we won't) evaluate commutators involving operators at different times. In the presence of interaction we are not, in

general, able to do this latter exactly. However, in a general way, we may expect that though the interaction may modify the commutators involving different times, it will not modify those involving a common time. We argue here by analogy with ordinary quantum mechanics. The rule (15) which relates the coordinate and momentum of a particle at the same time applies in all circumstances (i.e. whatever the interactions), and again at the same time, variables associated with different particles (or with different degrees of freedom of the same particle) always commute. However, if the particles interact then variables associated with different particles (or with different degrees of freedom of the same particle) at different times will, in general, not commute. Indeed, this is just an expression of the fact that the particles are interacting, i.e. that a measurement of, say, the coordinate of one particle can affect the coordinate of another particle at a later time. Also, as another example, the commutator of the momentum of a particle at one time and the coordinate of the same particle at another time will depend on the nature of the forces to which the particle is being subjected (with no forces, it is in fact independent of the time difference).

[20] The underlying philosophy of our discussion has been to view the formalism of quantum field theory as a direct extension of the formalism of particle mechanics to an infinite number of dynamical variables. We have tried to play down differences. The use of a finite L helps us here by making our ultimate choice of dynamical variables, the a_k and a_k^*, a discrete, though infinite, set. If we introduce interaction, then our procedure will be to express

the new Hamiltonian again in terms of the a_k and a_k^* (and usually variables describing the system with which the field is interacting) all referred to a fixed time - just as one expresses the Hamiltonian for interacting particles in terms of their x's and p's at a fixed time. Once this is done, we may use standard quantum mechanical procedures to carry out calculations. These calculations are usually most simple if, one way or another, we use the free field energy eigenstates as a basis since then we may use the simple results of [16.] to evaluate matrix elements. In these lectures we will use only perturbation methods, however one can also use variational methods, etc.

[21.] An Example: Suppose our string is perturbed in such a way that an extra term appears in H of the form $g\phi(0,t)$ where g is a constant, the coupling constant. Expressed in terms of the basic dynamical variables, then

$$H = \sum_k \hbar\omega_k \left(a_k^* a_k + \frac{1}{2}\right) + g \sum_k \sqrt{\frac{\hbar}{2\rho\omega_k L}} \left(a_k + a_k^*\right)$$

$$\equiv H_o + gV$$

where, to keep the problem simple, we have not introduced any dynamical variables associated with the perturber.

Actually, this Hamiltonian is sufficiently simple that we can find its eigenvalues exactly. However, let us treat it by

perturbation theory confining ourselves to the ground state, the vacuum. Denoting the unperturbed vacuum by ψ_o, the first order energy correction

$$E^{(1)} = g(\psi_o, V\psi_o)$$

is seen to vanish because $(\psi_o, a_k\psi_o) = 0$ and

$$(\psi_o, a_k^*\psi_o) = (a_k\psi_o, \psi_o) = 0$$

for all k.

The second order correction is

$$E^{(2)} = g^2 \sum_N \frac{|(\psi_o, V\psi_N)|^2}{E_o - E_N} .$$

From [16.] we see that the ψ_N which contribute are the one quantum states - there is one quantum in some mode k, no quanta in any other mode. For such a state, $E_0 - E_N = -h\omega_k$ (the zero-point energy cancelling), and $(\psi_o, V\psi_N) = \sqrt{\frac{\hbar}{2\rho\omega_k L}}$ since only the a_k term in V contributes and the matrix element of a_k is one ($N_k = 1$). Thus we have

$$E^{(2)} = -g^2 \sum_k \frac{1}{2\rho\omega_k^2 L}$$

Let us now take the limit $L \to \infty$. The spacing of successive k values then becomes very small (namely from eqn. (7) we have

$$\Delta k = \frac{2\pi}{L}$$

whence we can replace the sum by an integral according to

$$\sum_k \ldots = \frac{L}{2\pi} \sum_k \Delta k \ldots \to \frac{L}{2\pi} \int dk \ldots \quad . \qquad (22)$$

In particular, then, our second order energy becomes

$$E^{(2)} = - \frac{g^2}{4\pi \rho} \int \frac{dk}{\omega_k^2}$$

which is a divergent integral, because of the behavior of the integrand near $k = 0$ (infra-red catastrophe).

The main purpose of this example was to illustrate the application of conventional quantum-mechanical methods to field theory. It has also served to provide our second encounter with infinities in field theory.

SECOND LECTURE

[20.] Maxwell's equations for the electric and magnetic fields produced by charges are

$$\left.\begin{aligned} \nabla \times \mathcal{E} + \frac{1}{c}\frac{\partial B}{\partial t} &= 0 \\ \nabla \cdot B &= 0 \\ \nabla \times B - \frac{1}{c}\frac{\partial \mathcal{E}}{\partial t} &= \frac{4\pi}{c} j \\ \nabla \cdot \mathcal{E} &= 4\pi\rho \end{aligned}\right\} \qquad (23)$$

where j and ρ are the current and charge densities due to charges. To complete the dynamics, we must then adjoin Newton's equations describing the motion of the charges in response to the field. As is well-known, we can satisfy the first and second equations identically by introducing the vector and scalar potentials A and ϕ according to

$$\begin{aligned} B &= \nabla \times A \\ \mathcal{E} &= -\frac{1}{c}\frac{\partial A}{\partial t} - \nabla \phi \ . \end{aligned} \qquad (24)$$

Since we know further that $\underline{A}$ and ϕ will, presumably, occur in that part of the Hamiltonian describing the interaction of matter and field, since for example, for an electron in given external fields the Hamiltonian is

$$\frac{\left(\underline{p} + \frac{e}{c}\,\underline{A}^{(Ext)}\right)^2}{2m} - e\,\phi^{(Ext)} \quad .$$

Thus we are naturally led to use $\underline{A}$ and ϕ as dynamical variables rather than $\underline{\mathcal{E}}$ and $\underline{B}$.

The last two equations of the set (23) then become the equations of motion for $\underline{A}$ and ϕ :

$$\frac{1}{c^2}\,\frac{\partial^2 \underline{A}}{dt^2} - \nabla^2 \underline{A} + \underline{\nabla}\left(\underline{\nabla}\cdot\underline{A} + \frac{1}{c}\,\frac{\partial \phi}{\partial t}\right) = \frac{4\pi}{c}\,\underline{j}$$

$$-\nabla^2\phi - \frac{1}{c}\,\frac{\partial}{\partial t}\left(\underline{\nabla}\cdot\underline{A}\right) = 4\pi\rho \quad . \tag{25}$$

[21.] Given $\underline{A}$ and ϕ , eqn (24) determine $\underline{\mathcal{E}}$ and $\underline{B}$ uniquely and since $\underline{\mathcal{E}}$ and $\underline{B}$ are the physically measurable quantities (it is they, rather than $\underline{A}$ and ϕ which occur in Newton's equations of motion), this is fine. On the other hand given $\underline{B}$ and $\underline{\mathcal{E}}$, eqn. (24) do not determine $\underline{A}$ and ϕ uniquely. Namely, given a set of $\underline{A}$ and ϕ we can find any number of others which yield same $\underline{\mathcal{E}}$ and $\underline{B}$ according to

$$\underline{A} \rightarrow \underline{A} + \underline{\nabla} \Lambda$$

$$\phi \rightarrow \phi - \frac{1}{c} \frac{\partial \Lambda}{\partial t}$$

where Λ is an arbitrary function. The invariance of $\underline{B}$ and $\underline{\mathcal{E}}$, and hence of measurable quanties, to such transformations is called gauge invariance and such a transformation is called a gauge transformation.

[22.] Since we have decided to use $\underline{A}$ and ϕ as dynamical variables, the problem then arises of choosing a gauge in order to fix them uniquely. For our purposes it will be most convenient to assume that

$$\underline{\nabla} \cdot \underline{A} = 0 \quad . \tag{26}$$

This is the so-called Coulomb, or radiation, or transverse gauge. One can show that if one starts with an $\underline{A}$ which does not satisfy (26) then one can always find a Λ such that the transformed $\underline{A}$ will satisfy (26).

[25.] With this choice of gauge, the second equation (25) becomes

$$\nabla^2 \phi = -4\pi \rho$$

with the immediate solution

$$\phi(\underline{x},t) = \sum_i \frac{q_i}{|\underline{x} - \underline{x}_i(t)|}$$

where q_i is the charge on the i-th particle and $\underline{x}_i$ its position. Thus ϕ is no longer a dynamical variable as far as the field is concerned; it is completely expressed in terms of dynamical variables associated with the particles (all evaluated at the same time).

Thus we have further reduced the dynamical variablesof the field to $\underline{A}$, subject to the gauge condition (26) and its equation of motion,(the first of equations(25)) which is now

$$\frac{1}{c^2} \frac{\partial^2 \underline{A}}{\partial t^2} - \nabla^2 \underline{A} + \underline{\nabla} \frac{1}{c} \frac{\partial \phi}{\partial t} = 4\pi \frac{\underline{j}}{c} . \qquad (27)$$

[26.] Let us first consider free fields, $\varrho = \underline{j} = 0$. Then $\phi = 0$ and $\underline{A}$ satisfies the three dimensional wave equation

$$\frac{1}{c^2} \frac{\partial^2 \underline{A}}{\partial t^2} - \nabla^2 \underline{A} = 0 .$$

Quite in analogy to eqn. (13) we now analyze $\underline{A}$ into normal modes

$$\underline{A} = \sum_{\underline{k}} \sum_{s=1}^{2} \left[\frac{2\pi\hbar c^2}{\omega_k L^3} \right]^{\frac{1}{2}} \underline{\epsilon}_{\underline{k},s} \left[a_{\underline{k},s} e^{i\underline{k}\cdot\underline{x}} + a^*_{\underline{k},s} e^{-i\underline{k}\cdot\underline{x}} \right] \qquad (28)$$

where we have imposed periodic boundary conditions in a cube of volume L^3 so as to replace $\underline{A}$ by the discrete set of dynamical variables $a_{\underline{k},s}$, $a^*_{\underline{k},s}$, since from these boundary conditions it

then follows that $\underline{k}$ is discrete:

$$\underline{k} = \frac{2\pi}{L} \boldsymbol{\nu} \quad ; \quad \nu_x, \nu_y, \nu_z = 0, \pm 1, \pm 2, \ldots \tag{29}$$

In addition we have

$$\int \underline{dx}\, e^{i(\underline{k}-\underline{k}')\cdot\underline{x}} = L^3 \delta_{\underline{k},\underline{k}'} \tag{30}$$

The vector $\underline{k}$ tells us the direction of propagation of $\underline{A}$ in a normal mode and the unit vector $\underline{\epsilon}_{\underline{k},s}$ tells us its state of polarization. The gauge condition, equation (26), is then satisfied by having

$$\underline{k} \cdot \underline{\epsilon}_{\underline{k},s} = 0 \tag{31}$$

i.e. we are dealing with transverse waves. Since we can associate only two linearly independent polarizations s with each transverse wave the sum over s as indicated runs from 1 to 2. We assume (without loss of generality) that

$$\underline{\epsilon}_{\underline{k},s} \cdot \underline{\epsilon}_{\underline{k},s'} = \delta_{s,s'} \tag{31'}$$

i.e. the $\underline{\epsilon}$'s are orthogonal unit polarization vectors.

The fact that we are able to satisfy the gauge condition so simply - eq. (26) has now become simply an operator identity - is an additional reason for our choice of the radiation gauge over

other possibilities. In particular the more elegant and relativistic Lorentz gauge $\nabla\cdot\underline{A} + \frac{1}{c}\frac{\partial\phi}{\partial t} = 0$ cannot be readily incorporated as an operator equation and requires special conditions on the wave function (Fermi method) or an indefinite metric in Hilbert space (Gupta-Bleuler method).

Using the $a_{\underline{k},s}$ and $a^*_{\underline{k},s}$, as our dynamical variables the discussion now exactly parallels that for the string.

The wave equation for $\underline{A}$ now implies (and is implied by)

$$\frac{da_{\underline{k},s}}{dt} = -i\,\omega_k a_{\underline{k},s} \quad , \quad \frac{da^*_{\underline{k},s}}{dt} = i\omega_k a^*_{\underline{k},s} \tag{32}$$

where

$$\frac{\omega_k^2}{k^2} = c^2 \quad .$$

Further by direct calculation using (30) one readily shows that the constant factors in the square root in equation (28) have been chosen in such a way that the energy in the electromagnetic field,

$$H = \frac{1}{8\pi}\int (\mathcal{E}^2 + B^2)\ \underline{dx} \quad ,$$

takes the form

$$H = \tfrac{1}{2}\sum_{\underline{k}}\sum_{s} \hbar\omega_k (a^*_{\underline{k},s}\, a_{\underline{k},s} + a_{\underline{k},s}\, a^*_{\underline{k},s})$$

and the momentum

$$\underline{\mathcal{P}} = \frac{1}{c^2} \int \frac{\underline{\mathcal{E}} \times \underline{B}}{4\pi c} \, d\underline{x}$$

takes the form

$$\underline{\mathcal{P}} = \tfrac{1}{2} \sum_{\underline{k}} \sum_{s} \hbar \underline{k} \; (a^*_{\underline{k},s} \, a_{\underline{k},s} + a_{\underline{k},s} \, a^*_{\underline{k},s}) \quad .$$

[27.] The Analogy with the string is now complete making due allowance for three dimensions and two polarizations per normal mode. We can now go over directly to quantum mechanics. The dynamical variables $a_{\underline{k},s}$ and $a^*_{\underline{k},s}$ become operators which are one another's Hermitian conjugates and which satisfy the commutation rules (similar to equations (16) and (17)).

$$[a_{\underline{k},s} \; , \; a^*_{\underline{k}',s'}] = \delta_{\underline{k},\underline{k}'} \, \delta_{s,s'} \tag{33}$$

$$[a_{\underline{k},s} \; , \; a_{\underline{k}',s}] = 0 = [a^*_{\underline{k},s} \; , \; a^*_{\underline{k}',s'}] \quad .$$

The energy and momentum eigenvalues become (similar to equations (18) and (19))

$$E \left\{ N_{\underline{k},s} \right\} = \sum_{\underline{k}} \sum_{s} \hbar \omega_k (N_{\underline{k},s} + \tfrac{1}{2})$$

$$\underline{\mathcal{P}} \left\{ N_{\underline{k},s} \right\} = \sum_{\underline{k}} \sum_{s} \hbar \, \underline{k} \; N_{\underline{k},s} \quad .$$

Thus we have photons! The dynamical variables $a_{\underline{k},s}$ and $a^*_{\underline{k},s}$ become destruction and creation operators respectively for photons of momentum $\hbar \underline{k}$, polarization s .

[28.] We now wish to introduce interaction with charged particles. With no interaction, i.e., with all charges equal to zero, the Hamiltonian would be, using non relativistic mechanics for the particles,

$$\sum_{\underline{k}}\sum_{s} \hbar\omega_k \left(a^*_{\underline{k},s}\, a_{\underline{k},s} + \tfrac{1}{2}\right) + \sum_i \frac{p_i^2}{2m_i} \quad .$$

The first term describes the free radiation field; the second, the free motion of the particles (we are assuming only electromagnetic interactions). When we put the charges different from zero, two sorts of interactions occur:

(i) the coulombic interaction of the <u>particles</u> among themselves. This is a direct interaction between the particles. <u>It has nothing to do with the dynamics of the field</u>. It is, of course, in a sense, "due to" ϕ. But in our gauge, ϕ is <u>not</u> a dynamical variable associated with the fields (recall [25]).

(ii) The interactions of the particles with the field. As we shall see, this interaction gives rise to <u>effective</u> magnetic interaction and retarded interaction between the particles, as well as describing the interaction of matter and photons.

[29] We now simply state that the appropriate Hamiltonian which describes the interacting matter and field is

$$H = \sum_{\underline{k}}\sum_{s} \hbar\omega_k \left(a^*_{\underline{k},s}\, a_{\underline{k},s} + \tfrac{1}{2}\right) + \sum_i \frac{\left(p_i - \frac{q_i}{c}\underline{A}_i\right)^2}{2m_i} + \tfrac{1}{2}\sum_{i\neq j}\sum \frac{q_i q_j}{|\underline{x}_i - \underline{x}_j|} \quad . \qquad (34)$$

Here $\underline{A}_i$ is the vector potential evaluated at the position of the ith charge i.e.

$$\underline{A}_i = \sum_{\underline{k}} \sum_{s} \left[\frac{2\pi hc^2}{\omega_k L^3}\right]^{\frac{1}{2}} \underline{\epsilon}_{\underline{k},s} \left[a_{\underline{k},s}\, e^{i\underline{k}\cdot\underline{x}_i} + a^*_{\underline{k},s}\, e^{-i\underline{k}\cdot\underline{x}_i}\right] \qquad (35)$$

and eqn. (31), (31') and (33) continue to hold (with regard to (33) recall [19]). If there are also external fields present, $\underline{A}_i^{(Ext)}$ should be added to $\underline{A}_i$ and $\sum_i q_i \phi_i^{(Ext)}$ should be added to H.

Note that the structure of this Hamiltonian is really quite familiar. It is gotten by simply adding the Hamiltonian of the radiation field to the familiar Hamiltonian of a number of charged particles interacting among themselves via coulomb forces and in addition interacting with a vector potential. The presence of the radiation field Hamiltonian insures this vector potential is a dynamical entity not only acting on the particles (as an external field does) but also reacting to them.

[30.] We have said that this is the "appropriate Hamiltonian". What we mean by this is simply that using the commutation rules and using the general operator equation of motion

$$\frac{dF}{dt} = \frac{i}{h}[H,F]$$

applied to $F = a_{\underline{k},s}$, $F = \underline{x}_i$, and $F = \underline{p}_i$ one will derive exactly the extension of (32) to the interacting case, i.e. one will derive Maxwell's equations, and one will derive Newton's

equation describing the motion of the i-th particle under the influence of its electrostatic interactions with the other particles, and under the influence of the electromagnetic field represented by $\underline{A}_i$.

[31] We now wish to apply our formalism to various problems. Our basic tool will be perturbation theory with the unperturbed Hamiltonian taken to be

$$H_o = \sum_{\underline{k}} \sum_{s} \hbar\omega_k (a^*_{\underline{k},s}\, a_{\underline{k},s} + \tfrac{1}{2}) + \sum_i \frac{\underline{p}_i^{\,2}}{2m_i} + \tfrac{1}{2} \sum_{i \neq j} \sum \frac{q_i q_j}{|\underline{x}_i - \underline{x}_j|} \tag{36}$$

and the perturbation is then (in our gauge, $\underline{p}_i$ and $\underline{A}_i$ commute)

$$= \sum_i - \frac{q_i}{m_i c}\, \underline{p}_i \cdot \underline{A}_i + \sum_i \frac{q_i^2}{2m_i c^2}\, \underline{A}_i^{\,2} \tag{37}$$

$$= V_1 + V_2$$

Thus the unperturbed eigenfunctions are simply products of eigenfunctions of the free radiation field and eigenfunctions describing charged particles interacting via coulomb forces.

Note that our expansion parameter is basically the charge (the dimensionless parameter is $\sqrt{\alpha}$ where α is the fine structure

constant

$$\alpha = \frac{e^2}{\hbar c} \sim \frac{1}{137} \quad)$$

and, in this sense, V_1 is of first order, V_2 is of second order.

[31*.] If we would also include spin explicitly there would be additional terms in V. For example, there would be terms of the $\underline{S}_i \cdot \underline{B}_i$ type representing the direct interaction of the spin with the magnetic field, and there would also be contributions from the spin-orbit interaction when one replaces the $\underline{p}_i$ in the orbital angular momentum operators by $\underline{p}_i + \frac{q_i}{c} \underline{A}_i$. We will not consider these terms any further.

[32.] We will assume familiarity with stationary state perturbation theory. Indeed, we have already used it in [21]. We will also need time-dependent perturbation theory, whose formulae we will derive below. We emphasize that this is a method, like stationary state perturbation theory, which is of general use in quantum mechanics, whenever one has time-dependent processes. It is not a technique which is peculiar to field theory.

[33.] One may well ask, why do we need time-dependent perturbation theory when our Hamiltonian H does not involve the time explicitly? To answer this, let us note that the kind of problems to which we will apply this approximation are in the nature of scattering problems -

problems in the continuous spectrum. Let us, therefore, consider a typical problem of this type (which is not a field-theory problem) - the scattering of a particle by a potential. One way of handling this problem is to deal with an energy eigenstate in the continuous spectrum and look for wave functions which, at large distances from the scattering center, have the form of a plane wave plus an outgoing spherical wave. The former one is identified with the incident wave, the latter, with the scattered wave.

Though this procedure leads in the end to correct results, note that it is not an accurate description of a physical scattering experiment:

(i). Energy eigenfunctions in the continuum are not normalizeable.

(ii). The plane and spherical waves overlap everywhere in space and, therefore can't, in fact, be disentangled.

(iii). The wave function is continually non-zero in the region of the potential, i.e. scattering is always going on.

The remedy for these conceptual difficulties is to use realistic wave packets which as in an actual experiment confine the incident particle to a normalized moving "lump". This then means a non-stationary (time dependent) state, and does permit a clean separation (except in the region of the forward direction) between incident and scattered waves again as in an actual experiment. However, wave packets are messy to deal with and, in the end, the details of the packet cancel out. (During the interaction the potential, if it is of atomic or molecular

dimensions, can't distinguish between an experimental beam of small cross-section, and a plane wave.) Another, formal, procedure which allows us to use plane waves, etc., but still allows a clear distinction between incident and scattered waves, is to make the <u>interaction</u> V <u>time dependent</u>,

$$V \rightarrow Ve^{-\eta|t|}$$

where η is a small positive number. This insures (as with a packet) that there is no interaction in the remote past in the remote future. At the end of the calculation, one may let $\eta \rightarrow 0$. Thus we are led to the need for time-dependent perturbation theory.

[34] Now to the <u>formalism</u>. Our Hamiltonian is

$$H = H_o + Ve^{-\eta|t|} .$$

We will denote the eigenstates of H_o by ψ_I, ψ_F, etc. so that $H_o\psi_F = E_F\psi_F$, etc. We wish to solve the <u>time-dependent Schroedinger equation</u>

$$H\psi = -\frac{\hbar}{i}\frac{\partial\psi}{\partial t} \qquad (38)$$

subject to the condition that in the remote past

$$\psi = \psi_I e^{-iE_I t/\hbar} .$$

To do this, we write

$$\psi = \sum_F g_F \psi_F e^{-iE_F t/\hbar}$$

If $V = 0$, the g_F are constants. Because $V \neq 0$, they are not constants. Hence this method is sometimes called by the curious name, "the method of variation of constants".

Inserting this expansion into (38) and using the orthonormality of the ψ_F one readily derives

$$-\frac{\hbar}{i}\frac{\partial g_F}{\partial t} = \sum_{F'} (F|V|F')\, e^{i(E_F - E_{F'})t/\hbar - \eta|t|} g_{F'} \qquad (39)$$

We now introduce perturbation theory by expanding in powers of V. The zero order approximation is, of course, simply $g_{F'} = \delta_{F',I}$. Inserting this on the right hand side of (39), we get the first approximation

$$-\frac{\hbar}{i}\frac{dg_F}{dt} = (F|V|I)\, e^{i(E_F - E_I)t/\hbar - \eta|t|}$$

which we can immediately integrate, subject to the initial condition, to find

$$g_F = \delta_{F,I} - \frac{i}{\hbar}(F|V|I)\int_{-\infty}^{t} e^{i(E_F - E_I)\,t'/\hbar - \eta|t'|}\, dt'. \qquad (40)$$

[35.] The quantity of actual interest is the transition rate into the state $F \neq I$ for positive values of t (the maximum interaction clearly occurs at $t = 0$). Thus we want

$$T_{FI} = \frac{\partial}{\partial t} |g_F|^2 = g_F^* \frac{\partial g_F}{\partial t} + \frac{\partial g_F^*}{\partial t} g_F \quad .$$

One splits the integral in (40) into an integral from $-\infty$ to 0, and an integral from 0 to t.
In the former $\eta |t'| = -\eta t'$, in the latter $\eta |t'| = \eta t'$.
One finds, after a bit of algebra

$$T_{FI} = \frac{1}{\hbar} \frac{2\eta\hbar}{(E_F-E_I)^2 + (\eta h)^2} |(F|V|I)|^2 \left\{ e^{i(E_F-E_I)t/\hbar - \eta t} + e^{-i(E_F - E_I)t/\hbar - \eta t} - e^{-2\eta t} \right\} \quad .$$

We now let $\eta \to 0$. Note the first factor becomes zero if $E_F - E_I \neq 0$ and infinite if $E_F - E_I = 0$. Indeed,

$$\lim_{\epsilon \to 0} \frac{1}{\pi} \frac{\epsilon}{x^2 + \epsilon^2}$$

is a well-known representation for $\delta(x)$. Further, with $\eta = 0$ and $E_F - E_I$ effectively equally zero, the final bracketed factor becomes unity so we get the famous formula (the "golden rule") for the transition probability per unit time

$$T_{FI} = \frac{2\pi}{\hbar} |(F|V|I)|^2 \delta(E_F - E_I) \quad . \tag{41}$$

The δ function clearly expresses the overall conservation of energy. How one handles it to get finite measureable results will be discussed in the next lecture in connection with applications.

[36.] If one goes to second order in V , one finds a similar formula but with $(F|V|I)$ replaced by

$$(F|V|I) + \sum_{F'} \frac{(F|V|F')(F'|V|I)}{E_I - E_{F'}}$$

the states $\psi_{F'}$, appearing as virtual intermediate states. Since they are transitory, there is no contradiction with conservation of energy (recall $\Delta E \cdot \Delta t \sim \hbar$) in the fact that $E_{F'} \neq E_I$, i.e. energy "not conserved" in intermediate states.

[37.] In preparation for the applications, it is useful to note the nature of the non-zero photon matrix elements of V : Clearly V_1 can create or destroy any one photon $(\underline{k},s)$, we can represent this diagrammatically by (these are not Feynman diagrams)

creation of
a photon

destruction
of a photon

where one imagines <u>time</u> to increase from the bottom to the top of the diagram. Similarly V_2 can create any two photons, or destroy any two, or destroy one and create another.

creation
of two
photons

destruction
of two
photons

destruction
of one
photon and
creation of
another
photon.

THIRD LECTURE

[38.] As our first application of (41), we wish to discuss the spontaneous emission of light by a bound system (we will call it an atom) in an excited state. Let us first note that it is not at all clear that equation (41) applies since so far as the atom and the radiation is concerned this is not a collision process. Rather at some finite time (i.e. not $-\infty$) the atom is excited, say by collision, with another atom, and we want to know the rate at which it will emit light. We will return to this point of principle after we have completed the calculation.

[39.] Let us take the state ψ_I as a product of the photon vacuum and the wave function for an atom in state j while ψ_F is a product of a wavefunction describing one photon of momentum $\hbar\underline{k}$ with polarization s and the wave function for an atom in state f. For simplicity we will put the mass of the nucleus equal to ∞ so we are dealing only with the electrons. Thus, $q_i = -e$ and $m_i = m$. Also we have $E_F - E_I = \hbar\omega_k + E_f - E_j$.

From [37], it is clear that the only term in V which has a non-vanishing matrix element for this process is

$$\frac{e}{mc}\left[\frac{2\pi\hbar c^2}{\omega_{\underline{k}} L^3}\right]^{\frac{1}{2}} \sum_i \epsilon_{\underline{k},s} \cdot \underline{p}_i \; a^*_{\underline{k},s} \; e^{-i\underline{k}\cdot\underline{x}_i}$$

Since, further, the matrix element of $a^*_{\underline{k},s}$ between the two photon

states involved is unity (from equation (21)), we have in obvious notation

$$T_{fj}(\underline{k},s) = \frac{2\pi}{\hbar}\,\frac{e^2}{m^2c^2}\,\frac{2\pi\hbar c^2}{\omega_k L^3}\int \left|\underline{e}_{\underline{k},s}\cdot\langle f|\sum_\nu p_\nu\, e^{-i\underline{k}\cdot\underline{x}_\nu}|\, j\rangle\right|^2 \times \delta(E_f + \hbar\omega_k - E_j)$$

and we are still left with an electronic matrix element to calculate. It is the vanishing or non-vanishing of this matrix element which gives rise to all the familiar <u>selection rules</u>.

Now to "handle" the δ-function. We observe that in the (physical) limit, $L \to \infty$, we are not really interested in the probability that the photon emerge with a particular momentum $\hbar\underline{k}$, that is, in a particular direction since this is <u>impossible to measure</u>! No detector has infinitely sharp angular resolution. At best we want the probability that the photon will emerge in some range of solid angle. To infer a formula for this, let us sum our formula for T over <u>all</u> photons to find the <u>total transition</u> rate. In the limit as $L \to \infty$, this involves (generalizing equation (22) to three dimensions) $\frac{L^3}{(2\pi)^3}$ times an integral over $\underline{k}$ and a sum over s.

Because of the presence of the δ-function, we can readily carry out the integration over $\hbar\omega_k$ if we introduce it as a variable of integration. To do this, we introduce <u>spherical coordinates in $\underline{k}$ space</u>. Thus

$$\frac{L^3}{(2\pi)^3}\, d\underline{k} = \frac{L^3}{(2\pi)^3}\, k^2 dk\, d\Omega_{\underline{k}}$$

$$= \frac{L^3}{(2\pi)^3}\, \frac{\omega_k^2}{\hbar c^3}\, d(\hbar\omega_k)\, d\Omega_{\underline{k}} \equiv \rho\, d(\hbar\omega_k)$$

ρ is often called the density of final states or the phase space factor, the latter name because $L^3 d\underline{k}$ is ordinary space times momentum space = phase space. Carrying out the integration over $\hbar\omega_k$ we have, collecting all factors (note that the L^3 has cancelled out)

$$\text{Total transition rate} = \int d\Omega_{\underline{k}} \sum_s \frac{\omega}{(2\pi\hbar c^3)}\, \frac{e^2}{m^2}\, |\langle f| \cdots |j\rangle|^2$$

where now

$$\omega_k = \omega = (E_j - E_f)/\hbar$$

From this formula we infer that the differential transition rate for emission in the solid angle $d\Omega_{\underline{k}}$ with polarization s is

$$\frac{\omega}{(2\pi\hbar c^3)}\, \frac{e^2}{m^2}\, \left|\langle f| \underline{\epsilon}_{\underline{k},s} \cdot \sum_i p_i\, e^{-i\underline{k}\cdot\underline{x}_i} |\, j\rangle\right|^2 d\Omega_{\underline{k}}$$

This is the result we were after.

[40.] What we have calculated is a <u>specifically quantum mechanical effect</u>. We started with our atom in a <u>stationary state</u> (no oscillating charge or current densities) in the <u>dark</u> (no photons) and yet we have found that it radiates! Classically, in order to make such a system radiate, the presence of a field would be required. In fact, and it is here that the quantum mechanics enters, there <u>is such a field</u> even though there are no photons. Namely, one finds that although in the vacuum the average values of $\underline{\mathcal{E}}$ and $\underline{B}$ are zero (these operators are linear in $a_{\underline{k},s}$ and $a^{*}_{\underline{k},s}$) the averages of $\underline{\mathcal{E}}^2$ and $\underline{B}^2$ are not (recall the discussion in [15] of the nontrivial character of the "vacuum"). To put the matter another way, one readily verifies that $\underline{\mathcal{E}}$ and $\underline{B}$ do not commute with the $N_{\underline{k},s}$. Thus, <u>no photons does not mean no field</u>, and there <u>is</u> a fluctuating electro-magnetic field in the vacuum. It is this field then which can be said to "cause" spontaneous emission, though we will not attempt to show this in any further detail.

[41.] One further point. We have calculated the probability for the emission of <u>one</u> quantum. However, a system in general may also emit $2, 3, \cdots$ quanta provided only that

$$\sum_{k} \hbar\omega_{k} = E_{j} - E_{f}$$

Such <u>multiple quantum transitions</u> are well known in microwave and radio frequency spectroscopy, and, with the advent of lasers, can

also be seen in optical spectra (in absorption). As yet, none has been detected in nuclear transitions. As to the calculation of the probabilities for such transitions, V_2 clearly gives a possibility of 2 quantum emission already in 1st order (the $a^*_{\underline{k},s}\, a^*_{\underline{k}',s'}$ terms) while V_1, can give two quantum emission in second order.

Emission of Two Photons in Second Order

Two quantum emission is also of interest in astrophysics since in the transition $2^2S_{\frac{1}{2}} \longrightarrow 1^2S_{\frac{1}{2}}$ in hydrogen, the one quantum transition is very highly forbidden. More quanta become possible in higher order perturbation theory (and involve more powers of α).

[42.] For <u>optical transitions</u> it is usually a good approximation to put $e^{-i\underline{k}\cdot\underline{x}_i} = 1$. This is because the size of an atom is $\sim a_o$ while $\hbar\omega_k \sim \frac{e^2}{a_o}$ whence $\underline{k}\cdot\underline{x}_i \sim \frac{e^2}{\hbar c} = \alpha \sim \frac{1}{137}$.

This approximation is the familiar <u>dipole approximation</u> since then our electronic matrix element is

$$\left\langle f \left| \sum_i \underline{p}_i \right| j \right\rangle = im\omega \left\langle f \left| \sum_i \underline{x}_i \right| j \right\rangle \equiv im\omega\, \underline{R}_{fj}$$

$\underline{R}_{fj}$ being the <u>transition dipole matrix element</u>. In this approximation then, we get the familiar result that the differential transition rate is

$$\frac{e^2}{2\pi\hbar c^2}\omega^3\left|\underline{\epsilon}_{\underline{k},s}\cdot\underline{R}_{fj}\right|^2 \, d\Omega_{\underline{k}}$$

If we multiply this by $\hbar\omega$ to get the differential rate of energy emission then the explicit dependence on $\hbar$ disappears and we get a result identical in form to that for the radiation from a classical oscillating dipole.

[43.] Now let us return to the point of principle broached in [39]. The total transition rate, call it Γ_{fj}, is a finite number. Clearly then our result taken literally yields nonsense if applied for time intervals, t, longer than Γ_{fj}^{-1} since then the total probability of emission, $\Gamma_{fj}\, t$, will be larger than one!

Closer examination of the problem yields the following results: Let us first confine our attention to the atom, i.e., we sum over the photons, and let us suppose that the excitation occurs near time zero. Then what happens for very short times is strongly dependent on the details of the excitation mechanism. However, rather quickly the states f begin to build up according to the familiar rate equations which yield exponential behavior

$$\frac{d}{dt}|g_f|^2 = \sum_{f'}\Gamma_{ff'}|g_{f'}|^2 - \sum_{f''}\Gamma_{f''f}|g_f|^2$$

where $|g_f|^2$ is the probability that the atom is in state f (which may be j) and where $E_{f'} > E_f$ and $E_{f''} < E_f$. Thus $\Gamma_{ff'}$ is the intrinsic or partial transition rate from f' to f

and is therefore the physically measureable quantity, but it is only for times near zero that, for $f \neq j$ that $\frac{d|g_f|^2}{dt} = \Gamma_{fj}$. The rate equations of course guarantee that $\frac{d}{dt}\left(\sum |g_f|^2\right) = 0$, i.e. that probability is conserved. After very long times the behavior again deviates from that described by the rate equation.

If one also examines the photon state associated with the atomic transition $j \rightarrow f$ one finds that the photon need no longer be monochromatic. Rather there is a frequency distribution peaked very near to $\omega = (E_j - E_f)/\hbar$ with a (natural) width equal to $\sum_{f'} \Gamma_{f'j} + \sum_{f''} \Gamma_{f''f}$, where $E_{f'} < E_j$ and $E_{f''} < E_f$. One can reconcile this result with the conservation of energy by interpreting it as being due to a broadening of the levels f and j by the amounts $\hbar \sum_{f''} \Gamma_{f''f}$ and $\hbar \sum_{f'} \Gamma_{f'j}$ respectively, due to the interaction with the radiation field. More precisely, due to this interaction the states

j and f (unless the latter is the ground state) are no longer stable states, i.e. well defined energy eigenstates, but rather, depending on the numbers, are more or less long lived, more or less well-defined, metastable, resonant states in the continuum, their sharpness of definition being determined by the ratio of width to spacing.

[44.] As our second application, let us consider a problem of the type for which we did derive our approximation - the photoelectric effect in hydrogen. Thus

ψ_I = (photon $\underline{k}$, s) (atom in state o)

ψ_F = (photon vacuum) (atom ionized in state f)

Here clearly it is the $\underline{\epsilon}_{\underline{k},s} \cdot \underline{p}\ a_{\underline{k},s}$ term which contributes, the matrix element of $a_{\underline{k},s}$ being unity ($N_{\underline{k},s} = 1$). Further $E_I = E_o + \hbar\omega_k$ while $E_F = E_f$. Thus we have

$$T_{fo}(\underline{k},s) = \frac{2\pi\hbar c^2}{\omega_k L^3} \frac{e^2}{m^2c^2} \left| \underline{\epsilon}_{\underline{k},s} \cdot (f | \underline{p}\, e^{i\underline{k}\cdot\underline{x}} | o) \right|^2$$

$$\times \delta(E_f - E_o - \hbar\omega_k)$$

Now it is the electron we detect and it is the electron which is in the continuum (when $L \to \infty$). To first approximation its wave function is a plane wave

$$\psi_f = \frac{1}{\sqrt{L^3}} e^{i\underline{q}\cdot\underline{x}/\hbar}$$

$$E_f = q^2/2m$$

where $\underline{q}$ is its momentum. A more accurate approximation, to take account of the influence of the electric field of the proton is to replace the plane waves by a continuum wave function for hydrogen, which, at large distances from the proton, takes the form of a plane wave plus incoming spherical wave. That it is incoming rather

than outgoing is no doubt surprising but we will not pursue the matter further. The point we want to make is that in any case $T_{f0}(\underline{k},s)$ is proportional to $\frac{1}{L^6}$.

Now as we said the electron which we detect, like the photon in [39], is in the continuum. To get a formula to compare with experiment we proceed as we did there. We first sum over all final electron states. This involves $\frac{L^3}{(2\pi)^3}\int d\underline{q}$ (the derivation of this prescription had nothing to do with photons or quanta, only with plane waves and periodic boundary conditions). Writing

$$d\underline{q} = q^2 dq d\Omega_{\underline{q}} = q^2 \frac{dq}{dE_f} d\Omega_{\underline{q}} dE_f$$

$$= mq^2 d\Omega_{\underline{q}} dE_f$$

we can carry out the integration over E_f and then, as before, identify the integrand with a differential transition probability. The point we now want to emphasize (we will not write down the detailed formulae) is that the result is proportional to $\frac{1}{L^3}$ and therefore vanishes as $L \to \infty$!

[45.] On the one hand, this is a satisfying result. It means that there are no "time limitations" on our formula, no danger of transition probabilities becoming greater than one (recall [43]). The only limitation on the perturbation theory being the magnitude of V . On the other hand it does not seem very interesting physically.

To get an interesting result, let us note that the transition rate really involves two factors: (i) The probability that the photon will encounter the atom, (ii) The intrinsic rate at which a transition will then occur. It is the second factor which is interesting and it is the first which is small because we have (unphysically) described the photon "beam" by a plane wave in a box of volume L^3, therefore the photon density is $\sim \frac{1}{L^3} \to 0$.

A quantity which is <u>insensitive</u> to the <u>details</u> of the photon beam is the <u>differential cross-section</u>

$$d\sigma = \frac{\text{differential transition rate}}{\text{probability that a photon will cross unit area/sec.}}$$

and <u>is</u> representative of the physically interesting second factor. The denominator, the <u>photon flux</u>, can be calculated from the Poynting vector or by the following simple argument: The probability of crossing unit area/sec = probability that the photon is in a volume of unit cross-section and a depth of one second times c = ratio of that volume to $L^3 = c/L^3$. Thus, as expected, the L^3's do cancel out in $d\sigma$.

[46.] We have indicated how to calculate the photoelectric effect due to <u>one</u> quantum. One can also have an effect involving say <u>two quanta</u> and, indeed, such effects have been observed using lasers. Thus one might have

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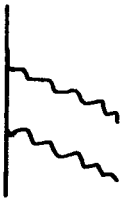


V_2 in 1st order + V_1 in 2nd order .

FOURTH LECTURE

[47.] We now will derive the (classical) Thomson Formula for the scattering of light by a charged particle. Here

$$\psi_I = (\text{photon } \underline{k},s\ )\ (\text{particle at rest})$$

$$\psi_F = (\text{photon } \underline{k}',s'\ )\ (\text{particle with momentum } \underline{q}\ ).$$

V_2 can produce this process in 1st order. As far as the photons are concerned V_1 can produce the process in second order (which is the same order in charge as V_2 - recall [36]) using the formula quoted in [36] . Here the states F' would involve either no quanta or two quanta (see [48] below). However, because the particle is initially at rest, and because V_1 involves the momentum operator, $(F \mid V_1 \mid I)$ is anyway zero. Thus we are left with the contribution of V_2 .

The terms which can contribute are clearly either the $a^*_{\underline{k}',s'} a_{\underline{k},s}$ or the $a_{\underline{k},s}\, a^*_{\underline{k}',s'}$ terms. Each yields the same electronic matrix element with the matrix elements of $a_{\underline{k},s}\, a^*_{\underline{k}',s'}$ and $a^*_{\underline{k}',s'} a_{\underline{k},s}$ equal to one. Thus we have

$$T(\underline{k}',s';\underline{k},s) = \frac{2\pi}{\hbar}\left[\frac{2\pi\hbar c^2}{L^3}\right]^2 \frac{1}{\omega_k \omega_{k'}} \left(\frac{e^2}{2mc^2}\right)^2 (2\,\underline{\epsilon}_{\underline{k}',s'} \cdot \underline{\epsilon}_{\underline{k},s})^2$$

$$\cdot \left| \int \frac{1}{\sqrt{L^3}}\, e^{-i\underline{q}\cdot\underline{x}/\hbar}\, e^{-i\,\underline{k}'\cdot\underline{x}}\, e^{i\,\underline{k}\cdot\underline{x}}\, \frac{1}{\sqrt{L^3}}\, d\underline{x} \right|^2$$

$$\cdot\, \delta\left(\frac{q^2}{2m} + \hbar\omega' - \hbar\omega\right)$$

where $\frac{1}{\sqrt{L^3}}$ is the wave function for the particle at rest and $\frac{1}{\sqrt{L^3}} e^{i\underline{q}\cdot\underline{x}/\hbar}$ is that for the particle with momentum $\underline{q}$. The integral is easily done and yields $\delta_{(\underline{q}/\hbar + \underline{k}'),\underline{k}}$ i.e. a Kronecker delta expressing conservation of momentum. From now on, we will assume momentum conservation, hence we may simply drop the Kronecker δ. For this process we have two particles in the continuum which we can detect in the final state. However, the conservation of energy and momentum fix the momentum (and energy) of one, given the momentum of the other. Thus if we sum over one of them, we have automatically summed over the other. Let us concentrate on the photon.

The conservation laws determine q^2 as a function of $\underline{k}'$ (given $\underline{k}$). Hence, if we denote $\frac{q^2}{2m} + \hbar\omega' - \hbar\omega$ by γ, in carrying out our sum over photons, prior to identifying the differential cross-section, we must write

$$d\underline{k}' = k'^2\, dk'\, d\Omega_{\underline{k}'}$$

$$= k'^2 \left(\frac{dk'}{d\gamma}\right)_{\underline{k}'} d\Omega_{\underline{k}'}\, d\gamma$$

so that we can carry out the γ integration using the δ-function. "Handling" the δ function is thus a bit more complicated here than it was in our earlier examples.

However, let us confine ourselves to $\hbar\omega_k \ll mc^2$. Then one readily shows, from the conservation laws that $q^2/2m$ is

negligible, i.e., $\omega_k \simeq \omega_{k'}$. Omitting the $\frac{q^2}{2m}$ then the complication just mentioned disappears and we infer, after doing the $\omega_{k'}$ integral and dividing by the incident photon flux that the differential cross-section is

$$d\sigma\ (\underline{k}', s'; \underline{k}, s) = \frac{2\pi}{\hbar}\left(\frac{2\pi\hbar c^2}{L^3}\right)^2 \frac{1}{\omega_k^2}\left(\frac{e^2}{2mc^2}\right)^2 \cdot$$

$$\frac{(2\,\underline{\epsilon}_{\underline{k}',s'} \cdot \underline{\epsilon}_{\underline{k},s})^2}{c/L^3} \frac{L^3}{(2\pi)^3} \frac{\omega_k^2}{\hbar c^3}\, d\Omega_{\underline{k}'}$$

$$= \left(\frac{e^2}{mc^2}\right)^2 (\underline{\epsilon}_{\underline{k}',s'} \cdot \underline{\epsilon}_{\underline{k},s})^2\, d\Omega_{\underline{k}'}$$

Note that this formula contains no $\hbar$. It is exactly the classical Thomson formula.

[48.] As our final scattering application we consider the scattering of light by an atom. This will lead to the Kramers-Heisenberg dispersion formula and the Raman effect. We are interested in the following process:

$$\psi_I = (\text{photon } \underline{k}, s)\ (\text{atom state } j)\ ,\ E_I = E_j + \hbar\omega_k$$

$$\psi_F = (\text{photon } \underline{k}'\ ,\ s'\ )\ (\text{atom state } f\ ),\ E_F = E_f + \hbar\omega_{k'}$$

V_2 can produce this in first order from either the $a^*_{\underline{k}',s'} a_{\underline{k},s}$ or the $a_{\underline{k},s}\, a^*_{\underline{k}',s'}$ terms just as in [47] , and each yields the same electronic matrix element, the matrix elements of $a_{\underline{k},s} a^*_{\underline{k}',s'}$ and $a^*_{\underline{k}',s'} a_{\underline{k},s}$ again being unity.

V_1 can produce this in second order (which is the same order in the charge as V_2 - recall [31]) the possible intermediate states in the formula of [36] being

$\psi_{F'}$ = (photon vacuum) (Atom in any state f')

with $E_I - E_{F'} = E_j + \hbar\omega_k - E_{f'}$ or

$\psi_{F'}$ = (photon $\underline{k},s$ and photon $\underline{k}',s'$) (atom in any state f')

with $E_I - E_{f'} = E_j + \hbar\omega_k - E_{f'} - \hbar\omega_k - \hbar\omega_{k'}$

$= E_j - E_{f'} - \hbar\omega_k$.

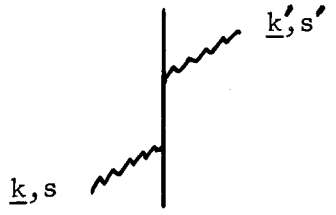
For the first type of intermediate state we have the matrix elements

$$(F \mid V_1 \mid F')(F' \mid V_1 \mid I) \sim (F \mid a^*_{\underline{k}',s'} \mid F')(F' \mid a_{\underline{k},s} \mid I)$$

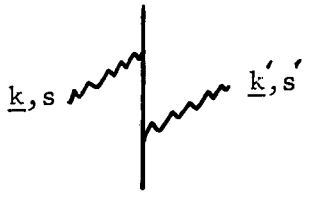
while for the second type,

$$(F \mid V_1 \mid F')(F' \mid V_1 \mid I) \sim (F \mid a_{\underline{k},s} \mid F')(F' \mid a^*_{\underline{k}',s'} \mid I) \ .$$

Diagrammatically (recall [37]) we can represent the first process by



and the second by



Again the matrix elements of the a and a^* are equal to one and we find for M defined by

$$M = (F|V_2|I) + \sum_{F'} \frac{(F|V_1|F')(F'|V_1|I)}{E_I - E_{F'}}$$

the following formula:

$$M = \left[\frac{2\pi\hbar c^2}{\omega_k L^3}\right]^{\frac{1}{2}} \left[\frac{2\pi\hbar c^2}{\omega_{k'} L^3}\right]^{\frac{1}{2}} \cdot$$

$$\left\{ 2 \cdot \frac{e^2}{2mc^2} \, \underline{\epsilon}_{\underline{k}',s'} \cdot \underline{\epsilon}_{\underline{k},s} \, (f| \sum_i e^{i(\underline{k}-\underline{k}')\cdot \underline{x}_i} |j) \right.$$

$$+ \frac{e^2}{m^2c^2} \sum_{f'} \frac{(f|\, \underline{\epsilon}_{\underline{k}',s'} \cdot \sum_i p_i \, e^{-i\underline{k}'\cdot \underline{x}_i} \, |f)(f'|\, \underline{\epsilon}_{\underline{k},s} \cdot \sum_\ell p_\ell \, e^{i\underline{k}\cdot \underline{x}_\ell} |j)}{E_j + \hbar\omega_k - E_{f'}}$$

$$\left. + \frac{e^2}{m^2c^2} \sum_{f'} \frac{(f|\, \underline{\epsilon}_{\underline{k},s} \cdot \sum_i p_i \, e^{i\underline{k}\cdot \underline{x}_i} |f')(f'|\, \underline{\epsilon}_{\underline{k}',s'} \cdot \sum_\ell p_\ell \, e^{-i\underline{k}'\cdot \underline{x}_\ell} |j)}{E_j - \hbar\omega_k - E_{f'}} \right\} .$$

Energy conservation now implies

$$E_j + \hbar\omega_k = E_f + \hbar\omega_{k'} \quad .$$

If $E_f = E_j$, we are dealing with elastic scattering - often called Rayleigh scattering.

If $E_f \neq E_j$, we have inelastic or Raman Scattering, $\hbar\omega_{k'} - \hbar\omega_k$ equalling some atomic energy difference.

If $E_f > E_j$ (atom originally in its ground state), $\omega_{k'} < \omega_k$ while if $E_f < E_j$ (atom originally in an excited state) $\omega_{k'} > \omega_k$.

In the by now we hope familiar fashion, we can infer the formula for the differential scattering cross-section:

$$d\sigma\,(\underline{k}',s',f\,;\,\underline{k},s,j) = \frac{2\pi}{\hbar}\,\frac{|M|^2}{\frac{c}{L^3}}\left(\frac{L}{2\pi}\right)^3\frac{\omega_{k'}^2}{\hbar c^3}\,d\Omega_{\underline{k}'}$$

We will not write it out in all detail.

[49.] We will, however, make several comments on the formula. First of all, if the dipole approximation is valid (all exponentials equal to unity) then it becomes the Kramers-Heisenberg formula (n is the number of electrons)

$$\frac{d\sigma}{d\Omega}\ (\underline{k}',s'f\ ;\underline{k},s,j) = \left(\frac{e^2}{mc^2}\right)^2 \Bigg[n\, \underline{\epsilon}_{\underline{k}',s'} \cdot \underline{\epsilon}_{\underline{k},s}\, \delta_{f,j}$$

$$+ \sum_{f'} \frac{(f \mid \underline{\epsilon}_{\underline{k}',s'} \cdot \sum_i \underline{p}_i \mid f')(f' \mid \underline{\epsilon}_{\underline{k},s} \cdot \sum_\ell \underline{p}_\ell \mid j)}{E_j + \hbar\omega_k - E_{f'}}$$

$$+ \sum_{f'} \frac{(f \mid \underline{\epsilon}_{\underline{k},s} \cdot \sum_i \underline{p}_i \mid f')(f' \mid \underline{\epsilon}_{\underline{k}',s'} \cdot \sum_\ell \underline{p}_\ell \mid j)}{E_j - \hbar\omega_{k'} - E_{f'}} \Bigg]^2 .$$

Note that in this approximation V_2 has become independent of the electronic coordinates and therefore contributes only to elastic scattering. It is the most important term in the x-ray region and yields just

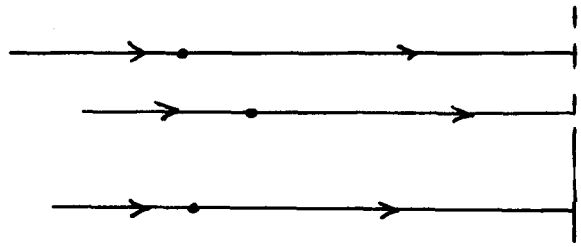
$$\frac{d\sigma}{d\Omega} = n^2 \frac{d\sigma\ (\text{Thomson})}{d\Omega}$$

i.e. at high frequencies the binding of the electrons is unimportant (hence the free Thomson cross-section) but the electrons do scatter coherently (n^2 rather than n).

Another point is that if $\hbar\omega_k$ is equal to $E_{f'} - E_j$ for some f' the corresponding term in the first sum in the formula for M blows up while if $\hbar\omega_k = E_f - E_{f'}$ for some f' (conservation of energy implies $E_j - \hbar\omega_{k'} - E_{f'} = E_f - \hbar\omega_k - E_{f'}$) the corresponding term in the second sum blows up - we have a resonance and clearly our formula is invalid (Actually this is the case only if f' is a discrete state. For states in the

continuum, the perturbation procedure automatically provides a prescription for avoiding the singularity) - the coupling has gotten too strong (recall remarks at beginning of [45]). However, methods can be found to deal with this situation.

[50.] There is a close connection between the forward elastic scattering in the dipole approximation and the index of refraction (Recall that forward elastic scattering from a number of centers is always coherent whatever the motion of the centers since the same optical path length is involved for all the centers:



Hence it is not surprising that it is this scattering which is involved in the coherent refraction phenomenon.) More precisely one can show that if we write $d\sigma \equiv |D|^2 \, d\Omega_{\underline{k}'}$, and if the index of refraction is close to unity, then

$$\text{index of refraction} = 1 + 2\pi N_o \frac{D(o)}{k^2}$$

where $D(o)$ is the value of D for forward elastic scattering, and where N_o is the number of atoms per unit volume. Since we also have

index of refraction = $1 + 2\pi N_o$ (Frequency dependent atomic polarizability)

it also follows that (as one can also show directly by manipulation of the formula for $D(o)$)

$$\text{Frequency dependent atomic polarizability} = \frac{D(o)}{k^2} .$$

[51.] Let us suppose that we were dealing with not one atom but two atoms. Then if we consider elastic scattering there are two ways of reaching the same final state, either by atom 1 scattering and 2 being unaffected, or by atom 2 scattering, and 1 being unaffected. Now in our discussion involving one atom we have, implicitly, referred electronic coordinates to the nucleus as an origin. With two atoms, suppose we use an arbitrary origin. Then it is clear from our formula for M, which is quite general, that we will now have

$$M = e^{i(\underline{k} - \underline{k}')\cdot\underline{R}_1} M_1 + e^{i(\underline{k} - \underline{k}')\cdot\underline{R}_2} M_2$$

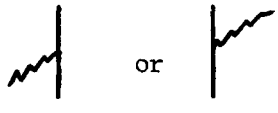
where $\underline{R}_1$ and $\underline{R}_2$ are the positions of the nuclei of atoms 1 and 2 and where M_1 is the M of (43) calculated for Atom 1 with electronic coordinates referred to its nucleus, and similarly for M_2. Since $d\sigma$ involves $|M|^2$ we see that, just as classically, we will get interferences effects.

[52.] We now turn from scattering problems to energy considerations - the shifts in atomic energy levels produced by V . Since, however, to do the job right one really needs relativistic mechanics for the electrons (the Dirac equation) and indeed - even better, the quantum field theory of electrons and positrons - we will merely indicate the results.

Suppose we simply just replace the non-relativistic electronic Hamiltonians for each electron by Dirac Hamiltonians. In addition to being more correct physically this also leads to a formal simplification - there is no term which looks like V_2 , only a term like V_1 , linear in the vector potential (and with $\underline{p}_i$ replaced by a Dirac Matrix $\underline{\alpha}_i$) and given as a sum over the particles. Let us write it as

$$V = \sum_i \underline{v}_i \cdot \underline{A}_i$$

where $\underline{v}_i$ involves $\underline{\alpha}_i$ and constants. Diagrammatically, it yields



Our unperturbed state is

$$\psi_I = \text{(photon vacuum) (atom in state } j \text{)}$$

and the energy shift through second order is given by the familiar formula

$$E^{(1)} + E^{(2)} = (I \mid V \mid I) + \sum{}' \frac{(I \mid V \mid F)(F \mid V \mid I)}{E_I - E_F}$$

Clearly $E^{(1)} = 0$ since the average value of $\underline{A}_i$ vanishes (recall [21]). The $E^{(2)}$, however, does not vanish; the intermediate states F for which $(F \mid V \mid I)$ is non zero are

$$\psi_F = (\text{any one photon } \underline{k},s\ )\ (\text{atom in any state } f\ )$$

with $E_I - E_F = E_j - E_f - \hbar\omega_k$. The $a^*_{\underline{k},s}$ parts of V_1 contribute to $(F \mid V \mid I)$ and the Hermitian conjugate $a_{\underline{k},s}$ part to $(I \mid V \mid F\ )$, and we can represent $E^{(2)}$ diagrammatically as

The sum over intermediate states thus means a sum over f and over $\underline{k}$ and s. Since the matrix elements of $a_{\underline{k},s}$ and $a^*_{\underline{k},s}$ yield unity we are left with (letting $L \to \infty$)

$$E^{(2)} = \frac{2\pi\hbar c^2}{(2\pi)^3} \sum_f \int \frac{d\underline{k}}{\omega_k} \sum_s \left(j \middle| \sum_i \underline{v}_i \cdot \underline{\epsilon}_{\underline{k},s}\ e^{i\underline{k}\cdot\underline{x}_i} \middle| f\right)$$

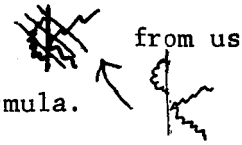
$$\cdot \frac{\left(f \middle| \sum_\ell \underline{v}_\ell \cdot \underline{\epsilon}_{\underline{k},s}\ e^{-i\underline{k}\cdot\underline{x}_\ell} \middle| j\right)}{E_j - E_f - \hbar\omega_k}$$

First consider the terms $i = \ell$ which one can think of as being produced by electron i emitting and absorbing the photon. One can show that they are <u>infinite</u>. We return to this point below. The terms $i \neq \ell$ are finite and one can think of them as being produced by electrons i and ℓ exchanging one photon. Formally one can write them as

$$(j \mid \tfrac{1}{2} \sum_{i \neq \ell} \sum b_{i\ell} \mid j)$$

where the $b_{i\ell}$ involve <u>only</u> electronic variables (we have "integrated out the photons"). Thus it is as though the photon exchange has produced an <u>additional interaction</u>, $b_{i\ell}$, over and above the coulomb interaction, $\frac{e^2}{|\underline{x}_i - \underline{x}_\ell|}$ between electrons and we were calculating its effects using first order perturbation theory. Under certain approximations $b_{i\ell}$ can be exhibited explicitly as the famous <u>Breit-Interaction</u>, which in turn can be approximated by the <u>Breit-Pauli</u> Interaction.

[53.] Before turning to the infinite terms $i = \ell$, let us remark that in all our calculations of <u>scattering</u> processes we calculated only to the <u>lowest nonvanishing order in the charge</u>, i.e. we used the lowest order of perturbation theory we could to get the effect. However, one can, of course carry perturbation theory to all orders in V. The results are most easily expressed in terms of diagrams.

Consider, for example, Thomson scattering again. Then in addition to a contribution  from V_2 in first order there are contributions like  from using V_2 once and V_1 twice in the third order formula.

Another way of stating the approximation we have made is that, except in our discussion of energy shifts, we have never introduced virtual quanta, i.e. quanta which do not appear in either initial or final states but which are created and then destroyed in intermediate states. If one does so, i.e. if one attempts to calculate higher order corrections ("Radiative corrections") one always gets divergences.

Now in fact, there is a way of handling these divergences. Using all the machinery of the Dirac equation and positron theory, one can show that there exist two (infinite) constants δm and δe, given as power series in the fine structure constant such that, if one expresses the divergent formulas consistently (i.e., to the appropriate power of the fine structure constant) in terms of $m_o \equiv m + \delta m$ and $e_o \equiv e + \delta e$ rather than in terms of m and e, then, a "miracle occurs": These formulas become finite functions of e_o and m_o. One may then identify the latter with the observed charge and mass, e and m being the "bare" charge and mass. This procedure is called charge and mass renormalization, e_o and m_o often being called the renormalized charge and mass, e and m the unrenormalized charge and mass.

Though clearly a bit suspicious (some call it "ugly"), this procedure has yielded very impressive results. The radiative corrections become small corrections when expressed in terms of e_o and m_o. Also, for example, the analogue of the $i = \ell$ terms mentioned earlier then yield with great accuracy the Lamb shifts in hydrogen and Helium and the anomalous magnetic moment of the electron.

Before the latter effects had been verified experimentally, around 1947, radiative corrections were almost universally ignored. However, some wise men warned that "just because they are infinite does not mean that they are zero". They were right!

THE END