Quantum Physics
Building From scratch

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Contents

Chapter 1

Quantum Theory of Radiation

1.1 Transverse and Longitudinal Fields

In non-relativistic Quantum Mechanics, the static Electric field is represented by a scalar potential, magnetic fields by the vector potential, and the radiation field also through the vector potential. It will be convenient to keep this separation between the large static atomic Electric field and the radiation fields, however, the equations we have contain the four-vector A_μ with all the fields mixed. When the quantize the field, all E and B fields as well as electromagnetic waves will be made up of photons. It is useful to be able to separate the E fields due to fixed charges from the EM radiation from moving charges. This separation is not Lorentz invariant, but it is still useful. Enrico Fermi showed, in 1930, that $A_\parallel$ together with A_0 give rise to Coulomb interactions between particles, whereas $A_\perp$ gives rise to the EM radiation from moving charges. With this separation, we can maintain the form of our non-relativistic Hamiltonian.

$$\boxed{\mathbf{H} = \sum_j \frac{1}{2m_j}\left(\vec{p} - \frac{e}{c}\vec{A}_\perp\left(\vec{x}_j\right)\right)^2 + \sum_{i>j}\frac{e_i e_j}{4\pi\,||\,\vec{x}_i - \vec{x}_j} + \mathbf{H_{rad}}} \tag{1.1}$$

Where $\mathbf{H_{rad}}$ is purely the Hamiltonian of the radiation (containing only $\vec{A}_\perp$) and $\vec{A}_\perp$ is the part of the vector potential which satisfies $\nabla \cdot \vec{A}_\perp = 0$. Note that $\vec{A}\|$ and A_4 appear nowhere in the Hamiltonian. Instead, we have the Coulomb potential. This separation allows us to continue with our standard Hydrogen solution and just add radiation. We will not derive this result.

In a region in which there are no source terms,

$$j_\mu = 0 \tag{1.2}$$

we can make a gauge transformation which eliminates A_0 by choosing Λ such that

$$\frac{1}{c}\frac{\partial \Lambda}{\partial t} = A_0 \tag{1.3}$$

Since the fourth component of A_μ is now eliminated, the Lorentz condition now implies that

$$\vec{\nabla} \cdot \vec{A} = 0 \tag{1.4}$$

Again, making one component of a 4-vector zero is not a Lorentz invariant way of working. We have to redo the gauge transformation if we move to another frame.

If $j_\mu \neq 0$, then we cannot eliminate A_0, since $\boxed{A}_0 = \frac{j_0}{c}$ and we are only allowed to make gauge transformation for which $\boxed{\Lambda} = 0$. In this case we must separate the vector potential into the transverse and longitudinal parts, with

$$\begin{aligned} \vec{A} &= \vec{A}_\perp + \vec{A}_\parallel \\ \vec{\nabla} \cdot \vec{A}_\perp &= 0 \\ \vec{\nabla} \times \vec{A}_\parallel &= 0. \end{aligned}$$

We will now study the radiation field in a region with no sources so that $\vec{\nabla} \cdot \vec{A} = 0$. We will use the equations

$$\begin{aligned} \vec{B} &= \vec{\nabla} \times \vec{A} \\ \vec{E} &= -\frac{1}{c}\frac{\partial \vec{A}}{\partial t} \\ \nabla^2 \vec{A} - \frac{1}{c^2}\frac{\partial \vec{A}}{\partial t} &= 0. \end{aligned}$$

1.2 Fourier Decomposition of Radiation Oscillators

Our goal is to write the Hamiltonian for the radiation field in terms of a sum of harmonic oscillators Hamiltonians. The first step is to write the radiation field in a simple way as possible, as a sum of harmonic components. We will work in a cubic volume $V = L^3$ and apply periodic boundary conditions on our electromagnetic waves. We also assume for now that there are no sources inside the region so that we can make a gauge transformation to make $A_0 = 0$ and hence $\vec{\nabla} \cdot \vec{A} = 0$. We decompose the field into its Fourier components at $t = 0$

$$\vec{A}\left(\vec{x}, t = 0\right) = \frac{1}{\sqrt{V}} \sum_k \sum_{\alpha=1}^{2} \hat{\epsilon}^{(\alpha)} \left(c_{k,\alpha}\left(t = 0\right) e^{i\vec{k}\cdot\vec{x}} + c^*_{k,\alpha}\left(t = 0\right) e^{-i\vec{k}\cdot\vec{x}} \right) \tag{1.5}$$

where $\hat{\epsilon}^{(\alpha)}$ are real unit vectors, and $c_{k,\alpha}$ is the coefficient of the wave with wave vector $\vec{k}$ and polarization vector $\hat{\epsilon}^{(\alpha)}$. Once the wave vector is chose, the two polarization vectors must be picked so that $\hat{\epsilon}^{(1)}$, $\hat{\epsilon}^{(2)}$, and $\vec{k}$ form a right handed orthogonal system. The components of the wave vector must satisfy

$$k_i = \frac{2\pi n_i}{L} \tag{1.6}$$

due to the periodic boundary conditions. The factor out front is set to normalize the states nicely since

$$\frac{1}{V}\int d^3x e^{i\vec{k}\cdot\vec{x}} e^{-i\vec{k}'\vec{x}} = \delta_{\vec{k}\vec{k}'} \tag{1.7}$$

and

$$\hat{\epsilon}^{(\alpha)} \cdot \hat{\epsilon}^{(\alpha')} = \delta_{\alpha\alpha'} \tag{1.8}$$

We know the time dependence of the waves from Maxwell's equation,

$$c_{k,\alpha}(t) = c_{k,\alpha}(0)\, e^{-i\omega t} \tag{1.9}$$

where $\omega = kc$. We can now write the vector potential as a function of position and time.

$$\vec{A}\left(\vec{x},\vec{t}\right) = \frac{1}{\sqrt{V}} \sum_{k} \sum_{\alpha=1}^{2} \hat{\epsilon}^{(\alpha)} \left(c_{k,\alpha}(t)\, e^{i\vec{k}\cdot\vec{x}} + c^{*}_{k,\alpha}(t)\, e^{-i\vec{k}\cdot\vec{x}} \right) \tag{1.10}$$

We may need to write this solution in several different ways, and use the best one for the calcualtion being performed. One nice way to write this is in terms 4-vector k_μ, the wave number,

$$k_\mu = \frac{p_\mu}{\hbar} = \left(k_x, k_y, k_z, ik\right) = \left(k_x, k_y, k_z, i\frac{\omega}{c}\right) \tag{1.11}$$

so that

$$k_p x_p = k \cdot x = \vec{k} \cdot \vec{x} - \omega t \tag{1.12}$$

We can then write the radiation field in a more covariant way

$$\vec{A}\left(\vec{x},t\right) = \frac{1}{\sqrt{V}} \sum_{k} \sum_{\alpha=1}^{2} \hat{\epsilon}^{(\alpha)} \left(c_{k,\alpha}(0)\, e^{ik_p x_p} + c^{*}_{k,\alpha}(0)\, e^{-ik_p x_p} \right) \tag{1.13}$$

A convenient shorthand for calculations is possible by noticing that the second term is just the complex conjugate of the first.

$$\vec{A}\left(\vec{x},t\right) = \frac{1}{\sqrt{V}} \sum_{k} \sum_{\alpha=1}^{2} \hat{\epsilon}^{(\alpha)} \left(c_{k,\alpha}(0)\, e^{ik_p x_p} + c.c. \right)$$

$$\vec{A}\left(\vec{x},t\right) = \frac{1}{\sqrt{V}} \sum_{k} \sum_{\alpha=1}^{2} \hat{\epsilon}^{(\alpha)} c_{k,\alpha}(0)\, e^{ik_p x_p} + c.c.$$

Note again that we have made this a transverse field by construction. The unit vectors $\hat{\epsilon}^{(\alpha)}$ are transverse to the deirection of propagation. Also note that we are working in a guage with $A_4 = 0$, so this can also represent

the 4-vector form of the potential. The Fourier Decomposition of the radiation field can be be be written very simply.

$$\boxed{A_\mu = \frac{1}{\sqrt{V}} \sum_k \sum_{\alpha=1}^{2} \epsilon_\mu^{(\alpha)} c_{k,\alpha}(0)\, e^{ik_p x_p} + c.c.} \tag{1.14}$$

This choice of guage makes switching between 4-vector and 3-vector expressions for the potential trivial. Let's verify that this decomposition of the radiation field satisfies the Maxwell equation, just for some practice. It's most convenient to use the covariant form of the equation and field.

$$\Box A_\mu = 0$$

$$\Box\left(\frac{1}{\sqrt{V}} \sum_k \sum_{\alpha=1}^{2} \epsilon_\mu^{(\alpha)} c_{k,\alpha}(0)\, e^{ik_p x_p} + c.c.\right) = \frac{1}{\sqrt{V}} \sum_k \sum_{\alpha=1}^{2} \epsilon_\mu^{(\alpha)} c_{k,\alpha}(0)\, \Box e^{ik_p x_p} + c.c.$$

$$= \frac{1}{\sqrt{V}} \sum_k \sum_{\alpha=1}^{2} \epsilon_\mu^{(\alpha)} c_{k,\alpha}(0)\, (-k_\nu k_\nu)\, e^{ik_p x_p} + c.c. = 0$$

The result is zero since $k_\nu k_\nu = k^2 - k^2 = 0$.

Let's also verify that $\vec{\nabla} \cdot \vec{A} = 0$

$$\vec{\nabla} \cdot \left(\frac{1}{\sqrt{V}} \sum_k \sum_{\alpha=1}^{2} \hat{\epsilon}^{(\alpha)} c_{k,\alpha}(t)\, e^{i\vec{k}\cdot\vec{x}} + c.c.\right) = \frac{1}{\sqrt{V}} \sum_k \sum_{\alpha=1}^{2} c_{k,\alpha}(t)\, \hat{\epsilon}^{(\alpha)} \cdot \vec{\nabla} e^{i\vec{k}\cdot\vec{x}} + c.c.$$

$$= \frac{1}{\sqrt{V}} \sum_k \sum_{\alpha=1}^{2} c_{k,\alpha}(t)\, \hat{\epsilon}^{(\alpha)} \vec{k} e^{i\vec{k}\cdot\vec{x}} + c.c. = 0.$$

The result here is zero because $\hat{\epsilon}^{(\alpha)} \cdot \vec{k} = 0$

1.3 The Hamiltonian for the Radiation Field

We now wish to compute the Hamiltonian in terms of the coefficients $c_{k,\alpha}(t)$. This is an important calculation because we will use the Hamiltonian formalism to do the quantization of the field. We will do the calculation using the covariant notaion (while Sakurai outlines an alternate calculation using 3-vectors). We have already calculated th Hamiltonian density of a classical EM field.

$$\boxed{\mathcal{H} = F_{\mu 4} \frac{\partial A_\mu}{\partial x_4} + \frac{1}{4} F_{\mu\nu} F_{\mu\nu}} \tag{1.15}$$

$$\mathcal{H} = \left(\frac{\partial A_4}{\partial x_\mu} - \frac{\partial A_4}{\partial x_4}\right) \frac{\partial A_\mu}{\partial x_4} + \frac{1}{4} \left(\frac{\partial A_\nu}{\partial x_\mu} - \frac{\partial A_\mu}{\partial x_\nu}\right) \left(\frac{\partial A_\nu}{\partial x_\mu} - \frac{\partial A_\mu}{\partial x_\nu}\right)$$

$$\mathcal{H} = -\frac{\partial A_4}{\partial x_\mu} \frac{\partial A_\mu}{\partial x_4} + \frac{1}{2} \left(\frac{\partial A_\nu}{\partial x_4} \frac{\partial A_\nu}{\partial x_4} - \frac{\partial A_\nu}{\partial x_\nu} \frac{\partial A_\mu}{\partial x_\nu}\right).$$

Now lets compute the basic element of the above formula for our decomposed radiation field.

$$
\begin{aligned}
A_\mu &= \frac{1}{\sqrt{V}} \sum_k \sum_{\alpha=1}^{2} \epsilon_\mu^{(\alpha)} \left(c_{k,\alpha}(0)\, e^{ik_p x_p} + c_{k,\alpha}^*(0)\, e^{-ik_p x_p} \right) \\
\frac{\partial A_\mu}{\partial x_\nu} &= \frac{1}{\sqrt{V}} \sum_k \sum_{\alpha=1}^{2} \epsilon_\mu^{(\alpha)} \left(c_{k,\alpha}(0)\, (ik_\nu)\, e^{ik_p x_p} + c_{k,\alpha}^*(0)\, (-ik_\nu)\, e^{-ik_p x_p} \right) \\
\frac{\partial A_\mu}{\partial x_\nu} &= i \frac{1}{\sqrt{V}} \sum_k \sum_{\alpha=1}^{2} \epsilon_\mu^{(\alpha)} \frac{\omega}{c} \left(c_{k,\alpha}(0)\, e^{ik_p x_p} - c_{k,\alpha}^*(0)\, e^{ik_p x_p} \right) \\
\frac{\partial A_\mu}{\partial x_4} &= -\frac{1}{\sqrt{V}} \sum_k \sum_{\alpha=1}^{2} \epsilon_\mu^{(\alpha)} \frac{\omega}{c} \left(c_{k,\alpha}(0)\, e^{ik_p x_p} - c_{k,\alpha}^*(0)\, e^{ik_p x_p} \right).
\end{aligned}
$$

We have all the elements to finish the calculation of the Hamiltonian. Before pulling this all together in a brute force way, it's good to realize that almost all the terms will give zero. We see that the derivative of A_μ is proportional to a 4-vector, say k_ν and to a polarization vector, say $\epsilon_\mu^{(\alpha)}$. The dot products of the 4-vectors, either k with itself, or k with ϵ are zero. Going back to out expression for the Hamiltonian density, we can eliminate some terms.

$$
\begin{aligned}
\mathcal{H} &= -\frac{\partial A_\mu}{\partial x_4} \frac{\partial A_\mu}{\partial x_4} + \frac{1}{2} \left(\frac{\partial A_\nu}{\partial x_\mu} \frac{\partial A_\nu}{\partial x_\mu} - \frac{\partial A_\nu}{\partial x_\mu} \frac{\partial A_\mu}{\partial x_\nu} \right) \\
\mathcal{H} &= -\frac{\partial A_\nu}{\partial x_4} \frac{\partial A_\mu}{\partial x_4} + \frac{1}{2} (0 - 0) \\
\mathcal{H} &= -\frac{\partial A_\mu}{\partial x_4} \frac{\partial A_\mu}{\partial x_4}.
\end{aligned}
$$

The remaining term has a dot product between polarization vectors which will be nonzero if the polarization vectors are the same. (Note that this simplification is possible because we have assumed no sources in the region.) The total Hamiltonian we are aiming at, is the integral of the Hamiltonian density.

$$
H = \int d^3x \mathcal{H} \tag{1.16}
$$

When we integrate over the volume only products like $e^{ik_p x_p} e^{-ik_p x_p}$ will give a nonzero result. So when we multiply one sum over k by another, only the terms with the same k will contribute to the integral, basically because the waves with different wave number are orthogonal.

$$
\frac{1}{V} \int d^3x e^{ik_p x_p} e^{-ik'_p x_p} = \delta_{kk'} \tag{1.17}
$$

$$
\begin{aligned}
H &= \int d^3x \mathcal{H} \\
\mathcal{H} &= -\frac{\partial A_\mu}{\partial x_4}\frac{\partial A_\mu}{\partial x_4} \\
\frac{\partial A_\mu}{\partial x_4} &= -\frac{1}{\sqrt{V}}\sum_k \sum_{\alpha=1}^{2} \epsilon_\mu^{(\alpha)} \left(c_{k,\alpha}(0)\frac{\omega}{c} e^{ik_p x_p} - c^*_{k,\alpha}(0)\frac{\omega}{c} e^{-ik_p x_p} \right) \\
H &= -\int d^3x \frac{\partial A_\mu}{\partial x_4}\frac{\partial A_\mu}{\partial x_4} \\
H &= -\int d^3x \frac{1}{V}\sum_k \sum_{\alpha}^{2} \left(c_{k,\alpha}(0)\frac{\omega}{c} e^{ik_p x_p} - c^*_{k,\alpha}(0) e^{-ik_p x_p} \right) \\
H &= -\sum_k \sum_{\alpha=1}^{2} \left(\frac{\omega}{c}\right)^2 \left[-c_{k,\alpha}(t) c^*_{k,\alpha}(t) - c^*_{k,\alpha}(t) c_{k,\alpha}(t) \right] \\
H &= \sum_k \sum_{\alpha}^{2} \left(\frac{\omega}{c}\right)^2 \left[c_{k,\alpha}(t) c^*_{k,\alpha}(t) + c^*_{k,\alpha}(t) c_{k,\alpha}(t) \right] \\
H &= \sum_{k,\alpha} \left(\frac{\omega}{c}\right)^2 \left[c_{k,\alpha}(t) c^*_{k,\alpha}(t) + c^*_{k,\alpha}(t) c_{k,\alpha}(t) \right].
\end{aligned}
$$

This is the result we will use to quantize the field. We have been careful not to commute C and $C*$ here in anticipation of the fact that they do not commute.

It should not be a surprise that the terms that made up the Lagrangian gave a zero contribution because $\mathcal{L} = \frac{1}{2}\left(E^2 - B^2\right)$ and we know that E and B have the same magnitude in radiation field. (There is one wrinkle we have glossed over; terms with $\vec{k}' = -\vec{k}$.)

1.4 Canonical Coordinates and Momenta

We now have the Hamiltonian for the radiation field

$$
\boxed{H = \sum_{k,\alpha} \left(\frac{\omega}{c}\right)^2 \left[c_{k,\alpha}(t) c^*_{k,\alpha}(t) + c^*_{k,\alpha}(t) c_{k,\alpha}(t) \right]} \tag{1.18}
$$

It was with the Hamiltonian that we first quantized the non-relativistic motion of particles. The position and momentum became operators which did not commute. Lets define $c_{k,\alpha}$ to be the time dependent Fourier coefficient.

$$
\ddot{c}_{k,\alpha} = -\omega^2 c_{k,\alpha} \tag{1.19}
$$

We can then simplify our notation a bit

$$
H = \sum_{k,\alpha} \left(\frac{\omega}{c}\right)^2 \left[c_{k,\alpha} c^*_{k,\alpha} + c^*_{k,\alpha} c_{k,\alpha} \right] \tag{1.20}
$$

This now clearly looks like the Hamiltonian for a collection of uncoupled oscillators; one oscillator for each wave vector and polariation.

We wish th write the Hamiltonian in terms of a coordinate for each oscillator and the conjugate momenta. The coordinate should be real so it can be represented by a Hermitian operator and have a physical meaning. The simplest choice for a read coordinates is $c + c^*$. With a little effort we can identify the coordinate

$$Q_{k,\alpha} = \frac{1}{c}\left(c_{k,\alpha} + c^*_{k,\alpha}\right) \tag{1.21}$$

and its conjugate momentum for each oscillator,

$$P_{k,\alpha} = -\frac{i\omega}{c}\left(c_{k,\alpha} - c^*_{k,\alpha}\right) \tag{1.22}$$

The Hamiltonian can be written in terms of these

$$\begin{aligned}
H &= \frac{1}{2}\sum_{k,\alpha}\left[P^2_{k,\alpha} + \omega^2 Q^2_{k,\alpha}\right] \\
&= \frac{1}{2}\sum_{k,\alpha}\left[-\left(\frac{\omega}{c}\right)^2\left(c_{k,\alpha} - c^*_{k,\alpha}\right)^2 + \left(\frac{\omega}{c}\right)^2\left(c_{k,\alpha} + c^*_{k,\alpha}\right)^2\right] \\
&= \frac{1}{2}\sum_{k,\alpha}\left(\frac{\omega}{c}\right)^2\left[-\left(c_{k,\alpha} - c^*_{k,\alpha}\right)^2 + \left(c_{k,\alpha} + c^*_{k,\alpha}\right)^2\right] \\
&= \frac{1}{2}\sum_{k,\alpha}\left(\frac{\omega}{c}\right)^2 2\left[c_{k,\alpha}c^*_{k,\alpha} + c^*_{k,\alpha}c_{k,\alpha}\right] \\
&= \sum_{k,\alpha}\left(\frac{\omega}{c}\right)^2\left[c_{k,\alpha}c^*_{k,\alpha} + c^*_{k,\alpha}c_{k,\alpha}\right].
\end{aligned}$$

This verifies that this choice gives the right Hamiltonian. We should also check that this choice of coordinates and momenta satisfy Hamiltonian's equations to identify them as the canonical coordinates. The first equation is

$$\begin{aligned}
\frac{\partial H}{\partial Q_{k,\alpha}} &= -\dot{P}_{k,\alpha} \\
\omega^2 Q_{k,\alpha} &= \frac{i\omega}{c}\left(\dot{c}_{k,\alpha} - \dot{c}^*_{k,\alpha}\right) \\
\frac{\omega^2}{c}\left(c_{k,\alpha} + c^*_{k,\alpha}\right) &= \frac{i\omega}{c}\left(-i\omega c_{k,\alpha} - i\omega c^*_{k,\alpha}\right) \\
\frac{\omega^2}{c}\left(c_{k,\alpha} + c^*_{k,\alpha}\right) &= \frac{\omega^2}{c}\left(c_{k,\alpha} + c^*_{k,\alpha}\right).
\end{aligned}$$

This one checks out OK.

The other equation of Hamiltonian is

$$\begin{aligned}
\frac{\partial H}{\partial P_{k,\alpha}} &= Q_{k,\alpha} \\
P_{k,\alpha} &= \frac{1}{c}\left(\dot{c}_{k,\alpha} + \dot{c}^*_{k,\alpha}\right) \\
-\frac{-i\omega}{c}\left(c_{k,\alpha} - c^*_{k,\alpha}\right) &= \frac{1}{c}\left(-i\omega c_{k,\alpha} + i\omega c^*_{k,\alpha}\right) \\
\frac{-i\omega}{c}\left(c_{k,\alpha} - c^*_{k,\alpha}\right) &= -\frac{i\omega}{c}\left(c_{k,\alpha} - c^*_{k,\alpha}\right).
\end{aligned}$$

This also checks out, so we have identified the canonical coordinates and momenta of our oscillators.

We have a collection of uncoupled oscillators with identified canonical coordinate and mementum. The next step is to quantize the oscillators.

1.5 Quantization of the Oscillators

To summarize the result of the calculatons of the last section we have the Hamiltonian for the radiation field.

$$\boxed{\mathbf{H} = \sum_{k,\alpha}\left(\frac{\omega}{c}\right)^2\left[c_{k,\alpha}c^*_{k,\alpha} + c^*_{k,\alpha}c_{k,\alpha}\right]}$$

$$\boxed{Q_{k,\alpha} = \frac{1}{c}\left(c_{k,\alpha} + c^*_{k,\alpha}\right)} \tag{1.23}$$

$$\boxed{P_{k,\alpha} = -\frac{i\omega}{c}\left(c_{k,\alpha} - c^*_{k,\alpha}\right)}$$

$$\boxed{H = \frac{1}{2}\sum_{k,\alpha}\left[P^2_{k,\alpha} + \omega^2 Q^2_{k,\alpha}\right]}$$

Soon after the development of non-relativistic quantum mechanics, Dirac proposed that the canonical variables of the radiation oscillators be reated like p and x in the quantum mechanics we know. The place to start is with the commutators. The coordinate and its corresponding momentum do not commute. For example $\left[p_x, x\right] = \frac{\hbar}{i}$. Coordinates and momenta that do not correspond, do not commute. For example $\left[p_y, x\right] = 0$. Different coordinates vommute with each other as do different momenta. We will impose the same rules here.

$$\begin{aligned}
\left[Q_{k,\alpha}, P_{k',\alpha'}\right] &= i\hbar\delta_{kk'}\delta_{\alpha\alpha'} \\
\left[Q_{k,\alpha}, Q_{k',\alpha'}\right] &= 0 \\
\left[P_{k,\alpha}, P_{k',\alpha'}\right] &= 0.
\end{aligned}$$

By now we know that if the Q and P do not commute, neither do the c and c^* so we should continue to avoid commuting them.

Since we are dealing with harmonic oscillators, we want to find the analog of the raising and lowering operators. We developed the raising and lowering operators by trying to write the Hamiltonian as $H = A^\dagger A\hbar\omega$. Follwing the same idea, we get

$$\begin{aligned}
a_{k,\alpha} &= \frac{1}{\sqrt{2\hbar\omega}}\left(\omega Q_{k,\alpha} + iP_{k,\alpha}\right)\\
a^\dagger_{k,\alpha} &= \frac{1}{\sqrt{2\hbar\omega}}\left(\omega Q_{k,\alpha} - iP_{k,\alpha}\right)\\
a^\dagger_{k,\alpha}a_{k,\alpha} &= \frac{1}{2\hbar\omega}\left(\omega Q_{k,\alpha} - iP_{k,\alpha}\right)\left(\omega Q_{k,\alpha} + iP_{k,\alpha}\right)\\
&= \frac{1}{2\hbar\omega}\left(\omega^2 Q^2_{k,\alpha} + P^2_{k,\alpha} + i\omega Q_{k,\alpha}P_{k,\alpha} - i\omega P_{k,\alpha}Q_{k,\alpha}\right)\\
&= \frac{1}{2\hbar\omega}\left(\omega^2 Q^2_{k,\alpha} + P^2_{k,\alpha} + i\omega Q_{k,\alpha}P_{k,\alpha} - i\omega\left(Q_{k,\alpha}P_{k,\alpha} + \frac{\hbar}{i}\right)\right)\\
&= \frac{1}{2\hbar\omega}\left(\omega^2 Q^2_{k,\alpha} + P^2_{k,\alpha} - \hbar\omega\right)\\
a^\dagger_{k,\alpha}a_{k,\alpha} + \frac{1}{2} &= \frac{1}{2\hbar\omega}\left(\omega^2 Q^2_{k,\alpha} + P^2_{k,\alpha}\right)\\
\left(a^\dagger_{k,\alpha}a_{k,\alpha} + \frac{1}{2}\right)\hbar\omega &= \frac{1}{2}\left(\omega^2 Q^2_{k,\alpha} + P^2_{k,\alpha}\right) = \mathbf{H}.
\end{aligned}$$

$$\boxed{\mathbf{H} = \left(a^\dagger_{k,\alpha}a_{k,\alpha} + \frac{1}{2}\right)\hbar\omega} \tag{1.24}$$

This is just the same as the Hamiltonian that we had for the one dimensional harmonic oscillator. We therefore have the raising and lowering operators, as long as $\left[a_{k,\alpha}, a^\dagger_{k,\alpha}\right] = 1$, as we had for the 1D harmonic oscillator.

$$\begin{aligned}
\left[a_{k,\alpha}, a^\dagger_{k,\alpha}\right] &= \left[\frac{1}{\sqrt{2\hbar\omega}}\left(\omega Q_{k,\alpha} + iP_{k,\alpha}\right), \frac{1}{\sqrt{2\hbar\omega}}\left(\omega Q_{k,\alpha} - iP_{k,\alpha}\right)\right]\\
&= \frac{1}{2\hbar\omega}\left[\omega Q_{k,\alpha} + iP_{k,\alpha}, \omega Q_{k,\alpha} - iP_{k,\alpha}\right]\\
&= \frac{1}{2\hbar\omega}\left(-i\omega\left[Q_{k,\alpha}, P_{k,\alpha}\right] + i\omega\left[P_{k,\alpha}, Q_{k,\alpha}\right]\right)\\
&= \frac{1}{2\hbar\omega}\left(\hbar\omega + \hbar\omega\right)\\
&= 1.
\end{aligned}$$

So these are definitely the raising and loweing operators. Of course the commutator would be zero if the operators were not for the same oscillator.

$$\left[a_{k,\alpha}, a^\dagger_{k',\alpha'}\right] = \delta_{kk'}\delta_{\alpha\alpha'} \tag{1.25}$$

(Note that all of our commutators are assumed to be taken at equal time.) The Hamiltonian is written in terms a and $a^\dagger$ in the same way as for the 1D harmonic oscillator. Therefore, everything we know about the raising and lowering operators applies here, including the commutator with the Hamiltonian, the raising and lowering of energy eigenstates, and even the constants.

$$a_{k,\alpha}|n_{k,\alpha}\rangle = \sqrt{n_{k,\alpha}}|n_{k,\alpha}-1\rangle$$
$$a^\dagger_{k,\alpha}|n_{k,\alpha}\rangle = \sqrt{n_{k,\alpha}+1}|n_{k,\alpha}\rangle\,.$$

The $n_{k,\alpha}$ can only take on integer values as with the harmonic oscillator we knw.

As with the 1D harmonic oscillator, we also casn define the number operator.

$$\mathbf{H} = \left(a^\dagger_{k,\alpha}a_{k,\alpha} + \frac{1}{2}\right)\hbar\omega = \left(N_{k,\alpha} + \frac{1}{2}\right)\hbar\omega.$$

The last step is to compute the raising and lowering operators in terms of the original coefficients.

$$\begin{aligned}
a_{k,\alpha} &= \frac{1}{\sqrt{2\hbar\omega}}\left(\omega Q_{k,\alpha} + iP_{k,\alpha}\right)\\
Q_{k,\alpha} &= \frac{1}{c}\left(c_{k,\alpha} + c^*_{k,\alpha}\right)\\
P_{k,\alpha} &= -\frac{i\omega}{c}\left(c_{k,\alpha} - c^*_{k,\alpha}\right)\\
&= \frac{1}{\sqrt{2\hbar\omega}}\frac{\omega}{c}\left(\left(c_{k,\alpha} + c^*_{k,\alpha}\right) + \left(c_{k,\alpha} - c^*_{k,\alpha}\right)\right)\\
&= \frac{1}{\sqrt{2\hbar\omega}}\frac{\omega}{c}\left(c_{k,\alpha} + c^*_{k,\alpha} + c_{k,\alpha} - c^*_{k,\alpha}\right)\\
&= \sqrt{\frac{\omega}{2\hbar c^2}}\left(2c_{k,\alpha}\right)\\
&= \sqrt{\frac{2\omega}{\hbar c^2}c_{k,\alpha}}.
\end{aligned}$$

$$\boxed{c_{k,\alpha} = \sqrt{\frac{\hbar c^2}{2\omega}}a_{k,\alpha}} \tag{1.26}$$

Similarly we can compute that

$$\boxed{c^*_{k,\alpha} = \sqrt{\frac{\hbar c^2}{2\omega}}a^\dagger_{k,\alpha}} \tag{1.27}$$

Since we now have the coefficients in our decomposition of the field equal to a constant times the raising or lowering operators, it is clear that these coefficients have themselves operators.

1.6 Photon States

It is now obvious that the integer $n_{k,\alpha}$ is the number of photons in the volume with wave number $\vec{k}$ and polarization $\hat{\epsilon}^{(\alpha)}$. It is called the occupation number for the state designated by the wave number $\vec{k}$ and polarization $\hat{\epsilon}^{(\alpha)}$. We can represent the state of the entire volume by giving the number of photons of each type (and some phases). The state vector for the volume is given by the direct product of the states for each type of photon.

$$\left|n_{k_1,\alpha_1}, n_{k_2,\alpha_2}, \ldots, n_{k_i,\alpha_i}, \ldots\right\rangle = \left|n_{k_1,\alpha_1}\right\rangle \left|n_{k_2,\alpha_2}\right\rangle \ldots \left|n_{k_i,\alpha_i}\right\rangle \ldots \tag{1.28}$$

The ground state for a particular oscillator cannot be lowered. The state in which all the oscilltors are in the ground state is called the vacuum state and can be written simply as $|0\rangle$

$$\left|n_{k_1,\alpha_1}, n_{k_2,\alpha_2}, \ldots, n_{k_i,\alpha_i}, \ldots\right\rangle = \prod_i \frac{\left(a^\dagger_{k_i,\alpha_i}\right)^{n_{k_i,\alpha_i}}}{\sqrt{n_{k_i,\alpha_i}!}} \tag{1.29}$$

The factorial on the bottom cancels all the $\sqrt{n+1}$ we get from the raising operators.

Any multi-photon state we construct is automatically symmetric under the interchange of pairs of photons. For example if we want to raise two photons out of the vacuum, we apply two raising operators. Since $\left[a^\dagger_{k,\alpha}, a^\dagger_{k',\alpha'}\right] = 0$, interchanging the photons gives the same state.

$$a^\dagger_{k,\alpha}, a^\dagger_{k',\alpha'}\left|0\right\rangle = a^\dagger_{k',\alpha'}, a^\dagger_{k,\alpha}\left|0\right\rangle \tag{1.30}$$

So the fact that the creation operators commute dictates that photon states are symmetricunder interchange.

1.7 Fermion Operators

At this point, we can hypothesize that the operators that create fermion states do not commute. In fact, if we assume the operators fermion states anti-commute (as do the Pauli matricies), then we can show that fermion states are antisymmetric under interchange. Assume $b^\dagger_r$ and b_r are the creation and annihilation operators for fermions and that they anti-commute.

$$\boxed{\left\{b^\dagger_r, b^\dagger_{r'}\right\} = 0} \tag{1.31}$$

The states are then antisymmetric under interchange of pairs of fermions.

$$b^\dagger_r b^\dagger_{r'}\left|0\right\rangle = -b^\dagger_{r'} b^\dagger_r\left|0\right\rangle \tag{1.32}$$

It's not hard to show that the occupation number for fermion states is either zero or one.

1.8 Quantized Radiation Field

The Fourier coefficients of the expansion of the classical radiation field should now be replaced by operators.

$$c_{k,\alpha} \to \sqrt{\frac{\hbar c^2}{2\omega}} a_{k,\alpha}$$
$$c^*_{k,\alpha} \to \sqrt{\frac{\hbar c^2}{2\omega}} a^\dagger_{k,\alpha}$$
$$A_\mu = \frac{1}{\sqrt{V}} \sum_{k,\alpha} \sqrt{\frac{\hbar c^2}{2\omega}} \epsilon^{(\alpha)}_\mu \left(a_{k,\alpha}(t)\, e^{i\vec{k}\cdot\vec{x}} + a^\dagger_{k,\alpha}(t)\, e^{-i\vec{k}\cdot\vec{x}} \right).$$

A is now an operator that acts on state vectors in occupation number space. The operator is parameterized in terms of $\vec{x}$ and t. This type of operator is called a field operator or a quantized field. The Hamiltonian operator can also be written in terms of the creation and annihilation operators.

$$\begin{aligned}
\mathbf{H} &= \sum_{k,\alpha} \left(\frac{\omega}{c}\right)^2 \left[c_{k,\alpha} c^*_{k,\alpha} + c^*_{k,\alpha} c_{k,\alpha} \right] \\
&= \sum_{k,\alpha} \left(\frac{\omega}{c}\right)^2 \frac{\hbar c^2}{2\omega} \left[a_{k,\alpha} a^\dagger_{k,\alpha} + a^\dagger_{k,\alpha} a_{k,\alpha} \right] \\
&= \frac{1}{2} \sum_{k,\alpha} \hbar\omega \left[a_{k,\alpha} a^\dagger_{k,\alpha} + a^\dagger_{k,\alpha} a_{k,\alpha} \right].
\end{aligned}$$

$$\boxed{\mathbf{H} = \sum_{k,\alpha} \hbar\omega \left(N_{k,\alpha} + \frac{1}{2} \right)} \tag{1.33}$$

For our purposes, we may remove the (infinite) constant energy due to the ground state enrgy of all the oscillators. It is simply the energy of the vacuum which we may define as zero. Note that the field fluctuations that cause this energy density, also cause the spontaneous decay of states of atoms. One thing that must be done is to cut off the sum at some maximum value of k. We so not expect electricity and magnetism to be completely valid up to infinite energy. Certainly by the gravitational or grand unified enrgy scale there must be important corrections to our formulas. The energy density of the vacuum is hard to define but plays an important role in cosmology. At this time, physicists have difficulty explaining how small the energy density in the vacuum is. Until recent experiments showed otherwise, most physicists thought it was actually zero due to some unknown symmetry. In any case we are not ready to consider this problem.

$$\mathbf{H} = \sum_{k,\alpha} \hbar\omega N_{k,\alpha} \tag{1.34}$$

With this subtraction, the enrgy of the vacuum state has been defined to be zero.

$$\mathbf{H}\,|0\rangle = 0 \tag{1.35}$$

This time the $\frac{1}{2}$ can really be dropped since the sum is over positive and negative $\vec{k}$, so it sums to zero.

$$\vec{P} = \sum_{k,\alpha} \hbar \vec{k} N_{k,\alpha} \tag{1.36}$$

The total momentum in the (transverse) radiation field can also be computed (from the classical formula for the Poynting vector)

$$\vec{P} = \frac{1}{c} \int \vec{E} \times \vec{B} d^3x = \sum_{k,\alpha} \hbar \vec{k} \left(N_{k,\alpha} + \frac{1}{2} \right) \tag{1.37}$$

We can compute the energy and momentum of a single photon state by operating on the state with the Hamiltonian and with the total momentum operator. The state for a single photon with a given momentum and polarization can be written as $a^\dagger_{k,\alpha} |0\rangle$

$$\mathbf{H} a^\dagger_{k,\alpha} |0\rangle = \left(a^\dagger_{k,\alpha} \mathbf{H} + \left[\mathbf{H}, a^\dagger_{k,\alpha} \right] \right) |0\rangle = 0 + \hbar\omega a^\dagger_{k,\alpha} |0\rangle = \hbar\omega a^\dagger_{k,\alpha} |0\rangle \tag{1.38}$$

The energy of single photon state is $\hbar\omega$

$$P a^\dagger_{k,\alpha} |0\rangle = \left(a^\dagger_{k,\alpha} P + \left[P, a^\dagger_{k,\alpha} \right] \right) |0\rangle = 0 + \hbar\vec{k} a^\dagger_{k,\alpha} |0\rangle = \hbar\vec{k} a^\dagger_{k,\alpha} |0\rangle \tag{1.39}$$

The momentum of the single photon state is $\hbar\vec{k}$. The mass of the photon can be computed.

$$\begin{aligned} E^2 &= p^2 c^2 + \left(mc^2 \right)^2 \\ mc^2 &= \sqrt{(\hbar\omega)^2 - (\hbar k)^2 c^2} = \hbar\sqrt{\omega^2 - \omega^2} = 0. \end{aligned}$$

The polarization $\hat{\epsilon}^{(\pm)}$ is associated with the $m = \pm 1$ component of the photon's spin. These are the transverse mode of the photon, $\vec{k} \cdot \hat{\epsilon}^{(\pm)} = 0$. We have separated the field into transverse and longitudinal parts. The longitudinal part is partially responsible for static E and B fields, while the transverse part makes up radiation. The $m = 0$ component of the photon is not present in radiation but is important in understanding static fields.

By assuming the canonical coordinates and momenta in the Hamiltonian have commutators like those of the position and momentum of a particle, led to an understanding that radiation is made up of spin-1 particles with mass zero. All fields correspond to a particle of definite mass and spin. We now have a pretty good idea how to quantize the field for any particle.

1.9 The Time Development of Field Operators

The creation and annihilation operators are related to the time dependent coefficients in our Fourier expansion of the radiation field.

$$c_{k,\alpha}(t) = \sqrt{\frac{\hbar c^2}{2\omega}} a_{k,\alpha}$$
$$c^*_{k,\alpha}(t) = \sqrt{\frac{\hbar c^2}{2\omega}} a^\dagger_{k,\alpha}.$$

This means that the creation, annihilation, and other operators are time dependent operators as we have studied the Heisenberg representation. In particular, we derived the canonical equation for the time dependence of an operator.

$$\begin{aligned}
\frac{d}{dt}B(t) &= \frac{i}{\hbar}[H, B(t)] \\
\dot{a}_{k,\alpha} &= \frac{i}{\hbar}[H, a_{k,\alpha}(t)] = \frac{i}{\hbar}(-\hbar\omega) a_{k,\alpha}(t) = -i\omega a_{k,\alpha}(t) \\
\dot{a}^\dagger_{k,\alpha} &= \frac{i}{\hbar}\left[H, a^\dagger_{,k,\alpha}(t)\right] = i\omega a^\dagger_{k,\alpha}(t).
\end{aligned}$$

So the operators have the same time dependence as did the coefficients in the Fourier expansion.

$$\begin{aligned}
a_{k,\alpha} &= a_{k,\alpha}(0) e^{-i\omega t} \\
a^\dagger_{k,\alpha}(t) &= a^\dagger_{k,\alpha}(0) e^{i\omega t}.
\end{aligned}$$

We can now write the quantized radiation field in terms of the operators at $t = 0$.

$$\boxed{A_\mu = \frac{1}{\sqrt{V}} \sum_{k,\alpha} \sqrt{\frac{\hbar c^2}{2\omega}} \epsilon^{(\alpha)}_\mu \left(a_{k,\alpha}(0) e^{ik_p x_p} + a^\dagger_{k,\alpha}(0) e^{-ik_p x_p} \right)} \tag{1.40}$$

Again, the 4-vector x_p is a parameter of this field, not the location of a photon. The field operator is Hermitial and the field itself is real.

1.10 Uncertainty relations and RMS Field Fluctuations

since the fields are sum of creation and annihilation operators, they do not commute with the occupation number operators

$$N_{k,\alpha} = a^\dagger_{k,\alpha} a_{k,\alpha} \tag{1.41}$$

Observables corresponding to operators which do not commute have an uncertainty principle between them. So we can't fix the number of photons and know the fields exactly. Fluctuations in the field take place even in the vacuum state, where we know there are no photons.

Of course the average value of the Electric or Magnetic field vector is zero by symmetry. To get an idea about the size of the field fluctuations, we should look at the mean square value of the field, for example in the vacuum state. We compute $\left\langle \left| \vec{E} \cdot \vec{E} \right| 0 \right\rangle$.

$$\vec{E} = -\frac{1}{c}\frac{\partial \vec{A}}{\partial t}$$

$$A_\mu = \frac{1}{\sqrt{V}}\sum_{k,\alpha}\sqrt{\frac{\hbar c^2}{2\omega}}\epsilon_\mu^{(\alpha)}\left(a_{k,\alpha}(0)\,e^{ik_p x_p}0a_{k,\alpha}^\dagger(0)\,e^{-ik_p x_p}\right)$$

$$\vec{A} = \frac{1}{\sqrt{V}}\sum_{k,\alpha}\sqrt{\frac{\hbar c^2}{2\omega}}\hat{\epsilon}^{(\alpha)}\left(a_{k,\alpha}(0)\,e^{ik_p x_p} + a_{k,\alpha}^\dagger(0)\,e^{-ik_p x_p}\right)$$

$$\vec{E} = -i\frac{1}{c}\frac{1}{\sqrt{V}}\sum_{k,\alpha}\sqrt{\frac{\hbar c^2}{2\omega}}\hat{\epsilon}^{(\alpha)}\left(-\omega a_{k,\alpha}(0)\right)e^{ik_p x_p} + \omega a_{k,\alpha}^\dagger(0)\,e^{-ik_p x_p}$$

$$\vec{E} = \frac{i}{\sqrt{V}}\sum_{k,\alpha}\sqrt{\frac{\hbar\omega}{2}}\hat{\epsilon}^{(\alpha)}\left(a_{k,\alpha}(0)\,e^{ik_p x_p} - a_{k,\alpha}^\dagger(0)\,e^{-ik_p x_p}\right)$$

$$\vec{E}\,|0\rangle = \frac{i}{\sqrt{V}}\sum_{k,\alpha}\sqrt{\frac{\hbar\omega}{2}}\hat{\epsilon}^{(\alpha)}\left(-a_{k,\alpha}^\dagger e^{-ik_p x_p}\right)|0\rangle$$

$$\left\langle 0\left|\vec{E}\cdot\vec{E}\right|0\right\rangle = \frac{1}{v}\sum_{k,\alpha}\frac{\hbar\omega}{2}1$$

$$\left\langle 0\left|\vec{E}\cdot\vec{E}\right|0\right\rangle = \frac{1}{V}\sum_{k}\hbar\omega \to \infty.$$

(Notice that we are basically taking the absolute square of $\vec{E}\,|0\rangle$ and that the orthogonality of the states collapses the result down to a single sum.)

The calculation is illustrative even though the answer is infinite. Basically, a term proportial to $aa^\dagger$ first creates one photon absorbs it giving a nonzero contribution for every oscillator mode. The terms sum to infinity but really it is the infinitesimally short wavelengths that cause this. Again, some cut off in the maximum energy would make sense.

The effect of these field fluctuations on particles is mitigated by quantum mechanics. In reality, any quantum particle will be spread out over a finite volume and it's the average field over the volume that might cause the particle to experience a force. So we could average the Electric field over a volume, then take the mean square of the average. If we average over a cubic volume $\Delta V = \Delta l^3$, when we find that.

$$\left\langle 0\left|\vec{E}\cdot\vec{e}\right|0\right\rangle \approx \frac{\hbar c}{\Delta l^4} \tag{1.42}$$

Thus if we can probe short distances, the effective size of the fluctuations increases.

Even the E and B fields do not commute. It can be shown that

$$\left[E_x(x)\,B_y(x')\right] = ic\hbar\delta\left(ds = \sqrt{(x-x')_p\,(x-x')_p}\right) \tag{1.43}$$

There is a nonzero commutator of the two spacetime points are connected by a light-like vector. Another way to say this is that the commutor is non-zero if the coordinates are simultaneous. This is a reasonable result considering causality.

To make a narrow beam of light, one must adjust the phases of various components of the beam carefully. Another version ofg the uncertainty relation is that $\Delta N \Delta\phi \geq 1$, where ϕ is the phase of the Fourier component and N is the number of photons.

Of course the Electromagnetic waves of classical physics usually have large numbers of photons and the quantum effects are not apparent. A good condition to identify the boundary between classical and quantum behavior is that for the classical E&M to be correct the number of photons per cubic wavelength should be much greater than 1.

1.11 Emission and Absorption of Photons by Atoms

The interaction of an electron with the quantized field is already in the standard Hamiltonian

$$\begin{aligned}\mathbf{H} &= \frac{1}{2m}\left(\vec{p} + \frac{e}{c}\vec{A}\right)^2 + V(r) \\ \mathbf{H}_{\text{int}} &= -\frac{e}{2mc}\left(\vec{p}\cdot\vec{A} + \vec{A}\cdot\vec{p}\right) + \frac{e^2}{2mc^2}\vec{A}\cdot\vec{A} \\ &= -\frac{e}{mc}\vec{A}\cdot\vec{p} + \frac{e^2}{2mc^2}\vec{A}\cdot\vec{A}.\end{aligned}$$

For completeness we should add the interaction with the spin of the electron $\mathbf{H} = -\vec{\mu}\cdot\vec{B}$

$$\boxed{\mathbf{H}_{\text{int}} = -\frac{e}{mc}\vec{A}\cdot\vec{p} + \frac{e^2}{2mc^2}\vec{A}\cdot\vec{A} - \frac{e\hbar}{2mc}\vec{\sigma}\cdot\vec{\nabla}\times\vec{A}} \tag{1.44}$$

For an atom with many electrons, we must sum over all the electrons. The field is evaluated at the coordinate x which should be that of the electron. This interaction Hamiltonian contains operators to create and annihilate photons with transitions between atomic states. From our previous study of time dependant perturbation theory, we know that transitions between initial and final states are proporional to the matrix element of the perturbing Hamiltonian between states, $\langle n|\mathbf{H}_{\text{int}}|i\rangle$. The initial state $|i\rangle$ should include a direct product of the atomic state and the photon state. Lets concentrate on one type of photon for now. We then could write

$$|i\rangle = \left|\psi_i; \vec{n}_{k,\alpha}\right\rangle \tag{1.45}$$

with a similar expression for the final state.

We will first consider the absorption of the one photon from the field. Assume there are $n_{\vec{k},\alpha}$ photons of this type in the initial state and that one photon is absorbed. We therefore will need a term in the interaction Hamiltonian that contains on annihitation operators (only). This will just come from the linear term in A.

$$
\begin{aligned}
\langle n\left|\mathbf{H}_{int}\right|i\rangle &= \left\langle \psi_n; n_{\vec{k},\alpha}-1\left|-\frac{e}{mc}\vec{A}\cdot\vec{p}\right|\psi_i; n_{\vec{k},\alpha}\right\rangle \\
&= -\frac{e}{mc}\left\langle \psi_n; n_{\vec{k},\alpha}-1\left|\frac{1}{\sqrt{V}}\sqrt{\frac{\hbar c^2}{2\omega}}\hat{\epsilon}^{(\alpha)}\left(a_{k,\alpha}(0)\,e^{ik_p x_p}+a^{\dagger}_{k,\alpha}(0)\,e^{-ik_p x_p}\right)\cdot\vec{p}\right|\psi_i; n_{\vec{k},\alpha}\right\rangle \\
\left\langle n\left|\mathbf{H}^{(abs)}_{int}\right|i\right\rangle &= -\frac{e}{mc}\frac{1}{\sqrt{V}}\sqrt{\frac{\hbar c^2}{2\omega}}\left\langle \psi_n; n_{\vec{k},\alpha}-1\left|\hat{\epsilon}^{(\alpha)}\cdot\vec{p}\left(a_{k,\alpha}(0)\,e^{ik_p x_p}\right)\right|\psi_i; n_{\vec{k},\alpha}\right\rangle \\
&= -\frac{e}{m}\frac{1}{\sqrt{V}}\sqrt{\frac{\hbar}{2\omega}}\left\langle \psi_n; n_{\vec{k},\alpha}-1\left|\hat{\epsilon}^{(\alpha)}\cdot\vec{p}\sqrt{n_{\vec{k},\alpha}}e^{ik_p x_p}\right|\psi_i; n_{\vec{k},\alpha}-1\right\rangle \\
&= -\frac{e}{m}\frac{1}{\sqrt{V}}\sqrt{\frac{\hbar n_{\vec{k},\alpha}}{2\omega}}\left\langle \psi_n\left|e^{i\vec{k}\cdot\vec{r}}\hat{\epsilon}^{(\alpha)}\cdot\vec{p}\right|\psi_i\right\rangle e^{-i\omega t}.
\end{aligned}
$$

Similarly, for the emission of a photon the matrix element is.

$$
\begin{aligned}
\langle n\left|\mathbf{H}_{int}\right|i\rangle &= \left\langle \psi_n; n_{\vec{k},\alpha}+1\left|-\frac{e}{mc}\vec{A}\cdot\vec{p}\right|\psi_i; n_{\vec{k},\alpha}\right\rangle \\
\left\langle n\left|\mathbf{H}^{(emit)}_{int}\right|i\right\rangle &= -\frac{e}{mc}\frac{1}{\sqrt{V}}\sqrt{\frac{\hbar c^2}{2\omega}}\left\langle \psi_n; n_{\vec{k},\alpha}+1\left|\hat{\epsilon}^{(\alpha)}\cdot\vec{p}\,a^{\dagger}_{k,\alpha}(0)\,e^{-ik_p x_p}\right|\psi_i; n_{\vec{k},\alpha}\right\rangle \\
&= -\frac{e}{m}\frac{1}{\sqrt{V}}\sqrt{\frac{\hbar\left(n_{\vec{k},\alpha}+1\right)}{2\omega}}\left\langle \psi_n\left|e^{-i\vec{k}\cdot\vec{r}}\hat{\epsilon}^{(\alpha)}\cdot\vec{p}\right|\psi_i\right\rangle e^{i\omega t}.
\end{aligned}
$$

These give the same result as our earlier guess to put an $n+1$ in the emission operator.something

Chapter 2

Electron Self Energy Corrections

2.1 Introduction and Physical Motivation

If one calculates the energy of a point charge using classical electromagnitism, the result is infinate, yet as far as we know, the electron is point charge. One can calculate the energy needed to assemble an electron due, essentially, to the interaction of the electron with its own field. A uniform charge distribution with the classical radius of an electron, we have an energy $m_e c^2$. Experiments have probed the electron's charge distribution and found that it is consistent with a point charge down to distances much smallen than the classical radius. Beyond classical calculations, the self energy of the electron calculated in the quantum theory of Dirac is still infinate but the divergences are less severe.

At this pint we must take the unpleasant position (constant) infinate energy should just be subtracted when we consider the overall zero of energy (as we did for the field energy in the vacuum). Electrons exist and don't carry infinate amount of energy baggage so we just subtract off the infinate constant. Nevertheless, we will find that the electron's self energy may change when it is a bound state and we should account for this change in out energy level calculations. This calculation will also give us the opportunity to understand resonant behaviour in scattering.

We can calculate the lowest order self energy corrections represented by the two Feynman diagrams below.

In these, a photon is emitted then reabsorbed. As we now know, both of these amplitutesare in order e^2. The first one comes from the A^2 term in which the number of photons changes by zero or two and the second comes from the $\vec{A}\cdot\vec{p}$ term in second order time dependent pertubation theory. A calculation of the first diagram will give the same result for a free electron and a bound electron, while the second diagram will give different results because the intermediate states are different if an electron is bound than they are if it is free. We will therefore compute the amplitude from the second diagram.

2.2 Perturbation Theory Setup

$$H_{\text{int}} = -\frac{e}{mc}\vec{A}\cdot\vec{p}$$

$$\vec{A} = \frac{1}{\sqrt{V}}\sum_{\vec{k},\alpha}\sqrt{\frac{\hbar c^2}{2\omega}}\hat{\epsilon}^{(\alpha)}\left(a_{\vec{k},\alpha}e^{i\left(\vec{k}\cdot\vec{x}-\omega t\right)}+a^{\dagger}_{\vec{k},\alpha}e^{-i\left(\vec{k}\cdot\vec{x}-\omega t\right)}\right).$$

This contains a term causing absorption of a photon and another term causing emission. We separate the terms for absorption and emission and pull out the time dependence.

$$\mathbf{H}_{\text{int}} = \sum_{\vec{k},\alpha}\left(H^{\text{abs}}_{\vec{k},\alpha}e^{-i\omega t}+H^{\text{emit}}_{\vec{k},\alpha}e^{i\omega t}\right)$$

$$\mathbf{H}^{\text{abs}} = -\sqrt{\frac{\hbar e^2}{2m^2\omega V}}a_{\vec{k},\alpha}e^{i\vec{k}\cdot\vec{x}}\vec{p}\cdot\hat{\epsilon}^{(\alpha)}$$

$$\mathbf{H}^{\text{emit}} = -\sqrt{\frac{\hbar e^2}{2m^2\omega V}}a^{\dagger}_{\vec{k},\alpha}e^{i\vec{k}\cdot\vec{x}}\vec{p}\cdot\hat{\epsilon}^{(\alpha)}.$$

The initial and final state is the same $|n\rangle$, and second order pertubation theory will involve a sum over intermediate, and second order pertubation theory will involve a sum over intermediate atomic states, $\left|j\right\rangle$ and photon states. We will use the matrix elementsof the interaction Hamiltonian between those states.

$$\begin{aligned}\mathbf{H}_{\mathrm{jn}} &= \left\langle j \left| \mathbf{H}^{\mathrm{emit}}_{\vec{k},\alpha} \right| n \right\rangle \\ \mathbf{H}_{\mathrm{nj}} &= \left\langle n \left| \mathbf{H}^{\mathrm{abs}}_{\vec{k},\alpha} \right| j \right\rangle \\ \mathbf{H}_{\mathrm{nj}} &= \mathbf{H}^{*}_{\mathrm{jn}}.\end{aligned}$$

In this case, we want to use the equations for the state we are studying, ψ_n, and all intermediate states, ψ_j plus a photon. Transitions can be made by emitting a photon from ψ_n to an intermediate state and transitions can be made back to the state ψ_n from any intermediate state. We neglect transitions from one intermediate state to another as they are higher order. (The diagram is emit a photon from $\psi_n then reabsorbit.$)
The differential equations for the amplitudes are then.

$$\begin{aligned}i\hbar\frac{dc_j}{dt} &= \sum_{\vec{k},\alpha} \mathbf{H}_{jn} e^{i\omega t} c_n e^{i\omega_{nj} t} \\ i\hbar\frac{dc_n}{dt} &= \sum_{\vec{k},\alpha}\sum_{j} \mathbf{H}_{nj} e^{i\omega t} c_j e^{i\omega t}.\end{aligned}$$

In the equations for c_n, we explicitly account for the fact that an intermediate state can make a transition back to the initial state. Transitions through another intermediate state would be higher order and thus should be neglected. Note that the matrix elements for the transitions to and from the initial state are closely related. We also include the effect that the initial state can become depleted as intermediate states are populated by using c_n (instead of 1) in the equation for c_j. Note also that all the photon states will make nonzero contributions to the sum.

2.3 Solving the Coupled Equations

Our task is to solve these coupled equations. Previously, we did this by integration, but needed the assumption that the amplitude to be in the initial state was 1. Since we are attempting to calculate an energy shift, let us make that assumption and plug it into the equations to verify the solution.

$$c_n = e^{\frac{-i\Delta E_n t}{\hbar}} \tag{2.1}$$

ΔE_n will be a complex number, the real part of which represents an energy shift, and the imaginary part of which represents the lifetime (and energy width) of the state.

$$\begin{aligned}i\hbar\frac{dc_j}{dt} &= \sum_{\vec{k},\alpha} \mathbf{H}_{jn} e^{i\omega t} c_n e^{-i\omega_{nj} t} \\ c_n &= e^{\frac{-i\Delta E_n t}{\hbar}} \\ c_j(t) &= \frac{1}{i\hbar}\sum_{\vec{k},\alpha}\int_0^t dt' \mathbf{H}_{jn} e^{i\omega t'} e^{\frac{-i\Delta E_n t'}{\hbar}} e^{-i\omega_{nj} t'} \\ c_j(t) &= \frac{1}{i\hbar}\sum_{\vec{k},\alpha}\int_0^t dt' \mathbf{H}_{jn} e^{i\left(-\omega_{nj}-\Delta\omega_n+\omega\right)t'} \\ c_j(t) &= \sum_{\vec{k},\alpha} \mathbf{H}_{jn}\left[\frac{e^{i\left(-\omega_{nj}-\Delta\omega_n+\omega\right)t'}}{\hbar\left(\omega_{nj}+\Delta\omega_n-\omega\right)}\right]_0^t \\ c_j(t) &= \sum_{\vec{k},\alpha} \mathbf{H}_{jn}\frac{e^{i\left(-\omega_{nj}-\Delta\omega_n+\omega\right)t-1}}{hbar\left(\omega_{nj}+\Delta\omega_n-\omega\right)}.\end{aligned}$$

Substitute this back into the differential equation for c_n to verify the solution and to find out what ΔE_n is. Note that the double sum over photons reduces to a single sum because we must absorb the same type of photon that was emitted. (We have not explicitly carried along the photon state for economy.)

$$
\begin{aligned}
i\hbar\frac{dc_n}{dt} &= \sum_{\vec{k},\alpha}\sum_j \mathbf{H}_{nj}e^{-i\omega t}c_j e^{i\omega_{nj}t} \\
c_j(t) &= \sum_{\vec{k},\alpha}\mathbf{H}_{jn}\frac{e^{i\left(-\omega_{nj}-\Delta\omega_n+\omega\right)t}-1}{\hbar\left(\omega_{nj}+\Delta\omega_n-\omega\right)} \\
i\hbar\frac{dc_n}{dt} &= \Delta E_n e^{-i\Delta E_n t/\hbar} = \sum_{\vec{k},\alpha}\sum_j \mathbf{H}_{nj}\mathbf{H}_{jn}e^{-i\omega t}e^{i\omega_{nj}t}\frac{e^{i\left(-\omega_{nj}-\Delta\omega_n+\omega\right)t}-1}{\hbar\left(\omega_{nj}+\Delta\omega_n-\omega\right)} \\
\Delta E_n &= \sum_{\vec{k},\alpha}\sum_j \left|\mathbf{H}_{nj}\right|^2 e^{i\left(\omega_{nj}+\Delta\omega_n-\omega\right)t}\frac{e^{i\left(-\omega_{nj}-\Delta\omega_n+\omega\right)t}-1}{\hbar\left(\omega_{nj}+\Delta\omega_n-\omega\right)} \\
\Delta E_n &= \sum_{\vec{k},\alpha}\sum_j \left|\mathbf{H}_{nj}\right|^2 \frac{1-e^{i\left(\omega_{nj}+\Delta\omega_n-\omega\right)t}}{\hbar\left(\omega_{nj}+\Delta\omega_n-\omega\right)}.
\end{aligned}
$$

Dince this is a calculation to order e^2 and the interaction Hamiltonian squared contains a factor of e^2 we should drop the $\Delta\omega_n = \Delta E_n/\hbar$ s from the right hand side of this equation.

$$\Delta E_n = \sum_{\vec{k},\alpha}\sum_j \left|\mathbf{H}_{nj}\right|^2 \frac{1-e^{i\left(\omega_{nj}-\omega\right)t}}{\hbar\left(\omega_{nj}-\omega\right)} \tag{2.2}$$

We have a solution to the coupled differential equations to order e^2. We should let $t\to\infty$ since the self energy is not a time dependent thing, however, the result oscillates as a function of time. This has been the case for many of out important delta functions, like the dot product of states with definite momentum. Let us analyze this self energy expression for large time.

2.4 Energy Shift and Width

We have something of the form.

$$-i\int_0^t e^{ixt'}\,dt' = \frac{1-e^{ixt}}{x} \tag{2.3}$$

If we think of x as a complex number, our integral goes along the real axis. In the upper hald plane, just above the real axis, $x\to x+i\epsilon$, the function goes to zero at infinity. In the lower half plane it blows up at infinity and on the axis, it's not well defined. We will calculate our result in the upper half plane and take the limit as we approach the real axis.

$$\lim_{t\to\infty}\frac{1-e^{ixt}}{x} = \lim_{\epsilon\to 0+} i\int_0^\infty e^{ixt'}\,dt' = \lim_{\epsilon\to 0+}\frac{1}{x+i\epsilon} = \lim_{\epsilon\to 0+}\left[\frac{x}{x^2+\epsilon^2}-\frac{i\epsilon}{x^2+\epsilon^2}\right] \tag{2.4}$$

This is well behaved everywhere expect at $x=0$. The second term goes to $-\infty$ there. A little further analasys could show that the second term is a delta function.

$$\lim_{t\to\infty}\frac{1-e^{ixt}}{x} = \frac{1}{x}-i\pi\delta(x) \tag{2.5}$$

Recalling that $c_n e^{-iE_n r/\hbar} = e^{\frac{-i\Delta E_n t}{\hbar}}e^{-iE_n t/\hbar} = e^{-i(E_n+\Delta E_n)t/\hbar}$, the real part of ΔE_n corresponds to an energy shift in

the state $|n\rangle$ and the imaginary part corresponds to a width.

$$\Re\left(\Delta E_n\right) = \sum_{\vec{k},\alpha}\sum_{j}\frac{\left|\mathbf{H}_{nj}\right|^2}{\hbar\left(\omega_{nj}-\omega\right)}$$

$$\Im\left(\Delta E_n\right) = -\pi\sum_{\vec{k},\alpha}\sum_{j}\frac{\left|\mathbf{H}_{nj}\right|^2}{\hbar}\delta\left(\omega_{nj}-\omega\right) = -\pi\sum_{\vec{k},\alpha}\sum_{j}\left|\mathbf{H}_{nj}\right|^2\delta\left(E_n-E_j-\hbar\omega\right).$$

All photon energies contribute to the real part. Only photons that satisfy the delta function constraint to the imaginary part. Moreover, there will only be an imaginary part if there is a lower energy state into which the state in question can decay. We can relate this width o those we previously calculated.

$$-\frac{2}{\hbar}\Im\left(\Delta E_n\right) = \sum_{\vec{k},\alpha}\sum_{j}\frac{2\pi\left|\mathbf{H}_{nj}\right|^2}{\hbar}\delta\left(E_n-E_j-\hbar\omega\right) \tag{2.6}$$

The time dependence of the wavefunction for the state n is modified by the self energy correction.

$$\psi_n\left(\vec{x},t\right) = \psi_n\left(\vec{x}\right)e^{-i(E_n+\Re(\Delta E_n))t/\hbar}e^{\frac{-\Gamma_n t}{2}} \tag{2.7}$$

This also gives us the exponential decay behaviour that we expect, keeping resonant scattering cross sections from going to infinity. So, the width just goes into the time dependence as expected and we don't have to worry about it anymore. We can now concentrate on the energy shift due to the real part of ΔE_n.

2.5 Evaluation of the Energy Shift

$$\begin{aligned}
\Delta E_n \equiv \Re\left(\Delta E_n\right) &= \sum_{\vec{k},\alpha}\sum_{j}\frac{\left|\mathbf{H}_{nj}\right|^2}{\hbar\left(\omega_{nj}-\omega\right)}\\
\mathbf{H}_{nj} &= \left\langle n\left|\mathbf{H}^{\text{abs}}_{\vec{k},\alpha}\right|j\right\rangle\\
\mathbf{H}^{\text{abs}} &= -\sqrt{\frac{\hbar e^2}{2m^2\omega V}}E^{i\vec{k}\cdot\vec{x}}\vec{p}\cdot\hat{\epsilon}^{(\alpha)}\\
\Delta E_n &= \frac{\hbar e^2}{2m^2V}\sum_{\vec{k},\alpha}\sum_{j}\frac{\left|\left\langle n\left|e^{i\vec{k}\cdot\vec{x}}\vec{p}\cdot\hat{\epsilon}^{(\alpha)}\right|j\right\rangle\right|^2}{\hbar\omega\left(\omega_{nj}-\omega\right)}\\
&= \frac{e^2}{2m^2V}\int\frac{Vd^3k}{(2\pi)^3}\sum_{\alpha}\sum_{j}\frac{\left|\left\langle n\left|e^{i\vec{k}\cdot\vec{x}}\vec{p}\cdot\hat{\epsilon}^{(\alpha)}\right|j\right\rangle\right|^2}{\omega\left(\omega_{nj}-\omega\right)}\\
&= \frac{e^2}{(2\pi)^3\,2m^2}\sum_{\alpha}\sum_{j}\int d\Omega\,\frac{k^2dk}{\omega}\frac{\left|\left\langle n\left|e^{i\vec{k}\cdot\vec{x}}\vec{p}\cdot\hat{\epsilon}^{(\alpha)}\right|j\right\rangle\right|^2}{\left(\omega_{nj}-\omega\right)}\\
&= \frac{e^2}{(2\pi)^3\,2m^2c^3}\sum_{j}\sum_{\alpha}\int d\Omega\int\frac{\omega\left|\left\langle n\left|e^{i\vec{k}\cdot\vec{x}}\vec{p}\right|j\right\rangle\cdot\hat{\epsilon}^{(\alpha)}\right|^2}{\left(\omega_{nj}-\omega\right)}d\omega.
\end{aligned}$$

In our calculation of the total decay rate summed over polarization and integrated over photon direction we computed the cosine of the angle between each polarization vector and the (vector) matrix element. Summing these two and integrating over photon direction we got a factor of $\frac{8\pi}{3}$ and the polarization is eliminated from the

matrix element. The same calculation applies here.

$$\begin{aligned}\Delta E_n &= \frac{e^2}{(2\pi)^3 2m^2c^3}\sum_j \frac{8\pi}{3}\int \frac{\omega\left|\left\langle n\left|e^{i\vec{k}\cdot\vec{x}}\vec{p}\right|j\right\rangle\right|^2}{(\omega_{nj}-\omega)}\,d\omega \\ &= \frac{e^2}{6\pi^2m^2c^3}\sum_j \int \frac{\omega\left|\left\langle n\left|e^{i\vec{k}\cdot\vec{x}}\vec{p}\right|j\right\rangle\right|^2}{(\omega_{nj}-\omega)}\,d\omega \\ &= \frac{2\alpha\hbar}{3\pi m^2c^2}\sum_j \int \frac{\omega\left|\left\langle n\left|e^{i\vec{k}\cdot\vec{x}}\vec{p}\right|j\right\rangle\right|^2}{(\omega_{nj}-\omega)}\,d\omega.\end{aligned}$$

Note that we wish to use the electric dipole approximation which is not valid for large $k = \frac{\omega}{c}$. It is valid up to about 2000 eV so we wish to cut off the calculation around there. While this calculation clearly diverges, things are less clear here because of the eventually rapid oscillation of the $e^{i\vec{k}\cdot\vec{x}}$ term in the integrand as the E1 approximation fails. Nevertheless, the largest differences in corrections between free electrons and bound electrons occur in the region in which the E1 approximation is valid. For now we will just use it and assume the cut-off is low enough.

2.6 Free Electron Self Energy

It is the difference between the bound electron's self energy and that for a free electron in which we are interested. Therefore, we will start with the free electron with a definite momentum $\vec{p}$. The normalized wave function for the free electron is $\frac{1}{\sqrt{V}}e^{i\vec{p}\cdot\vec{x}}/\hbar$.

$$\begin{aligned}\Delta E_{\text{free}} &= \frac{2\alpha\hbar}{3\pi m^2c^2V^2}\sum_{\vec{p}'}\int \frac{\omega}{(\omega_{nj}-\omega)}\left|\int e^{-i\vec{p}\cdot\vec{x}/\hbar}\vec{p}e^{i\vec{p}'\cdot\vec{x}/\hbar}d^3\right|^2 d\omega \\ &= \frac{2\alpha\hbar}{3\pi m^2c^2V^2}\left|\vec{p}\right|^2\sum_{\vec{p}}\int \frac{\omega}{(\omega_{nj}-\omega)}\left|\int e^{i(\vec{p}'/\hbar-\vec{p}\cdot\vec{x}/\hbar)}d^3x\right|^2 d\omega \\ &= \frac{2\alpha\hbar}{3\pi m^2c^2V^2}\left|\vec{p}\right|^2\sum_{\vec{p}'}\int \frac{\omega}{(\omega_{nj}-\omega)}\left|V\delta_{\vec{p}',\vec{p}}\right|^2 d\omega \\ &= \frac{2\alpha\hbar}{3\pi m^2c^2}\left|\vec{p}\right|^2\int_0^\infty \frac{\omega}{(\omega_{nj}-\omega)}\,d\omega \\ &= \frac{2\alpha\hbar}{3\pi m^2c^2}\left|\vec{p}\right|^2\int_0^\infty \frac{\omega}{(\omega_{nj}-\omega)}d\omega \to -\infty.\end{aligned}$$

It's easy to see that this will go to negative infinity if the limit on the integral is infinite. It is quite reasonable to cut off the integral at some enrgy beyond which the theory we are using is invalid. Since we are still using non-relativistic quantum mechanics, the cut-off should have $\hbar\omega \ll mc^2$. For the E1 approximation, it should be $\hbar\omega \ll 2\pi\hbar c/1 = 10keV$. We will approximate $\frac{\omega}{(\omega_{nj}-\omega)} \approx -1$ since the integral is just giving us a number and we are not interested in high accuracy here. We will be more interested in accuracy in the next

section when we compute the difference between free electron and bound electron self energy corrections.

$$\begin{aligned}
\Delta E_{free} &= \frac{2\alpha\hbar}{3\pi m^2c^2}\left|\vec{p}\right|^2\int_0^{E_{cut-off}/\hbar}\frac{\omega}{\left(\omega_{nj}-\omega\right)}\,d\omega \\
&= -\frac{2\alpha\hbar}{3\pi m^2c^2}\left|\vec{p}\right|^2\int_0^{E_{cut-off}/\hbar}\frac{\omega}{\left(\omega_{nj}-\omega\right)}\,d\omega \\
&= -\frac{2\alpha\hbar}{3\pi m^2c^2}\left|\vec{p}\right|^2 E_{cut-off}/\hbar \\
&= -\frac{2\alpha}{3\pi m^2c^2}\left|\vec{p}\right|^2 E_{cut-off} \\
&= -C\left|\vec{p}\right|^2.
\end{aligned}$$

If we were hoping for little dependence on the cut-off we should be disappointed. This self energy calculated is linear in the cut-off.

2.7 Mass Renormalization

For a non-relativisitc free electron the energy $\frac{p^2}{2m}$ decreases as the mass of the electron increases, so the negative sign corresponds to a positive shift in the electron's mass, and hence an increase in the real energy of the electron. Later, we will think of this as a renormalization of the electron's mass. The electron starts off with some bare mass. The self-energy due to the interaction of the electron's charge with its own radiation field increases the mass to what is observed.

Note that the correction to the energy is a constant times p^2, like the non-relativistic formula for the kinetic energy.

$$\begin{aligned}
C &= \frac{2\alpha}{3\pi m^2c^2}E_{cut-off} \\
\frac{p^2}{2m_{obs}} &= \frac{p^2}{2m_{bare}} - Cp^2 \\
\frac{1}{m_{obs}} &= \frac{1}{m_{bare}} - 2C \\
m_{obs} &= \frac{m_{bare}}{1-2Cm_{bare}} \approx \left(1+2Cm_{bare}\right)m_{bare} \approx \left(1+2Cm\right)m_{bare} \\
&= \left(1+\frac{4\alpha E_{cut-off}}{3\pi mc^2}\right)m_{bare}.
\end{aligned}$$

If we cut off the integral at m_ec^2, the correction to the mass is only about 0.3 percent, but if we don't cut off, its infinite. It makes no sense to trust our non-relativistic calculation up to infinite energy, so we must proceed with the cut-off integral.
If we use the Dirac theory, then we will be justified to move the cut-off up to very high energy. It turns out that the relativistic correction diverges logarithmically (instead of linearly) and the difference between bound and free electrons is finite relativistically (while it diverges logarithmically for out non-relativistic calculation).
Note that the self-energy of the free electron depends on the momentum of the electron, so we cannot simply subtract it from out bound state calculation. (What p^2 would we choose?) Rather we must account for the mass renormalization. We used the observed electron mass in the calculation of the Hydrogen bound state energies. In doing so, we have already included some of the self energy correction and we must not double correct. This is the subtraction we must make.

It's hard to keep all the minus signs straight in this calculation, particularly if we consider the bound and continuum electron states separately. The free particle correction to the electron mass is positive. Because we ignore the rest energy of the electron in our non-relativistic calculations. This makes a negative energy correction to both the bound $E = \frac{1}{2n^2}\alpha^2mc^2$ and the continuum $E \approx \frac{p^2}{2m}$. Bound states and continuum states have the

same fractional change in the energy. We need to add back in a positive term in ΔE_n to avoid double counting of the self-energy correction. Since the bound state and continuum state terms have the same fractional, it is convecient to just use $\frac{p^2}{2m}$ for all the corrections.

$$\frac{p^2}{2m_{obs}} = \frac{p^2}{2m_{bare}} - Cp^2$$
$$\Delta E_n^{(obs)} = \Delta E_n + C\left\langle n\left|p^2\right|n\right\rangle = \Delta E_n + \frac{2\alpha}{3\pi m^2 c^2} E_{cut-off}\left\langle n\left|p^2\right|n\right\rangle.$$

Because we are correcting for the mass used to calculate the base enrgy of the state $|n\rangle$, our corrections is written in terms of the electron's momentum in that state.

Chapter 3

The Lamb Shift

3.1 Experimental Discovery

In 1947, Willis E. Lamb and R. C Retherford used microwave techniques to determine the splitting between the $2S_{\frac{1}{2}}$ and $2P_{\frac{1}{2}}$ states in Hydrogen to have a frequency of 1.06 GHz, (a wavelenght of about 30 cm). (The shift is now accurately measured to be 1057.864 MHz.) This is abour the same size as the hyperfine splitting of the ground state.

The technique used was quite interesting. They made a beam of Hydrogen atoms in the $2S_{\frac{1}{2}}$ state, which has a very long lifetime because of selection rules. Microwave radiation with a (fixed) frequency of 2395 MHz was used to cause transitions to the $2P_{\frac{3}{2}}$ state and a magnetic field was adjusted to shift the enrgy of the states until the rate was largest. The decay of the $2P_{\frac{3}{2}}$ state to the ground state was observed to determine the transition rate. From this, they were able to deduce the shift between the $2S_{\frac{1}{2}}$ and $2P_{\frac{1}{2}}$ states. Hans Bethe used non-relativistic quantum mechanics to calculate the self-energy correction to account for this observation.

3.2 Bethe's Calculation

We now can compute the correction the same way he did.

$$\Delta E_n^{(obs)} = \Delta E_n + C \left\langle n \left| p^2 \right| n \right\rangle = \Delta E_n + \frac{2\alpha}{3\pi m^2 c^2} E_{cut-off} \left\langle n \left| p^2 \right| n \right\rangle$$

$$\Delta E_n = \frac{2\alpha\hbar}{3\pi m^2 c^2} \sum_j \int \frac{\omega \left| \left\langle n \left| e^{i\vec{k}\cdot\vec{x}} \vec{p} \right| j \right\rangle \right|^2}{(\omega_{nj} - \omega)} \, d\omega$$

$$\begin{aligned}
\Delta E_n^{(obs)} &= \frac{2\alpha\hbar}{3\pi m^2 c^2} \int_0^{\omega_{cut-off}} \left(\frac{\omega}{(\omega_{nj} - \omega)} \left| \left\langle n \left| e^{i\vec{k}\cdot\vec{p}} \vec{p} \right| j \right\rangle \right|^2 + \left\langle n \left| p^2 \right| n \right\rangle \right) d\omega \\
&= \frac{2\alpha\hbar}{3\pi m^2 c^2} \int_0^{\omega_{cut-off}} \sum_j \left(\frac{\omega}{(\omega_{nj} - \omega)} \left| \left\langle n \left| e^{i\vec{k}\cdot\vec{x}} \vec{p} \right| j \right\rangle \right|^2 + \left\langle n \left| \vec{p} \right| j \right\rangle \left\langle j \left| \vec{p} \right| n \right\rangle \right) d\omega \\
&= \frac{2\alpha\hbar}{3\pi m^2 c^2} \int_0^{\omega_{cut-off}} \sum_j \left(\frac{\omega}{(\omega_{nj} - \omega)} \left| \left\langle n \left| e^{i\vec{k}\cdot\vec{x}} \vec{p} \right| j \right\rangle \right|^2 + \left| \left\langle n \left| \vec{p} \right| j \right\rangle \right|^2 \right) d\omega.
\end{aligned}$$

It is now necessary to discuss approximate needed to complete this calculation. In particular, the electric dipole approximationwill be of great help, however, it is certainly not warranted for large photon energies. For a good E1 approximation we need $E_\gamma << 1973$ eV. On the other hand, we want the cut-off for the calculation to be of order $\omega_{cut-off} \approx mc^2/\hbar$. We will use the E1 approximation and the high cut-off, as Bethe did, to get the right answer. At the end, the result from a relativistic calculation can be tacked on to show why it turns out to be the

right answer. (We aren't aiming for the worlds best calculation anyway.)

$$\begin{aligned}
\Delta E_n^{(obs)} &= \frac{2\alpha\hbar}{3\pi m^2c^2}\int_0^{\omega_{cut-off}} \sum_j \left(\frac{\omega}{(\omega_{nj}-\omega)} \left|\left\langle n\left|\vec{p}\right|j\right\rangle\right|^2 + \left|\left\langle n\left|\vec{p}\right|j\right\rangle\right|^2 \right) d\omega \\
&= \frac{2\alpha\hbar}{3\pi m^2c^2}\int_0^{\omega_{cut-off}} \sum_j \frac{\omega + (\omega_{nj}-\omega)}{(\omega_{nj}-\omega)} \left|\left\langle n\left|\vec{p}\right|j\right\rangle\right|^2 d\omega \\
&= -\frac{2\alpha\hbar}{3\pi m^2c^2}\sum_j \int_0^{\omega_{cut-off}} \frac{\omega_{nj}}{\omega-\omega_{nj}} \left|\left\langle n\left|\vec{p}\right|j\right\rangle\right|^2 d\omega \\
&= -\frac{2\alpha\hbar}{3\pi m^2c^2}\sum_j \omega_{nj}\left[\log\left(\omega-\omega_{nj}\right)\right]_0^{\omega_{cut-off}} \left|\left\langle n\left|\vec{p}\right|j\right\rangle\right|^2 \\
&= \frac{2\alpha\hbar}{3\pi m^2c^2}\sum_j \omega_{nj}\left[\log\left(\left|\omega_{nj}\right|\right) - \log\left(\omega_{cut-off}\right)\right] \left|\left\langle n\left|\vec{p}\right|j\right\rangle\right|^2 \\
&\approx \frac{2\alpha\hbar}{3\pi m^2c^2}\sum_j \omega_{nj}\left[\log\log\left(\left|\omega_{nj}\right|\right) - \log\left(\omega_{cut-off}\right)\right] \left|\left\langle n\left|\vec{p}\right|j\right\rangle\right|^2 \\
&= \frac{2\alpha\hbar}{3\pi m^2c^2}\sum_j \omega_{nj}\log\left(\frac{\left|\omega_{nj}\right|}{\omega_{cut-off}}\right) \left|\left\langle n\left|\vec{p}\right|j\right\rangle\right|^2 .
\end{aligned}$$

The long term varies more slowly than the rest of the terms in the sum. We can approximate it by an average. Bethe used numerical calculations to determine that the effective average of $\hbar\omega_{nj}$ is $8.9\alpha^2mc^2$. We will do the same and pull the log term out as a constant.

$$\Delta E_n^{(obs)} = \frac{2\alpha\hbar}{3\pi m^2c^2}\log\left(\frac{|\overline{\omega}|}{\omega_{cut-off}}\right)\sum_j \omega_{nj}\left|\left\langle n\left|\vec{p}\right|j\right\rangle\right|^2 \tag{3.1}$$

3.3 Commutator Simplification

This sum can now be reduced further to a simple expression proportional to the $\left|\psi_n(0)\right|^2$ using a typical clever quantum mechanics calculation. The basic Hamitonian for the Hydrogen atom is $\mathbf{H}_0 = \frac{p^2}{2m} + V(r)$.

$$\begin{aligned}
\left[\vec{p}, \mathbf{H}_0\right] &= \left[\vec{p}, V\right] = \frac{\hbar}{i}\vec{\nabla}V \\
\left\langle j\left|\left[\vec{p}, \mathbf{H}_0\right]\right|n\right\rangle &= \frac{\hbar}{i}\left\langle j\left|\vec{\nabla}V\right|n\right\rangle \\
\sum_j \left\langle n\left|\vec{p}\right|j\right\rangle\left\langle j\left|\left[\vec{p}, \mathbf{H}_0\right]\right|n\right\rangle &= \frac{\hbar}{i}\sum_j \left\langle n\left|\vec{p}\right|j\right\rangle \cdot \left\langle j\left|\vec{\nabla V}\right|n\right\rangle \\
\sum_j (E_i - E_n)\left\langle n\left|\vec{p}\right|j\right\rangle\left\langle j\left|\vec{p}\right|n\right\rangle &= \frac{\hbar}{i}\sum_j \left\langle n\left|\vec{p}\right|j\right\rangle\left\langle j\left|\vec{\nabla V}\right|n\right\rangle .
\end{aligned}$$

This must be a real number so we may use its complex conjugate.

$$\left(\sum_j (E_i - E_n) \langle n|\vec{p}|j\rangle \langle j|\vec{p}|n\rangle\right)^* = \sum_j (E_i - E_n) \langle n|\vec{p}|j\rangle \langle j|\vec{p}|n\rangle$$
$$= -\frac{\hbar}{i} \sum_j \left\langle n\left|\vec{\nabla}V\right|j\right\rangle \langle j|\vec{p}|n\rangle$$
$$\sum_j (E_i - E_n) \langle n|\vec{p}|j\rangle \langle j|\vec{p}|n\rangle = \frac{\hbar}{2i}\left[\sum_j \langle n|\vec{p}|j\rangle \left\langle j\left|\vec{\nabla}V\right|n\right\rangle - \left\langle n\left|\vec{\nabla}V\right|j\right\rangle \langle j|\vec{p}|n\rangle\right]$$
$$= \frac{\hbar}{2i}\left\langle n\left|\left[\vec{p}, \vec{\nabla}V\right]\right|n\right\rangle$$
$$= -\frac{\hbar^2}{2}\langle n|\nabla^2 V|n\rangle$$
$$= -\frac{\hbar^2}{2}\langle n|e^2\delta^3(\vec{x})|n\rangle$$
$$= -\frac{e^2\hbar^2}{2}|\psi_n(0)|^2.$$

3.4 Result for S-States

Only the s states will have a non-vanishing probability to be at the origin with $|\psi_{n00}(0)|^2 = \frac{1}{\pi n^3 a_0^3}$ and $a_0 = \frac{\hbar}{\alpha mc}$. Therefore, only the s states will shift in energy appreciably. The shift will be.

$$\Delta E_n^{(obs)} = -\frac{2\alpha\hbar}{3\pi m^2 c^2}\log\left(\frac{|\overline{\omega}_{nj}|}{\omega_{cut-off}}\right)\frac{e^2\hbar}{2}\frac{1}{\pi n^3}\left(\frac{\alpha mc}{\hbar}\right)^3$$
$$= \frac{\alpha^4 e^2 mc}{3\pi^2\hbar n^3}\log\left(\frac{\omega_{cut-off}}{|\overline{\omega}_{nj}|}\right)$$
$$= \frac{4\alpha^5 mc^2}{6\pi}\log\left(\frac{mc^2}{8.9\alpha^2 mc^2}\right)$$
$$\Delta E_{2s}^{(obs)} = \frac{\alpha^5 mc^2}{6\pi}\log\left(\frac{mc^2}{8.9\alpha^2 mc^2}\right)$$
$$\nu = \frac{\Delta E_{2s}^{(obs)}}{2\pi\hbar} = \frac{\alpha^5 mc^2 c}{12\pi^2\hbar c}\log\left(\frac{1}{8.9\alpha^2}\right) = 1.041GHz.$$

3.5 Relativistic Correction and Combined Result

This agrees far too well with the measurement, considering the approximations made and the dependence on the cut-off. There is, however, justification in the relativistic calculation. Typically, the full calculation was made by using this non-relativistic approach up to some energy of the order of αmc^2, and using the relativistic calculation above that. The relativistic free electron self-energy correction diverges only logarithmically and a very high cutoff can be used without a problem. The mass of the electron is renormalized as above. The Lamb shift does not depend on the cutoff and hence it is well calculated. We only need the non-relativistic part of the calculation up to photon energies for which the E1 approximations is OK. The relativistic part of the calculation down to ω_{min} yields.

$$\Delta E_n = \frac{4\alpha^5}{3\pi n^3}\left(\log\left(\frac{mc^2}{2\hbar\omega_{min}}\right) + \frac{11}{24} - \frac{1}{5}\right)mc^2 \tag{3.2}$$

The non-relativistic calculation gave.

$$\Delta E_n = \frac{4\alpha^5}{3\pi n^3}\log\left(\frac{\omega_{min}}{|\overline{\omega}_{nj}|}\right)mc^2 \tag{3.3}$$

So the sum of the two gives.

$$\Delta E_n^{(obs)} = \frac{4\alpha^5}{3\pi n^3}\left(\log\left(\frac{mc^2}{2\hbar\overline{\omega}_{nj}}\right) + \frac{11}{24} - \frac{1}{5}\right)mc^2 \tag{3.4}$$

The dependence on ω_{min} cancels. In this calculation, the mc^2 in the log is the outcome of the relativistic calculation, not the cutoff. The electric dipole approximation is even pretty good since we did not need to go up to large photon energies non-relativistically and no E1 approximation is needed for the relativistic part. That's how we (and Bethe) got about the right answer.

3.6 Physical Interpretation

The Lamb shift splits the $2S_{\frac{1}{2}}$ and $2P_{\frac{1}{2}}$ states which are otherwise degenerate. Its origin is purely from field theory. The experimental measurement of the Lamb shift stimulated theorists to develop Quantum ElectroDynamics. The correction increases the energy of s states. One may think of the physical origin as the electron becoming less point-like as virtual photons are emitted and reabsorbed. Spreading the electron out a bit decreases the effect of being in the deepest part of the potential, right at the origin. Based on the energy shift, I estimate that the electron in the 2s state is spread out about 0.005 Angtroms, much more than the size of the nucleus.

The anomalous magnetic moment of the electron, $g - 2$, which can also be calculated in field theory, makes a small contribution to the Lamb shift.

Chapter 4

Scattering of Photons

4.1 Scattering of Photons

In the scattering of photons, for example from an atom, an initial state photon with wave-number $\vec{k}$ and polarization $\hat{\epsilon}$ is absorbed by the atom and a final state photon with wave-number $\vec{k}'$ and polarization $\hat{\epsilon}'$ is emitted. The atom may remain in the same state (elastic scattering) or it may change to another state (inelastic). Any calculation we will do will use the matrix element of the interaction Hamiltonian between initial and final states.

$$\mathbf{H}_{ni} = \left\langle n; \vec{k}'\hat{\epsilon}^{(\alpha')} \left| \mathbf{H}_{int} \right| i; \vec{k}\hat{\epsilon}^{(\alpha)} \right\rangle$$
$$\mathbf{H}_{int} = -\frac{e}{mc}\vec{A}(x)\cdot\vec{p} + \frac{e^2}{2mc^2}\vec{A}\cdot\vec{A}.$$

The scattering process clearly requires terms in $\mathbf{H}_{int}$ that annihilate one photon and create another. The order does not matter. The $\frac{e^2}{2mc^2}\vec{A}\cdot\vec{A}$ is the square of the Fourier decomposition of the radiation field so it contains terms like $a^\dagger_{k',\alpha'}a_{k,\alpha}$, which are just what we want. The $-\frac{e}{mc}\vec{A}\cdot\vec{p}$ term has both creation and annihilation operators in it but not profucts of them. It changes the number of photons by plus or minus one, not by zero as required for the scattering process. Nevertheless this part of the interaction could contribute in second order perturbation theory, by absorbing one photon in a transition from the initial atomic state to an intermediate state, then emitting another photon and making a transition to the final atomic state. While this is higher order in perturbation theory, it is the same order in the electromagnetic coupling constant e, which is what really counts when expanding in powers of α. Therefore, we will need to consider the $\frac{e^2}{2mc^2}\vec{A}\cdot\vec{A}$ term in first order and the $-\frac{e}{mc}\vec{A}\cdot\vec{p}$ term in the second order perturbation theory to get an order α calculation of the matrix element. Start with the first order perturbation theory term. All the terms in the sum that do not annihilate the initial state photon and create the final state photon give zero. We will assume that the wavelength of the photon's is long compared to the size of the atom so that $e^{i\vec{k}\cdot\vec{r}} \approx 1$

$$A_\mu(x) = \frac{1}{\sqrt{V}}\sum_{k\alpha}\sqrt{\frac{\hbar c^2}{2\omega}}\epsilon^{(\alpha)}_\mu\left(a_{k,\alpha}(0)\,e^{ik_px_p} + a^\dagger_{k,\alpha}(0)\,e^{-ik_px_p}\right)$$

$$\begin{aligned}
\frac{e^2}{2mc^2}\left\langle n; \vec{k}'\hat{\epsilon}^{(\alpha')}\left|\vec{A}\cdot\vec{A}\right| i; \vec{k}\hat{\epsilon}^{(\alpha)}\right\rangle &= \frac{e^2}{2mc^2}\frac{1}{V}\frac{\hbar c^2}{2\sqrt{\omega'\omega}}\epsilon^{(\alpha)}_\mu\epsilon^{(\alpha')}_\mu\left\langle n; \vec{k}'\hat{\epsilon}^{(\alpha')}\left|\left(a_{k,\alpha}a^\dagger_{k',\alpha'} + a^\dagger_{k'\alpha'}a_{k,\alpha}\right)e^{i(k_p-k'_p)x_p}\right| i; \vec{k}\hat{\epsilon}^{(\alpha)}\right\rangle \\
&= \frac{e^2}{2mc^2}\frac{1}{V}\frac{\hbar c^2}{2\sqrt{\omega'\omega}}\epsilon^{(\alpha)}_\mu\epsilon^{(\alpha')}_\mu e^{-i(\omega-\omega')t}\left\langle n; \vec{k}'\hat{\epsilon}^{(\alpha')}\left|2\right| i; \vec{k}'\hat{\epsilon}^{(\alpha')}\right\rangle \\
&= \frac{e^2}{2mc^2}\frac{1}{V}\frac{\hbar c^2}{2\sqrt{\omega'\omega}}\epsilon^{(\alpha)}_\mu\epsilon^{(\alpha')}_\mu e^{-i(\omega-\omega')t}2\left\langle n|i\right\rangle \\
&= \frac{e^2}{2mc^2}\frac{1}{V}\frac{\hbar c^2}{\sqrt{\omega'\omega}}\epsilon^{(\alpha)}_\mu\epsilon^{(\alpha')}_\mu e^{-i(\omega-\omega')t}\delta_{ni}.
\end{aligned}$$

This is the matrix element $\mathbf{H}_{ni}(t)$. The amplitude to be in the final state $\left|n;\vec{k}'\hat{\epsilon}^{(\alpha')}\right\rangle$ is given by first order time dependent perturbation theory.

$$
\begin{aligned}
c_n^{(1)}(t) &= \frac{1}{i\hbar}\int_0^t e^{i\omega_{ni}t'}\mathbf{H}_{ni}(t')\,dt' \\
c^{(1)}_{n;\vec{k}'\hat{\epsilon}^{(\alpha')}}(t) &= \frac{1}{i\hbar}\frac{e^2}{2mc^2}\frac{1}{V}\frac{\hbar c^2}{\sqrt{\omega'\omega}}\epsilon_\mu^{(\alpha)}\epsilon_\mu^{(\alpha')}\delta_{ni}\int_0^t e^{i\omega_{ni}t'}e^{-i(\omega-\omega')t}\,dt' \\
&= \frac{e^2}{2imV\sqrt{\omega'\omega}}\hat{\epsilon}^{(\alpha)}\cdot\hat{\epsilon}^{(\alpha')}\delta_{ni}\int_0^t e^{i(\omega_{ni}+\omega'\omega)t'}\,dt'.
\end{aligned}
$$

Recall that the absoulte square of the time integral will turn into $2\pi t\delta(\omega_{ni}+\omega'-\omega)$. We will carry along the integral for now, since we are not yet ready to square it.

Now we very carefully put the interaction term into the formula for second order time dependent perturbation theory, again using $e^{i\vec{k}\cdot\vec{x}}\approx 1$. Our notation is that the intermediate state of atom and field is called $|I\rangle = \left|j, n_{\vec{k},\alpha}, n_{\vec{k}',\alpha'}\right\rangle$ where $\mathbf{j}$ represents the state of the atom and we may have zero or two photons, as indicated in the diagram.

$$
\begin{aligned}
\mathcal{V} &= -\frac{e}{mc}\vec{A}\cdot\vec{p} \equiv -\frac{e}{mc}\frac{1}{\sqrt{V}}\sum_{\vec{k}\alpha}\sqrt{\frac{\hbar c^2}{2\omega}}\hat{\epsilon}^{(\alpha)}\cdot\vec{p}\left(a_{k,\alpha}e^{-i\omega t}+a_{k,\alpha}^\dagger e^{i\omega t}\right) \\
c_n^{(2)}(t) &= -\frac{1}{\hbar^2}\sum_{j,\vec{k},\alpha}\int_0^t dt_2\mathcal{V}_{nI}(t_2)\,e^{i\omega_{nj}t_2}\int_0^{t_2}dt_1 e^{i\omega_{ji}t_1}\mathcal{V}_{Ii}(t_1) \\
c^{(2)}_{n;\vec{k}'\hat{\epsilon}^{(\alpha')}}(t) &= -\frac{e^2}{m^2c^2\hbar^2}\sum_I\frac{1}{V}\frac{\hbar c^2}{2\sqrt{\omega'\omega}}\int_0^t dt_2\left\langle n;\vec{k}'\hat{\epsilon}^{(\alpha')}\left|\left(\hat{\epsilon}^{(\alpha)}a_{k,\alpha}e^{-i\omega t_2}+\hat{\epsilon}^{(\alpha')}a_{k',\alpha'}^\dagger e^{i\omega' t_2}\right)\cdot\vec{p}\right|I\right\rangle e^{i\omega_{nj}t_2} \\
&\quad\times\int_0^{t_2}dt_1 e^{i\omega_{ji}t_1}\left\langle I\left|\hat{\epsilon}^{(\alpha)}a_{k,\alpha}e^{-iomet_1}+\hat{\epsilon}^{(\alpha')}a_{k',\alpha'}^\dagger e^{i\omega' t}\cdot\vec{p}\right|i;\vec{k}\hat{\epsilon}^{(\alpha)}\right\rangle.
\end{aligned}
$$

We can understand this formula as a second order transition from state $|i\rangle$ to state $|n\rangle$ through all possible intermediate states. The transition from the initial state to the intermediate state takes place at time t_1. The transition from the intermediate state to the final state takes place at time t_2.

The space-time diagram below shows the three terms in $c_n(t)$ Time is assumed to run updwards in the diagrams.

Diagram (c) represents the A^2 term in which one photon is absorbed and one emitted at the same piont. Diagrams (a) and (b) represent two second order terms. In diagram (a) the initial state photon is absorbed at time t_1, leaving the atom in an intermediate state which may or may not be the same as the initial (or final) atomic state. This intermediate state has no photons in the field. In digram (b), the atom emits the final state photon at time t_1, leaving the atom in some intermediate state. The intermediate state $|I\rangle$ includes two photons in the field for this diagram. At time t_2 the atom absorbs the initial state photon.

Looking again at the formula for the second order scattering amplitude, note that we integrate over the times t_1 and t_2 and that $t_1 < t_2$. For diagram (a), the annihilation operator $a_{k,\alpha}$ is active at time t_1 and the creation operator is active at time t_2. For diagram (b) it's just the opposite. The second order formula above contains four terms as written. The $a^\dagger a$ and $aa^\dagger$ terms are the ones described by the diagram. The aa and $a^\dagger a^\dagger$ terms will clearly give zero. Note that we are just picking the terms that will survive the calculation, not changing any formulas. Now, reduce to the two nonzero terms. The operators give a factor of 1 and make the photon states work out. If $\left|j\right\rangle$ is the intermediate atomic state, the second order term reduces to.

$$c^{(2)}_{n;\vec{k}'\hat{\epsilon}^{(\alpha')}} = -\frac{e^2}{2Vm^2\hbar\sqrt{\omega'\omega}}\sum_j \int_0^t dt_2 \int_0^{t_2} dt_1 \left[e^{i\left(\omega'+\omega_{nj}\right)t_2} \left\langle n \left| \hat{\epsilon}^{(\alpha')} \cdot \vec{p} \right| j \right\rangle e^{i\left(\omega_{ji}-\omega\right)t_1} \right.$$
$$\left. + e^{i\left(\omega_{nj}-\omega\right)t_2} \left\langle n \left| \hat{\epsilon}^{(\alpha)} \cdot \vec{p} \right| j \right\rangle e^{i\left(\omega'+\omega_{ji}\right)t_1} \right]$$

$$c^{(2)}_{n;\vec{k}'\hat{\epsilon}'}(t) = -\frac{e^2}{2Vm^2\hbar\sqrt{\omega'\omega}}\sum_j \int_0^t dt_2 \left[e^{i\left(\omega'+\omega_{nj}\right)t_2} \left\langle n \left| \hat{\epsilon}' \cdot \vec{p} \right| j \right\rangle \left\langle j \left| \hat{\epsilon} \cdot \vec{p} \right| i \right\rangle \left[\frac{e^{i\left(\omega_{nj}-\omega\right)t_1}}{i\left(\omega_{ji}-\omega\right)} \right]_0^{t_2} \right.$$
$$\left. + e^{i\left(\omega_{nj}-\omega\right)t_2} \left\langle n \left| \hat{\epsilon} \cdot \vec{p} \right| j \right\rangle \left\langle j \left| \hat{\epsilon}' \cdot \vec{p} \right| i \right\rangle \left[\frac{e^{i\left(\omega'+\omega_{ji}\right)t_1}}{i\left(\omega'+\omega_{ji}\right)} \right]_0^{t_2} \right]$$

$$c^{(2)}_{n;\vec{k}'\hat{\epsilon}'}(t) = -\frac{e^2}{2Vm^2\hbar\sqrt{\omega'\omega}}\sum_j \int_0^t dt_2 \left[e^{i\left(\omega'+\omega_{nj}\right)t_2} \left\langle n \left| \hat{\epsilon}' \cdot \vec{p} \right| j \right\rangle \left\langle j \left| \hat{\epsilon} \cdot \vec{p} \right| j \right\rangle \left[\frac{e^{i\left(\omega_{ji}-\omega\right)t_2}-1}{i\left(\omega_{ji}-\omega\right)} \right] \right.$$
$$\left. e^{i\left(\omega_{nj}-\omega\right)t_2} \left\langle n \left| \hat{\epsilon} \cdot \vec{p} \right| j \right\rangle \left\langle j \left| \hat{\epsilon}' \cdot \vec{p} \right| i \right\rangle \left[\frac{e^{i\left(\omega'+\omega_{ji}\right)t_2}-1}{i\left(\omega'+\omega_{ji}\right)} \right] \right].$$

The -1 terms coming from the integration over t_1 can be dropped. We can anticipate that the integral over t_2 will eventually give us a delta function of energy conservation, going to infinity when energy is conserved and going to zero when it is not. Those -1 terms can never go to infinity and can therefore be neglected. When the energy conservation is satisfied, those terms are negligible and when it is not, the whole thing goes to zero.

$$c^{(2)}_{n;\vec{k}'\hat{\epsilon}'}(t) = -\frac{e^2}{2Vm^2\hbar\sqrt{\omega'\omega}}\sum_j \int_0^t dt_2 \left[e^{i\left(\omega_{ni}+\omega'-\omega\right)t_2} \left\langle n \left| \hat{\epsilon}' \cdot \vec{p} \right| j \right\rangle \left\langle j \left| \hat{\epsilon} \cdot \vec{p} \right| i \right\rangle \left[\frac{1}{i\left(\omega_{ji}-\omega\right)} \right] \right.$$
$$\left. + e^{i\left(\omega_{ni}+\omega'-\omega\right)t_2} \left\langle n \left| \hat{\epsilon} \cdot \vec{p} \right| j \right\rangle \left\langle j \left| \hat{\epsilon}' \cdot \vec{p} \right| i \right\rangle \left[\frac{1}{i\left(\omega'+\omega_{ji}\right)} \right] \right]$$

$$c^{(2)}_{n;\vec{k}'\hat{\epsilon}'}(t) = -\frac{e^2}{2iVm^2\hbar\sqrt{\omega'\omega}}\sum_j \left[\frac{\left\langle n \left| \hat{\epsilon}' \cdot \vec{p} \right| j \right\rangle \left\langle j \left| \hat{\epsilon} \cdot \vec{p} \right| i \right\rangle}{\omega_{ji}-\omega} + \frac{\left\langle n \left| \hat{\epsilon} \cdot \vec{p} \right| j \right\rangle \left\langle j \left| \hat{\epsilon}' \cdot \vec{p} \right| i \right\rangle}{\omega'+\omega_{ji}} \right]$$
$$\times \int_0^t dt_2 e^{i\left(\omega_{ni}+\omega'-\omega\right)t_2}.$$

We have calculated all the amplitudes. The first order and second order amplitudes should be combined,

then squared.

$$
\begin{aligned}
c_n(t) &= c_n^{(1)}(t) + c_n^{(2)}(t) \\
c^{(1)}_{n;\vec{k}'\hat{\epsilon}'}(t) &= \frac{e^2}{2iVm\sqrt{\omega'\omega}}\hat{\epsilon}\cdot\hat{\epsilon}'\delta_{ni}\int_0^t e^{i(\omega_{ni}+\omega'-\omega)t'}\,dt' \\
c^{(2)}_{n;\vec{k}'\hat{\epsilon}'}(t) &= -\frac{e^2}{2iVm^2\hbar\sqrt{\omega'\omega}}\sum_j\left[\frac{\langle n|\hat{\epsilon}'\cdot\vec{p}|j\rangle\langle j|\hat{\epsilon}\cdot\vec{p}|i\rangle}{\omega_{ji}-\omega}+\frac{\langle n|\hat{\epsilon}\cdot\vec{p}|j\rangle\langle j|\hat{\epsilon}'\cdot\vec{p}|i\rangle}{\omega'+\omega_{ji}}\right]\int_0^t dt_2 e^{i(\omega_{ni}+\omega'-\omega)t_2} \\
c_{n;\vec{k}'\hat{\epsilon}'}(t) &= \left(\delta_{ni}\hat{\epsilon}\cdot\hat{\epsilon}'-\frac{1}{m\hbar}\sum_j\left[\frac{\langle n|\hat{\epsilon}'\cdot\vec{p}|j\rangle\langle j|\hat{\epsilon}\cdot\vec{p}|i\rangle}{\omega_{ji}-\omega}+\frac{\langle n|\hat{\epsilon}\cdot\vec{p}|j\rangle\langle j|\hat{\epsilon}'\cdot\vec{p}|i\rangle}{\omega'+\omega_{ji}}\right]\right) \\
&\quad\times\frac{e^2}{2iVm\sqrt{\omega'\omega}}\int_0^t dt_2 e^{i(\omega_{ni}+\omega'-\omega)t_2} \\
|c(t)|^2 &= \left|\delta_{ni}\hat{\epsilon}\cdot\hat{\epsilon}'-\frac{1}{m\hbar}\sum_j\left[\frac{\langle n|\hat{\epsilon}'\cdot\vec{p}|j\rangle\langle j|\hat{\epsilon}\cdot\vec{p}|i\rangle}{\omega_{ji}-\omega}+\frac{\langle n|\hat{\epsilon}\cdot\vec{p}|j\rangle\langle j|\hat{\epsilon}'\cdot\vec{p}|i\rangle}{\omega'+\omega_{ji}}\right]\right|^2 \\
&\quad\times\frac{e^4}{4V^2m^2\omega'\omega}\left|\int_0^t dt_2 e^{i(\omega_{ni}+\omega'-\omega)t_2}\right|^2 \\
|c(t)|^2 &= \left|\delta_{ni}\hat{\epsilon}\cdot\hat{\epsilon}'-\frac{1}{m\hbar}\sum_j\left[\frac{\langle n|\hat{\epsilon}'\cdot\vec{p}|j\rangle\langle j|\hat{\epsilon}\cdot\vec{p}|i\rangle}{\omega_{ji}-\omega}+\frac{\langle n|\hat{\epsilon}\cdot\vec{p}|j\rangle\langle j|\hat{\epsilon}'\cdot\vec{p}|i\rangle}{\omega'+\omega_{ji}}\right]\right|^2 \\
&\quad\times\frac{e^4}{4V^2m^2\omega'\omega}2\pi t\,\delta(\omega_{ni}+\omega'-\omega)
\end{aligned}
$$

$$
\begin{aligned}
\Gamma &= \int\frac{Vd^3k'}{(2\pi)^3}\left|\delta_{ni}\hat{\epsilon}\cdot\hat{\epsilon}'-\frac{1}{m\hbar}\sum_j\left[\frac{\langle n|\hat{\epsilon}'\cdot\vec{p}|j\rangle\langle j|\hat{\epsilon}\cdot\vec{p}|i\rangle}{\omega_{ji}-\omega}+\frac{\langle n|\hat{\epsilon}\cdot\vec{p}|j\rangle\langle j|\hat{\epsilon}'\cdot\vec{p}|i\rangle}{\omega'+\omega_{ji}}\right]\right|^2 \\
&\quad\times\frac{e^4}{4V^2m^2\omega'\omega}2\pi\delta(\omega_{ni}+\omega'-\omega) \\
\Gamma &= \int\frac{V\omega'^2d\omega'd\Omega}{(2\pi)^3}\left|\delta_{ni}\hat{\epsilon}\cdot\hat{\epsilon}'-\frac{1}{m\hbar}\sum_j\left[\frac{\langle n|\hat{\epsilon}'\cdot\vec{p}|j\rangle\langle j|\hat{\epsilon}\cdot\vec{p}|i\rangle}{\omega_{ji}-\omega}+\frac{\langle n|\hat{\epsilon}\cdot\vec{p}|j\rangle\langle j|\hat{\epsilon}'\cdot\vec{p}|i\rangle}{\omega'+\omega_{ji}}\right]\right|^2 \\
&\quad\times\frac{e^4}{4V^2m^2\omega'\omega}2\pi\delta(\omega_{ni}+\omega'-\omega) \\
\Gamma &= \int d\Omega\left|\delta_{ni}\hat{\epsilon}\cdot\hat{\epsilon}'-\frac{1}{m\hbar}\sum_j\left[\frac{\langle n|\hat{\epsilon}'\cdot\vec{p}|j\rangle\langle j|\hat{\epsilon}\cdot\vec{p}|i\rangle}{\omega_{ji}-\omega}+\frac{\langle n|\hat{\epsilon}\cdot\vec{p}|j\rangle\langle j|\hat{\epsilon}'\cdot\vec{p}|i\rangle}{\omega'+\omega_{ji}}\right]\right|^2 \\
&\quad\times\frac{V\omega'^2}{(2\pi c)^3}\frac{e^4}{4V^2m^2\omega'\omega}2\pi \\
\frac{d\Gamma}{d\Omega} &= \frac{e^4\omega'}{(4\pi)^2Vm^2c^3\omega}\left|\delta_{ni}\hat{\epsilon}\cdot\hat{\epsilon}'-\frac{1}{m\hbar}\sum_j\left[\frac{\langle n|\hat{\epsilon}'\cdot\vec{p}|j\rangle\langle j|\hat{\epsilon}\cdot\vec{p}|i\rangle}{\omega_{ji}-\omega}+\frac{\langle n|\hat{\epsilon}\cdot\vec{p}|j\rangle\langle j|\hat{\epsilon}'\cdot\vec{p}|i\rangle}{\omega'+\omega_{ji}}\right]\right|^2.
\end{aligned}
$$

Note that the delta function has enforced energy conservation requiring that $\omega' = \omega - \omega_{ni}$, but we have left ω' in the formula for convenince.

The final step to a differential cross section is to divide the transition rate by the incident flux of particled. This is a suprisingly easy step because we are using plane waves of photons. The initial state is one particle in

the volume V moving with velocity of c, so the flux is simply $\frac{c}{V}$.

$$\frac{d\sigma}{d\Omega} = \frac{e^4\omega'}{(4\pi)^2 m^2 c^4 \omega}\left|\delta_{ni}\hat{\epsilon}\cdot\hat{\epsilon}' - \frac{1}{m\hbar}\sum_j\left[\frac{\langle n|\hat{\epsilon}'\cdot\vec{p}|j\rangle\langle j|\hat{\epsilon}\cdot\vec{p}|i\rangle}{\omega_{ji}-\omega} + \frac{\langle n|\hat{\epsilon}\cdot\vec{p}|j\rangle\langle j|\hat{\epsilon}'\cdot\vec{p}|i\rangle}{\omega'+\omega_{ji}}\right]\right|^2 \tag{4.1}$$

The classical radius of the electron is defined to be $r_0 = \frac{e^2}{4\pi mc^2}$ in our units. We will factor the square of this out but leave the answer in terms of fundemental constants.

$$\frac{d\sigma}{d\Omega} = \left(\frac{e^2}{4\pi mc^2}\right)^2\left(\frac{\omega'}{\omega}\right)\left|\delta_{ni}\hat{\epsilon}\cdot\hat{\epsilon}' - \frac{1}{m\hbar}\sum_j\left[\frac{\langle n|\hat{\epsilon}'\cdot\vec{p}|j\rangle\langle j|\hat{\epsilon}\cdot\vec{p}|i\rangle}{\omega_{ji}-\omega} + \frac{\langle n|\hat{\epsilon}\cdot\vec{p}|j\rangle\langle j|\hat{\epsilon}'\cdot\vec{p}|i\rangle}{\omega_{ji}+\omega'}\right]\right|^2 \tag{4.2}$$

This is called the Kramers-Heisenberg Formula. Even now, the three (space-time) Feynman diagrams are visible as separate terms in the formula.

(They show up like $\left|c + \sum_j (a+b)\right|^2$ Note that, for the very short time that the system is in an intermediate state, energy conservation is not strictly enforced. The energy denominators in the formula suppress larger energy non-conservation. The formula can be applied to several physical situations as discusssed below.

Also note that the formula yields an infinite result if $\omega = \pm\omega_{ji}$. This is not a physical result. In fact the cross section will be large but not infinite when energy is conserved in the intermediate state. This condition is often referred to as 'the intermediate state being on the mass shell' because of the relation between energy and mass in four dimensions

4.2 Resonant Scattering

The Kramers-Heiseberg photon scattering cross section, below, has unphysical infinities if an intermediate state is on the mass shell.

$$\frac{d\sigma}{d\Omega} = \left(\frac{e^2}{4\pi mc^2}\right)^2\left(\frac{\omega'}{\omega}\right)\left|\delta_{ni}\hat{\epsilon}\cdot\hat{\epsilon}' - \frac{1}{m\hbar}\sum_j\left[\frac{\langle n|\hat{\epsilon}'\cdot\vec{p}|j\rangle\langle j|\hat{\epsilon}\cdot\vec{p}|i\rangle}{\omega_{ji}-\omega}\frac{\langle n|\hat{\epsilon}\cdot\vec{p}|j\rangle\langle j|\hat{\epsilon}'\cdot\vec{p}|i\rangle}{\omega_{ji}+\omega'}\right]\right|^2 \tag{4.3}$$

In reality, the cross section becomes large but not infinite. These infinites come about because we have not properly accounted for the finite lifetime of the intermediate state when we derived the second order perturbation theory formula. If the energy width of the intermediate states is included in the calculation, as we will attempt below, the cross section is large but not infinite.

The resonance in the cross section will exhibit the same shape and width as does the intermediate state. These resonances in the cross section can dominate scattering. Again both resonant terms in the cross section, occur if an intermediate state has the right energy so that the energy is conserved.

4.3 Elastic Scattering

In elastic scattering, the initial and final atomic states are the same, as are the initial and final photon energies.

$$\frac{d\sigma_{elastic}}{d\Omega} = \left(\frac{e^2}{4\pi mc^2}\right)^2\left|\delta_{ii}\hat{\epsilon}\cdot\hat{\epsilon}' - \frac{1}{m\hbar}\sum_j\left[\frac{\langle i|\hat{\epsilon}'\cdot\vec{p}|j\rangle\langle j|\hat{\epsilon}\cdot\vec{p}|i\rangle}{\omega_{ji}-\omega} + \frac{\langle i|\hat{\epsilon}\cdot\vec{p}|j\rangle\langle j|\hat{\epsilon}'\cdot\vec{p}|i\rangle}{\omega_{ji}+\omega}\right]\right|^2 \tag{4.4}$$

The commutator $\left[\vec{x},\vec{p}\right]$ (with no dot products) can be very useful in calculations. When the two vectors are multiplied directly, we get something with two Cartesian indices.

$$x_i p_j - p_j x_i = i\hbar\delta_{ij} \tag{4.5}$$

The commutator of the vectors is $i\hbar$ times the identity. This can be used to cast the first term above into something like the other two.

$$\begin{aligned} x_i p_j - p_j x_i &= i\hbar\delta_{ij} \\ \hat{\epsilon}\cdot\hat{\epsilon}' &= \hat{\epsilon}_i\hat{\epsilon}'_j\delta_{ij} \\ i\hbar\hat{\epsilon}\cdot\hat{\epsilon}' &= \hat{\epsilon}_i\hat{\epsilon}'_j\left(x_i p_j - p_j x_i\right) \\ &= \left(\hat{\epsilon}\cdot\vec{x}\right)\left(\hat{\epsilon}'\cdot p\right)\left(\hat{\epsilon}'\cdot\vec{p}\right)\left(\hat{\epsilon}\cdot\vec{x}\right). \end{aligned}$$

Now we need to put the states in using an identity, then use the commutator with $\mathbf{H}$ to change $\vec{x}$ to $\vec{p}$.

$$\begin{aligned} 1 &= \sum_j \left\langle i|j\right\rangle\left\langle j|i\right\rangle \\ i\hbar\hat{\epsilon}\cdot\hat{\epsilon}' &= \sum_j\left[\left(\hat{\epsilon}\cdot\vec{x}\right)_{ij}\left(\hat{\epsilon}'\cdot\vec{p}\right)_{ji} - \left(\hat{\epsilon}'\cdot\vec{p}\right)_{ij}\left(\hat{\epsilon}\cdot\vec{x}\right)_{ji}\right] \\ \left[\mathbf{H},\vec{x}\right] &= \frac{\hbar}{im}\vec{p} \\ \frac{\hbar}{im}\left(\hat{\epsilon}\cdot\vec{p}\right)_{ij} &= \left(\hat{\epsilon}\left[\mathbf{H},\vec{x}\right]\right)_{ij} \\ &= \hbar\omega_{ij}\left(\hat{\epsilon}\cdot\vec{p}\right)_{ij} \\ \left(\hat{\epsilon}\cdot\vec{x}\right)_{ij} &= -\frac{i}{m\omega_{ij}}\left(\hat{\epsilon}\cdot\vec{p}\right)_{ij} \\ i\hbar\hat{\epsilon}\cdot\hat{\epsilon}' &= \sum_j\left[\frac{-i}{m\omega_{ij}}\left(\hat{\epsilon}\cdot\vec{p}\right)_{ij}\left(\hat{\epsilon}'\cdot\vec{p}\right)_{ij} - \frac{-i}{m\omega_{ji}}\left(\hat{\epsilon}'\cdot\vec{p}\right)_{ij}\left(\hat{\epsilon}\cdot\vec{p}\right)_{ji}\right] \\ &= \sum_j\left[\frac{-i}{m\omega_{ij}}\left(\hat{\epsilon}\cdot\vec{p}\right)_{ij}\left(\hat{\epsilon}'\cdot\vec{p}\right)_{ji} + \frac{-i}{m\omega_{ij}}\left(\hat{\epsilon}'\cdot\vec{p}\right)_{ij}\left(\hat{\epsilon}\cdot\vec{p}\right)_{ji}\right] \\ &= \sum_j\frac{-i}{m\omega_{ij}}\left[\left(\hat{\epsilon}\cdot\vec{p}\right)_{ij}\left(\hat{\epsilon}'\cdot\vec{p}\right)_{ji} + \left(\hat{\epsilon}'\cdot\vec{p}\right)_{ij}\left(\hat{\epsilon}\cdot\vec{p}\right)_{ji}\right] \\ \hat{\epsilon}\cdot\hat{\epsilon}' &= \frac{-1}{m\hbar}\sum_j\frac{1}{\omega_{ij}}\left[\left(\hat{\epsilon}'\cdot\vec{p}\right)_{ij}\left(\hat{\epsilon}\cdot\vec{p}\right)_{ji} + \left(\hat{\epsilon}\cdot\vec{p}\right)_{ij}\left(\hat{\epsilon}'\cdot\vec{p}\right)_{ji}\right]. \end{aligned}$$

(Reminder: $\omega_{ij} = \dfrac{E_i - E_j}{\hbar}$ is just a number. $\left(\hat{\epsilon}\cdot\vec{p}\right)_{ij} = \left\langle i\left|\hat{\epsilon}\cdot\vec{p}\right|j\right\rangle$ is a matrix element between states.)

We may now combine the terms for elastic scattering.

$$\frac{d\sigma_{elas}}{d\Omega} = \left(\frac{e^2}{4\pi mc^2}\right)^2 \left|\delta_{ii}\hat{\epsilon}\cdot\hat{\epsilon}' - \frac{1}{\hbar}\left[\frac{\langle i|\hat{\epsilon}\cdot\vec{p}|j\rangle\langle j|\hat{\epsilon}\cdot\vec{p}|i\rangle}{\omega_{ji}-\omega} + \frac{\langle i|\hat{\epsilon}\cdot\vec{p}|j\rangle\langle j|\hat{\epsilon}'\cdot\vec{p}|i\rangle}{\omega_{ji}+\omega}\right]\right|^2$$

$$\delta_{ii}\hat{\epsilon}\cdot\hat{\epsilon}' = \frac{-1}{m\hbar}\sum_j\left[\frac{\langle i|\hat{\epsilon}'\cdot\vec{p}|j\rangle\langle j|\hat{\epsilon}\cdot\vec{p}|i\rangle}{\omega_{ij}} + \frac{\langle i|\hat{\epsilon}\cdot\vec{p}|j\rangle\langle j|\hat{\epsilon}'\cdot\vec{p}|i\rangle}{\omega_{ij}}\right]$$

$$\frac{1}{\omega_{ij}} + \frac{1}{\omega_{ji}\pm\omega} = \frac{\omega_{ji}\pm\omega+\omega_{ji}}{\omega_{ij}(\omega_{ji}\pm\omega)} = \frac{\mp\omega}{\omega_{ji}(\omega_{ji}\pm\omega)}$$

$$\frac{d\sigma_{elas}}{d\Omega} = \left(\frac{e^2}{4\pi mc^2}\right)^2\left(\frac{1}{m\hbar}\right)^2\left|\sum_j\left[\frac{\omega\langle i|\hat{\epsilon}'\cdot\vec{p}|j\rangle\langle j|\hat{\epsilon}\cdot\vec{p}|i\rangle}{\omega_{ji}(\omega_{ji}-\omega)} - \frac{\omega\langle i|\hat{\epsilon}\cdot\vec{p}|j\rangle\langle j|\hat{\epsilon}'\cdot\vec{p}|i\rangle}{\omega_{ji}(\omega_{ji}+\omega)}\right]\right|^2.$$

This is a nice symmetric form for elastic scattering. If computation of the matrix elements is planned, it's useful to again use the commutator to change $\vec{p}$ into $\vec{x}$.

$$\boxed{\frac{d\sigma_{elas}}{d\Omega} = \left(\frac{e^2}{4\pi mc^2}\right)^2\left(\frac{m\omega}{\hbar}\right)^2\left|\sum_j\omega_{ji}\left[\frac{\langle i|\hat{\epsilon}'\cdot\vec{x}|j\rangle\langle j|\hat{\epsilon}\cdot\vec{x}|i\rangle}{\omega_{ji}-\omega} - \frac{\langle i|\hat{\epsilon}\cdot\vec{x}|j\rangle\langle j|\hat{\epsilon}'\cdot\vec{x}|i\rangle}{\omega_{ji}+\omega}\right]\right|^2} \tag{4.6}$$

4.4 Rayleigh Scattering

Lord Rayleigh calculated low energy elastic scattering of light from atoms using classical electromagnetism. If the energy of the scattered photon is much less than the energy needed to excite an atom, $\omega \ll \omega_{ji}$, then the cross section may be approximated.

$$\frac{\mp\omega_{ji}}{\omega_{ji}\pm\omega} = \frac{\mp\omega_{ji}}{\omega_{ji}\left(1\pm\frac{\omega}{\omega_{ji}}\right)} = \mp\left(1\mp\frac{\omega}{\omega_{ji}}\right) = \mp 1\frac{\omega}{\omega_{ji}}$$

$$\frac{d\sigma_{elas}}{d\Omega} = \left(\frac{e^2}{4\pi mc^2}\right)^2\left(\frac{m\omega}{\hbar}\right)^2\left|\sum_j\frac{\omega_{ji}\langle i|\hat{\epsilon}'\cdot\vec{x}|j\rangle\langle j|\hat{\epsilon}\cdot\vec{x}|i\rangle}{\omega_{ji}-\omega} - \frac{\omega_{ji}\langle i|\hat{\epsilon}\cdot\vec{x}|j\rangle\langle j|\hat{\epsilon}'\cdot\vec{x}|i\rangle}{\omega_{ji}+\omega}\right|^2$$

$$= \left(\frac{e^2}{4\pi mc^2}\right)^2\left(\frac{m\omega}{\hbar}\right)^2\left|\sum_j\left[\left(\langle i|\hat{\epsilon}'\cdot\vec{x}|j\rangle\langle j|\hat{\epsilon}\cdot\vec{x}|i\rangle\right.\right.\right.$$

$$\left.\left.\left. - \langle i|\hat{\epsilon}\cdot\vec{x}|j\rangle\langle j|\hat{\epsilon}'\cdot\vec{x}|i\rangle\right) + \frac{\omega}{\omega_{ji}}\left(\langle i|\hat{\epsilon}'\cdot\vec{x}|j\rangle\langle j|\hat{\epsilon}\cdot\vec{x}|i\rangle + \langle i|\hat{\epsilon}\cdot\vec{x}|j\rangle\langle j|\hat{\epsilon}'\cdot\vec{x}|i\rangle\right)\right]\right|^2$$

$$= \left(\frac{e^2}{4\pi mc^2}\right)^2\left(\frac{m}{\hbar}\right)^2\omega^4\left|\sum_j\left[\frac{1}{\omega_{ji}}\left(\langle i|\hat{\epsilon}'\cdot\vec{x}|j\rangle\langle j|\hat{\epsilon}\cdot\vec{x}|i\rangle + \langle i|\hat{\epsilon}\cdot\vec{x}|j\rangle\langle j|\hat{\epsilon}'\cdot\vec{x}|i\rangle\right)\right]\right|^2.$$

For the colorless gasses (like the ones in our atmosphere), the first excited state in the UV, so the scattering of visible light with be proportional to ω^4, which explains why the sky is blue and sunsets are red. Atoms with intermediate states in the visible will appear to be colored due to the strong resonances in the scattering. Rayleigh got the same dependence from classical physics.

4.5 Thomson scattering

If the energy of the scattered photon is much bigger than the binding energy of the atom, $\omega \gg 1$ eV, then cross section approaches that for scattering from a free electron, Thoomson Scattering. We still neglect the effect of electron recoil so we should also requre that $\hbar\omega \ll m_e c^2$. Start from the Kramers-Heisenberg formula.

$$\frac{d\sigma}{d\Omega} = \left(\frac{e^2}{4\pi m c^2}\right)^2 \left(\frac{\omega'}{\omega}\right) \left| \delta_{ni} \hat{\epsilon} \cdot \hat{\epsilon}' - \frac{1}{m\hbar} \sum_j \left[\frac{\langle n | \hat{\epsilon}' \cdot \vec{p} | j \rangle \langle j | \hat{\epsilon} \cdot \vec{p} | i \rangle}{\omega_{ji} - \omega} + \frac{\langle n | \hat{\epsilon} \cdot \vec{p} | j \rangle \langle j | \hat{\epsilon}' \cdot \vec{p} | i \rangle}{\omega_{ji} + \omega} \right] \right|^2 \tag{4.7}$$

The $\hbar\omega = \hbar\omega'$ denominators are much larger than $\frac{\langle n | \hat{\epsilon}' \cdot \vec{p} | j \rangle \langle j | \hat{\epsilon} \cdot \vec{p} | i \rangle}{m}$ which is of the order of the electron's kinetic energy, so we can ignore the second two terms. (Even if the intermediate and final states have unbound electrons, the initial state wave function will keep these terms small.)

$$\frac{d\sigma}{d\Omega} = \left(\frac{e^2}{4\pi m c^2}\right)^2 \left| \hat{\epsilon} \cdot \hat{\epsilon}' \right|^2 \tag{4.8}$$

This scattering cross section is of the order of the classical radius of the electron squared, and is independent of the frequency of the light. The only dependence is on polarization. This is a good time to take a look at the meaning of the polarization vectors we've been carrying around in the calculation and at the lack of any wave-vectors for the initial and final state. A look back at the calculation shows that we calculated the transition rate from a state with one photon with wave-vector $\vec{k}$ and polarization $\epsilon^{(\alpha)}$ to a final state with polarization of $\epsilon^{(\alpha')}$. We have integrated over the final state wave vector magnitude, subject to the delta function giving energy conservation, but we have not integrated over final state photon direction yet, as indicated by the $\frac{d\sigma}{d\Omega}$.

There is no explicit angular dependence but there is some hidden in the dot product between initial and final polarization vectors, both of which must be transverse to the direction of propagation. We are ready to compute four different differential cross sections corresponding to two initial polarizations times two final state photon polarizations. Alternatively, we average and/or sum, if we so choose. In the high energy approximation we have made, there is no dependence on the state of the atoms, so we are free to choose our coordinate system any way we want. Set the z-axis to be along the direction of the initial photon and set the x-axis so that the scattered photon is in the x-z plane $(\phi = 0)$. The scattered photon is at an angle θ to the initial photon direction and at $\phi = 0$. A reasonable set of initial state polarization vectors is

$$\hat{\epsilon}^{(1)} = \hat{x}$$
$$\hat{\epsilon}^{(2)} = \hat{y}.$$

Pick $\hat{\epsilon}^{(1)'}$ to be in the scattering plane (x-z) defined as the plane containing both $\vec{k}$ and $\vec{k}'$ and $\hat{\epsilon}^{(2)'}$ to be perpendicular to the scattering plane. $\hat{\epsilon}^{(1)'}$ is then at an angle. θ to the x-axis. $\hat{\epsilon^{(2)'}}$ is along the y-axis. We can compute all the dot products.

$$\hat{\epsilon^{(1)}} \cdot \hat{\epsilon}^{(1)'} = \cos\theta$$
$$\hat{\epsilon}^{(1)} \cdot \hat{\epsilon}^{(2)'} = 0$$
$$\hat{\epsilon}^{(2)} \cdot \hat{\epsilon}^{(1)'} = 0$$
$$\hat{\epsilon}^{(2)} \cdot \hat{\epsilon}^{(2)'} = 1.$$

From these, we can compute any cross section we want. For example, averaging over initial state polarization and summing over final is just half the sum of the squares of the above.

$$\frac{d\sigma}{d\Omega} = \left(\frac{e^2}{4\pi mc^2}\right)^2 \frac{1}{2}\left(1 + \cos^2\theta\right) \tag{4.9}$$

Even if the initial state is unpolarized, the final state can be polarized. For example, for $\theta = \frac{\pi}{2}$, all of the above dot products are zero except $\hat{\epsilon}^{(2)} \cdot \hat{\epsilon}^{(2)'} = 1$. That means only the initial photons polarized along the y direction will scatter and that the scattered photon is 100% polarized transverse to the scattering plane (really just the same polarization as the initial state). The angular distribution could also be used to deduce the polarization of the initial state if a large ensemble of initial state photons were available.

For a definite initial state polarization (at an angle ϕ to the scattering plane, the component along $\hat{\epsilon}^{(1)}$ is $\cos\phi$ and along $\hat{\epsilon}^{(2)}$ is $\sin\phi$). If we don't observe final state polarization we sum $\left(\cos\theta\cos\phi\right) + \left(\sin\phi\right)^2$ and have

$$\frac{d\sigma}{d\Omega} = \left(\frac{e^2}{4\pi mc^2}\right)^2 \frac{1}{2}\left(\cos^2\theta\cos^2\phi + \sin^2\phi\right) \tag{4.10}$$

For atoms with more than one electron, this cross section will grow as Z^4

Chapter 5

Deriving the KG Equation

5.1 The Strategy: Combining Relativity and Quantum Mechanics

The goal is to derive a relativistic wave equation that respects both special relativity and quantum mechanics. The strategy is to:

1. Start with Einstein's relativistic energy-momentum relation
2. Replace classical quantities (energy, momentum) with quantum operators
3. Apply these operators to a wavefunction ψ

This "double derivative" approach (squaring the energy) will give us a second-order differential equation.

Definition 5.1.1: Relativity: the mass shell (Einstein's energy-momentum relation)

Einstein showed that energy and momentum are related by:
$E^2 = (pc)^2 + (mc^2)^2$

Rearranging in four-vector notation: $p \cdot p = (mc)^2 \rightarrow (mc)^2 = \left(\frac{E}{c}\right)^2 - p_x^2 - p_y^2 - p_z^2$

This is called the **mass shell** — it's a constraint that relates energy and momentum for a particle with mass m.

Definition 5.1.2: Quantum: energy and momentum operators

In quantum mechanics, we promote classical observables to operators that act on wavefunctions. From the Schrödinger equation and de Broglie relations:

- Energy operator: $\hat{E} = i\hbar\frac{\partial}{\partial t}$
- Momentum operator: $\hat{p} = -i\hbar\nabla$

To use these in Einstein's energy-momentum relation, we need to square them. When we square an operator, we apply it twice:

Energy term:

$$\left(\frac{E}{c}\right)^2 \to \left(\frac{\hat{E}}{c}\right)^2 = \left(\frac{i\hbar}{c}\frac{\partial}{\partial t}\right)^2 = -\frac{\hbar^2}{c^2}\frac{\partial^2}{\partial t^2} \tag{5.1}$$

Momentum terms:

$$\hat{p}_x = -i\hbar\frac{\partial}{\partial x} \to -p_x^2 \to \hbar^2\frac{\partial^2}{\partial x^2} \tag{5.2}$$

$$\text{Likewise: } -p_y^2 \to \hbar^2\frac{\partial^2}{\partial y^2} \quad \text{and} \quad -p_z^2 \to \hbar^2\frac{\partial^2}{\partial z^2} \tag{5.3}$$

5.2 Substituting Operators into Einstein's Relation

Now we substitute the quantum operators into the relativistic mass shell equation. Remember, these operators will act on a wavefunction ψ:

$$(mc)^2 = \left(\frac{E}{c}\right)^2 - p_x^2 - p_y^2 - p_z^2$$
$$(mc)^2 = -\frac{\hbar^2}{c^2}\frac{\partial^2}{\partial t^2} + \hbar^2\frac{\partial^2}{\partial x^2} + \hbar^2\frac{\partial^2}{\partial y^2} + \hbar^2\frac{\partial^2}{\partial z^2}.$$

Dividing through by $\hbar^2$ and rearranging:

$$\frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial y^2} - \frac{\partial^2}{\partial z^2} + \left(\frac{mc}{\hbar}\right)^2 = 0 \tag{5.4}$$

5.3 The Klein-Gordon Equation!

We've done it! This is the **Klein-Gordon equation** — the first successful attempt at a relativistic quantum wave equation.

Operating on a wavefunction ψ:

$$\left[\frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial y^2} - \frac{\partial^2}{\partial z^2} + \left(\frac{mc}{\hbar}\right)^2\right]\psi = 0 \tag{5.5}$$

Key features:

- Second-order in both time and space (treats them equally — relativistic!)
- Reduces to Schrödinger equation in the non-relativistic limit
- Contains the mass m explicitly

5.4 Compact Notation: Laplacian

We can write the spatial derivatives more compactly using the Laplacian operator:

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \tag{5.6}$$

Note the sign: in our equation we have $-\nabla^2$ because of the minus signs in the original expression.

Substituting this into our equation:

$$\left[\frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \nabla^2 + \left(\frac{mc}{\hbar}\right)^2\right]\psi = 0 \tag{5.7}$$

This is cleaner and makes the equation look more symmetric.

5.5 Even More Compact: d'Alembertian Notation

We can make this even more compact by defining two convenient symbols:

The d'Alembertian operator (wave operator):

$$\Box = \frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \nabla^2 \tag{5.8}$$

This is the relativistic generalization of the Laplacian. It's the natural wave operator in spacetime.

The mass parameter:

$$\mu = \frac{mc}{\hbar} \tag{5.9}$$

This has units of inverse length (like a wavenumber). It represents the "Compton wavenumber" of the particle.

Note:-

In natural units where $c = \hbar = 1$, we'd just write $\mu = m$. But we keep factors explicit for clarity.

With these definitions, the Klein-Gordon equation becomes beautifully simple:

$$\left[\Box + \mu^2\right]\psi = 0 \tag{5.10}$$

This compact form makes it easy to see: it's a wave equation (the $\Box$) with a mass term (μ^2).

Chapter 6

Four-momentum Eigenstates

Now that we have the Klein-Gordon equation, what are its solutions? The simplest solutions are plane waves — states with definite energy and momentum.

6.1 Klein-Gordon Plane Wave Solutions

Just like in non-relativistic quantum mechanics, we look for plane wave solutions. These represent particles with definite four-momentum.

Definition 6.1.1: Klein-Gordon Plane Wave function

The general form using four-vector notation:

$$\psi = A \exp\left(-\frac{i}{\hbar} p \cdot x\right) \tag{6.1}$$

where:

$$\begin{aligned} p &= \left[E/c, \vec{p}\right] && \text{(four-momentum)} \\ x &= \left[ct, \vec{x}\right] && \text{(four-position)} \\ A &\in \mathbb{C} && \text{(complex amplitude)} \\ p^0 = \frac{E}{c} &= \pm\sqrt{|\vec{p}|^2 + m^2c^2} && \text{(energy, with } \pm \text{ solutions!)} \end{aligned}$$

Expanding the four-vector dot product $p \cdot x = Et - \vec{p} \cdot \vec{x}$:

$$\psi = A \exp\left[\frac{i}{\hbar}\left(\vec{p} \cdot \vec{x} - Et\right)\right]$$

$$\psi = A \exp\left[\frac{i}{\hbar}\left(\vec{p} \cdot \vec{x} \pm c\sqrt{|\vec{p}|^2 + m^2c^2}t\right)\right]$$

This looks like $e^{i(\vec{k}\cdot\vec{x} - \omega t)}$ — a traveling wave!

6.2 Proof that plane waves satisfy Klein-Gordon

Let's verify that $\psi = A\exp[-ip\cdot x/\hbar]$ is indeed a solution.

Rewrite Klein-Gordon as:

$$\left[\Box + \mu^2\right]\psi = 0 \qquad \Longrightarrow \qquad \Box\psi = -\mu^2\psi \tag{6.2}$$

The question is: does the d'Alembertian acting on our plane wave give us $-\mu^2\psi$?

Apply the d'Alembertian to the plane wave:

$$\Box\left[\exp\left[\frac{i}{\hbar}\left(\vec{p}\cdot\vec{x} - Et\right)\right]\right] \tag{6.3}$$

Remember: $\Box = \frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \nabla^2$

Taking derivatives:

- Time derivative: $\frac{\partial}{\partial t}\exp[i(\vec{p}\cdot\vec{x} - Et)/\hbar] = -\frac{iE}{\hbar}\psi \Rightarrow \frac{\partial^2}{\partial t^2} = -\frac{E^2}{\hbar^2}\psi$
- Spatial derivatives: $\nabla^2\exp[i(\vec{p}\cdot\vec{x} - Et)/\hbar] = -\frac{|\vec{p}|^2}{\hbar^2}\psi$

Therefore:

$$\Box\psi = \left[-\frac{E^2}{c^2\hbar^2} + \frac{|\vec{p}|^2}{\hbar^2}\right]\psi = -\frac{1}{\hbar^2}\left[\frac{E^2}{c^2} - |\vec{p}|^2\right]\psi \tag{6.4}$$

Using the mass shell relation $E^2/c^2 - |\vec{p}|^2 = m^2c^2$:

$$\Box\psi = -\frac{m^2c^2}{\hbar^2}\psi = -\mu^2\psi \quad \checkmark \tag{6.5}$$

The plane wave satisfies Klein-Gordon! **And notice**: the mass shell relation is exactly what makes this work.

Chapter 7

Superposition

7.1 Linearity: Building Complex Solutions from Simple Ones

The Klein-Gordon equation is **linear** — this is a crucial property! It means if ψ_1 and ψ_2 are solutions, then any linear combination $c_1\psi_1 + c_2\psi_2$ is also a solution.

Why is this important? It lets us build arbitrarily complex wavefunctions from simple plane wave building blocks. This is how we describe localized particles, wave packets, and realistic physical situations.

Let's say that you have two functions that satisfy the Klein-Gordon Equation, call them ψ_1 and ψ_2

$$\left[\Box + \mu^2\right]\psi_1 = 0 \tag{7.1}$$

$$\left[\Box + \mu^2\right]\psi_2 = 0 \tag{7.2}$$

Let's call their sum ψ_3 so

$$\psi_3 = \psi_1 + \psi_2 \tag{7.3}$$

The question then arises: does ψ_3 satisfy the Klein-Gordon Equation?
Well, yes it does. We can show this with:

$$\begin{aligned}\left[\Box + \mu^2\right]\psi_3 &= \left[\Box + \mu^2\right](\psi_1 + \psi_3) \\ &= \left[\Box + \mu^2\right]\psi_1 + \left[\Box + \mu^2\right]\psi_2 = 0 + 0 = 0 \text{ ... also satisfies K.G..}\end{aligned}$$

The following reasoning does not just apply to the sum of two wave functions, but also scaling up a wave function or taking the arbitrary sum over many wave functions. Or even more usefully if you have a basis set of functions that satisfy the Klein-Gordon Equation, then you can make wave functions of that basis set by summing over them with some series of coefficients

Say we write a wavefunction ψ as a linear combination of $\{\psi_n\}$

$$\psi = \sum_n C_n\psi_n, \qquad C_n \in \mathbb{C} \tag{7.4}$$

Since each basis function in $\psi_n \in \{\psi_n\}$ satisfies K.G....

$$\left[\Box + \mu^2\right]\psi_n = 0 \rightarrow \left[\Box + \mu^2\right]\sum_n C_n\psi_n = 0 \tag{7.5}$$

And that's how we actually use energy and momentum in Eigen-states most of the time.

Chapter 8

Group Velocity and the Speed of Light Limit

8.1 What is Group Velocity?

A single plane wave $e^{i(kx-\omega t)}$ extends infinitely in space — not very physical! Real particles are localized wave packets made by superposing many plane waves with different k values.

For a wave packet:

- **Phase velocity:** $v_p = \omega/k$ — speed of individual wave crests
- **Group velocity:** $v_g = d\omega/dk$ — speed of the packet envelope (the actual particle!)

The group velocity is what we actually measure — it's the speed of information/energy transport. Let's calculate it for Klein-Gordon.

8.2 Step 1: Finding the Dispersion Relation

The **dispersion relation** $\omega(k)$ tells us how frequency depends on wavenumber. It encodes the physics of the wave.

General form of any plane wave:

$$\psi = A\exp\left(i\left(\vec{k}\cdot\vec{x}-\omega t\right)\right) \tag{8.1}$$

Our Klein-Gordon plane wave:

$$\psi = A\exp\left(\frac{i}{\hbar}\left(\vec{p}\cdot\vec{x}-Et\right)\right) \tag{8.2}$$

Comparing these, we identify:

$$\vec{k} = \frac{\vec{p}}{\hbar} \quad \text{(de Broglie relation)}$$
$$\omega = \frac{E}{\hbar} \qquad \text{(Planck relation)}$$

Using $E = c\sqrt{|\vec{p}|^2 + m^2c^2}$ and $|\vec{p}| = \hbar k$:

$$\omega(k) = \sqrt{(kc)^2 + \left(\frac{mc^2}{\hbar}\right)^2} \tag{8.3}$$

This is the dispersion relation! Notice:

- Massless ($m = 0$): $\omega = kc$ (linear — no dispersion)
- Massive ($m \neq 0$): $\omega \neq kc$ (nonlinear — dispersive!)

8.3 Step 2: Calculating the Group Velocity

Now we differentiate the dispersion relation to get the group velocity:

$$v_g = \frac{d\omega}{dk} \tag{8.4}$$

$$v_g = \frac{d}{dk}\left[\sqrt{(kc)^2 + (mc^2/\hbar)^2}\right] \tag{8.5}$$

Using the chain rule:

$$v_g = \frac{kc^2}{\sqrt{(kc)^2 + (mc^2/\hbar)^2}} = \frac{kc^2}{\omega} \tag{8.6}$$

Substituting $k = |\vec{p}|/\hbar$:

$$v_g = \frac{c|\vec{p}|}{\sqrt{|\vec{p}|^2 + (mc)^2}} \tag{8.7}$$

8.4 The Speed Limit: Why $v_g < c$

Look at what we just derived! The group velocity depends on momentum in a very special way.

For massive particles ($m \neq 0$):

- Low momentum ($|\vec{p}| \ll mc$): $v_g \approx |\vec{p}|/m$ (non-relativistic)
- High momentum ($|\vec{p}| \gg mc$): $v_g \approx c(|\vec{p}|/|\vec{p}|) = c$... but never quite reaches it!
- The denominator $\sqrt{|\vec{p}|^2 + (mc)^2}$ is always larger than $|\vec{p}|$, so $v_g < c$ always

For massless particles ($m = 0$):

$$v_g = \frac{c|\vec{p}|}{|\vec{p}|} = c \tag{8.8}$$

Massless particles always travel at exactly the speed of light, regardless of momentum!

The Klein-Gordon equation naturally enforces special relativity's speed limit. This is a beautiful consistency check — we started with relativistic energy-momentum, and we get relativistic velocities.

Chapter 9

Fourier Transforms and Antimatter

9.1 From Momentum Space to Position Space

We've been working with plane waves — states with definite momentum p. But real particles are localized in space! How do we describe them?

Answer: Fourier transform! We build a position-space wavefunction $\psi(x)$ by superposing plane waves with different momenta, weighted by a momentum-space wavefunction $\phi(p)$.

9.2 The Fourier Transform

$$\psi(x) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \phi(p) \exp\left[-\frac{i}{\hbar} p \cdot x\right] dp \tag{9.1}$$

- wavefunction in spacetime
- Normalization constant
- Add up eigenstate for each p, weighted $\phi(p)$
- Momentum-space wavefunction (complex numbers assigned to each momentum)
- p-eigenstate (plane wave with momentum p)

The key insight: $\phi(p)$ assigns a complex number (amplitude and phase) to each allowed momentum p. But what are the "allowed" values of p? They must satisfy the mass shell relation!

9.3 The Two Halves of the Mass Shell

There is a one-to-one connection between all possible wavefunctions that satisfy the Klein-Gordon equation in spacetime and all possible ways of decorating the mass shell with complex numbers.

The critical insight: You need *both halves* of the mass shell to have a complete basis set for Fourier transforms from momentum space to position space.

Recall from the plane wave solution that:

$$p^0 = \frac{E}{c} = \pm\sqrt{|\vec{p}|^2 + m^2c^2} \tag{9.2}$$

This ± sign gives us two branches:

- **Positive energy:** $E = +\sqrt{p^2c^2 + m^2c^4}$ (normal particles)
- **Negative energy:** $E = -\sqrt{p^2c^2 + m^2c^4}$ (antimatter!)

9.3.1 Reinterpreting Negative Energy: Feynman-Stueckelberg

Negative energy sounds strange. But there's a beautiful way to reinterpret this that doesn't require "negative energy" at all.

Recall the energy operator:

$$\hat{E} = i\hbar\frac{\partial}{\partial t} \tag{9.3}$$

Shift your perspective: Instead of thinking about negative energy, reinterpret what $-\hat{E}$ means:

$$-\hat{E} = -i\hbar\frac{\partial}{\partial t} \tag{9.4}$$

$$\text{Negative energy??} \quad \longrightarrow \quad \text{Time reversal!}$$

A *negative energy* particle moving *forward in time* is mathematically equivalent to a *positive energy* antiparticle moving *backward in time*.

This is the **Feynman-Stueckelberg interpretation**:

- Particles: positive energy, moving forward in time
- Antiparticles: positive energy, moving backward in time (which *looks like* negative energy forward in time)

When an electron and positron annihilate, you can picture the positron as an electron that reversed its direction in time!

The bottom line: The negative energy solutions represent *antimatter*. When you include both halves of the mass shell, you're accounting for both particles and antiparticles.

9.4 Dirac's Critique: The Fatal Flaws of Klein-Gordon

Dirac identified two deeply connected problems with the Klein-Gordon equation that made it unsuitable as a single-particle quantum theory.

9.4.1 Problem 1: Second-Order in Time

The Klein-Gordon equation is **second-order in time**.

Compare the time derivatives:

$$\text{Schrödinger:} \quad i\hbar\frac{\partial\psi}{\partial t} = \hat{H}\psi \quad \text{(first-order in time)}$$

$$\text{Klein-Gordon:} \quad \frac{1}{c^2}\frac{\partial^2\psi}{\partial t^2} - \nabla^2\psi + \left(\frac{mc}{\hbar}\right)^2\psi = 0 \quad \text{(second-order in time)}$$

Being second-order in time allows both positive and negative energy solutions and treats space and time on equal footing (manifestly relativistic). However, it creates a serious problem.

Too much freedom! Just like classical mechanics needs position AND velocity for second-order equations, Klein-Gordon requires *two* initial conditions:

- The wavefunction: $\psi(x, 0)$
- The time derivative: $\left.\frac{\partial\psi}{\partial t}\right|_{t=0}$

In quantum mechanics, the state should be completely determined by $\psi(x, 0)$ alone. Having $\partial\psi/\partial t$ as an independent initial condition violates this fundamental principle.

9.4.2 Problem 2: Negative Probability Density

This "too much freedom" problem directly causes the negative probability issue.

For Schrödinger, the probability density is simple:

$$\rho = |\psi|^2 = \psi^* \psi \geqslant 0 \quad \text{(always positive!)} \tag{9.5}$$

For Klein-Gordon, deriving the probability density from the continuity equation gives:

$$\rho = \frac{i\hbar}{2mc^2}\left(\psi^* \frac{\partial \psi}{\partial t} - \psi \frac{\partial \psi^*}{\partial t}\right) \tag{9.6}$$

This depends on both ψ and $\partial\psi/\partial t$! Since $\partial\psi/\partial t$ is an independent degree of freedom (Problem 1), we can choose it to make ρ negative. Negative probabilities are physically nonsensical.

The connection: The negative probability problem exists *because* the equation is second-order in time. These aren't separate issues — they're two sides of the same coin.

9.4.3 Dirac's Solution

Dirac wanted the impossible:

1. **First-order in time** (like Schrödinger) — needs only $\psi(x, 0)$, no extra freedom
2. **Relativistically correct** — treats energy and momentum on equal footing
3. **Positive definite probability** — $\rho \geqslant 0$ always

This seemingly impossible requirement led Dirac to discover the **Dirac equation**, which is first-order in *both* time and space. The price? The wavefunction becomes a multi-component spinor, and quantum mechanical spin emerges naturally!

However, even Dirac's equation still has negative energy solutions. The Feynman-Stueckelberg interpretation (discussed earlier) applies here too — those solutions represent antimatter. Klein-Gordon and Dirac equations aren't single-particle theories — they're fundamentally quantum field theory equations.

Chapter 10

Dirac Equation

10.1 Motivation and Strategy

Our goal is to find the analog of the Schrodinger equation of relativistic spin one-half particles, however, we should note that even in the Schrodinger equation, the interaction of the field with spin was rather ad hoc. There was no explanation of gyromagnetic ration of 2. One can incorporate spin into the non-relativistic equation by using the Schrodinger-Pauli Hamiltonian which contains the dot product of the Pauli matrices with the momentum operator.

$$H = \frac{1}{2m}\left(\vec{\sigma}\cdot\left[\vec{p}+\frac{e}{c}\vec{A}\left(\vec{r},t\right)\right]\right)^2 - e\phi\left(\vec{r},t\right) \tag{10.1}$$

A little computation shows that this gives the correct interaction with spin.

$$H = \frac{1}{2m}\left[\vec{p}+\frac{e}{c}\vec{A}\left(\vec{r},t\right)\right]^2 - e\psi\left(\vec{r},t\right) + \frac{e\hbar}{2mc}\vec{\sigma}\cdot\vec{B}\left(\vec{r},t\right) \tag{10.2}$$

This Hamiltonian acts on a two component spinor.

10.2 Deriving the Dirac Equation

We can extend this concept to use the relativistic energy equation. The idea is to replace $\vec{p}$ with $\vec{sigma}\cdot\vec{p}$

relativistic energy equation.

$$\left(\frac{E}{c}^2\right) - p^2 = (mc)^2$$

$$\left(\frac{E}{c} - \vec{\sigma}\cdot\vec{p}\right)\left(\frac{E}{c} + \vec{\sigma}\cdot\vec{p}\right) = (mc)^2$$

$$\left(i\hbar\frac{\partial}{\partial x_0} + i\hbar\vec{\sigma}\cdot\vec{\nabla}\right)\left(i\hbar\frac{\partial}{\partial x_0} - i\hbar\vec{\sigma}\cdot\vec{\nabla}\right)\phi = (mc)^2\,\phi.$$

Instead of an equation which is second order in time derivative, we can make a first order equation, like the Schrodinger equation, by extending this equation to four components.

$$\phi^{(L)} = \phi$$

$$\phi^{(R)} = \frac{1}{mc}\left(i\hbar\frac{\partial}{\partial x_0} - i\hbar\vec{\sigma}\cdot\vec{\nabla}\right)\phi^{(L)}.$$

Now rewriting in terms of $\psi A = \phi^{(R)} + \phi^{(L)}$ and $\psi B = \phi^{(R)} - \phi^{(L)}$ and ordering it as a matrix equation, we get an equation that can be written as a dot product between 4-vectors.

$$\begin{aligned}
\begin{pmatrix} -i\hbar\frac{\partial}{\partial x_0} & -i\hbar\vec{\sigma}\cdot\vec{\nabla} \\ i\hbar\vec{\sigma}\cdot\vec{\nabla} & i\hbar\frac{\partial}{\partial x_0} \end{pmatrix} &= \hbar\left[\begin{pmatrix} 0 & -i\vec{\sigma}\cdot\vec{\nabla} \\ i\vec{\sigma} & 0 \end{pmatrix} + \begin{pmatrix} \frac{\partial}{\partial x_4} & 0 \\ 0 & -\frac{\partial}{\partial x_4} \end{pmatrix}\right] \\
&= \hbar\left[\begin{pmatrix} 0 & -i\sigma_i \\ i\sigma_i & 0 \end{pmatrix}\frac{\partial}{\partial x_i} + \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\frac{\partial}{\partial x_4}\right] \\
&= \hbar\left[\gamma_\mu \frac{\partial}{\partial x_4}\right]
\end{aligned}$$

.

10.3 Gamma Matrices and Their Properties

Define the 4 by 4 matrices $\gamma\mu$ are by.

$$\begin{aligned}
\gamma_i &= \begin{pmatrix} + & i\sigma_i \\ i\sigma_i & 0 \end{pmatrix} \\
\gamma_4 &= \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.
\end{aligned}$$

With this definition, the relativistic equation can be simplified a great deal

$$\left(\gamma_\mu \frac{\partial}{\partial x_\mu} + \frac{mc}{\hbar}\right)\psi = 0 \tag{10.3}$$

where the gamma matrices are given by

$$\begin{aligned}
\gamma_1 &= \begin{pmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & -i & 0 \\ 0 & i & 0 & 0 \\ i & 0 & 0 & 0 \end{pmatrix} \\
\gamma_2 &= \begin{pmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix} \\
\gamma_3 &= \begin{pmatrix} 0 & 0 & -i & 0 \\ 0 & 0 & 0 & i \\ i & 0 & 0 & 0 \\ 0 & -i & 0 & 0 \end{pmatrix}.
\end{aligned}$$

and they satisfy anti-commutation relations.

$$\left\{\gamma_\mu, \gamma_v\right\} = 2\partial_{\mu v} \tag{10.4}$$

In fact any set of matrices satisfy the anti-commutation relations would yield equivalent physics results, however, we will work in the above explicit representation of the gamma matrices.

10.4 Conserved Current and Probability Density

defining $\overline{\psi} = \psi^\dagger \gamma_4$.

$$j_\mu = ic\overline{\psi}\gamma_\mu\psi \tag{10.5}$$

satisfies the equation of a conserved 4-vector current

$$\frac{\partial}{\partial x_\mu} j_\mu = 0 \tag{10.6}$$

and also transforms like a 4-vector. The fourth component of the vector shows that the probability density is $\psi^\dagger\psi$. This indicates that the normalization of the state includes all four components of the Dirac spinors

10.5 Non-Relativistic Limit

For non-relativistic electrons, the first two components of the Dirac spinor are large while the last two are small.

$$\psi = \begin{pmatrix} \psi_a \\ \psi_B \end{pmatrix}$$
$$\psi_B \approx \frac{c}{2mc^2}\vec{\sigma}\cdot\left(\vec{p} + \frac{e}{c}\vec{A}\right)\psi_A \approx \frac{pc}{2mc^2}\psi_A.$$

We use this fact to write an approximate two-component equation derived from the Dirac equation in the non-relativistic limit.

$$\left(\frac{p^2}{2m} - \frac{Ze^2}{4\pi r} - \frac{p^4}{8\pi m^2c^2r^3} + \frac{Ze^2\vec{L}\cdot\vec{S}}{8m^2c^2}\partial^3(\vec{r})\right)\psi = E\begin{pmatrix} N & R \end{pmatrix}\psi \tag{10.7}$$

This "Schrodinger equation", derived from the Dirac equation, agrees well with the one we used to understand the fine structure of Hydrogen. The first two terms are the kinetic and potential energy terms for the unperturbed Hydrogen Hamitonian. The third term is the relativistic correction to the kinetic energy. The fourth term is the correct spin-orbit interaction, including the Thomas Precession effect that we did not take time to understand when we did the NR fine structure. The fifth term is the so called Darwin term which we said would come from the Dirac equation; and now it has.

10.6 Plane Wave Solutions

For a free particle, each component of the Dirac spinor satisfies the Klein-Gordon equation.

$$\psi_{\vec{p}} = u_{\vec{p}} e^{i\left(\vec{p}\cdot\vec{x} - Et\right)/\hbar} \tag{10.8}$$

This is consistent with the relativistic energy relation.

The four normalized solutions for a Dirac particle at rest are.

$$\psi^{(1)} = \psi_E = +mc^2, +\hbar/2 \qquad = \qquad \frac{1}{\sqrt{V}}\begin{pmatrix}1\\0\\0\\0\end{pmatrix} e^{-imc^2 t/\hbar}$$

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.

The first and third have spin up while the second and fourth have spin down. The first and second are positive energy solutions while the third and fourth are "negative energy solutions", which we still need to understand.

10.6.1 Solutions with Definite Momentum

The next step is to find the solutions with definite momentum. The four plane wave solutions to the Dirac equation are:

$$\psi^{(r)}_{\vec{p}} = \sqrt{\frac{mc^2}{|E|\,V}}\, u^{(r)}_{\vec{p}}\, e^{i(\vec{p}\cdot\vec{x} - Et)/\hbar} \tag{10.9}$$

where the four spinors are given by:

$$u^{(1)}_{\vec{p}} = \sqrt{\tfrac{E+mc^2}{2mc^2}}\begin{pmatrix}1\\0\\\frac{p_z c}{E+mc^2}\\\frac{(p_x+ip_y)c}{E+mc^2}\end{pmatrix} \qquad u^{(2)}_{\vec{p}} = \sqrt{\tfrac{E+mc^2}{2mc^2}}\begin{pmatrix}0\\1\\\frac{(p_x-ip_y)c}{E+mc^2}\\\frac{-p_z c}{E+mc^2}\end{pmatrix}$$

$$u^{(3)}_{\vec{p}} = \sqrt{\tfrac{-E+mc^2}{2mc^2}}\begin{pmatrix}\frac{-p_z c}{-E+mc^2}\\\frac{-(p_x+ip_y)c}{-E+mc^2}\\1\\0\end{pmatrix} \qquad u^{(4)}_{\vec{p}} = \sqrt{\tfrac{-E+mc^2}{2mc^2}}\begin{pmatrix}\frac{-(p_x-ip_y)c}{-E+mc^2}\\\frac{p_z c}{-E+mc^2}\\0\\1\end{pmatrix} \tag{10.10}$$

E is positive for solutions 1 and 2 and negative for solutions 3 and 4. The spinors are orthogonal

$$u^{(r)\dagger}_{\vec{p}}\, u^{(r')}_{\vec{p}} = \frac{|E|}{mc^2}\partial_{rr'} \tag{10.11}$$

and the normalization constants have been set so that the states are properly normalized and the spinors follow

the convention given above, with the normalization proportional to energy.

The solutions are not in general eigenstates of any component of spin but are eigenstates of helicity, the component of spin along the direction of the momentum.

10.7 Reinterpreting Negative Energy Solutions

Note:-

with E negative, the exponential $e^{i(\vec{p}\cdot\vec{x}-Et)/\hbar}$ has the phase velocity, the group velocity and the probability flux all in the opposite direction of the momentum as we have defined it. This clearly doesn't make sense. Solutions 3 and 4 need to be understood in a way for which the non-relativistic operators have not prepared us. Let us simply relabel solutions 3 and 4 such that:

$$\vec{p} \to -\vec{p}$$
$$E \to -E.$$

so that all the energies are positive and the momenta point in the direction of the velocities. This mean we change the signs in solutions 3 and 4 as follows

$$\psi^{(1)}_{\vec{p}} = \sqrt{\frac{E+mc^2}{2EV}} \begin{pmatrix} 1 \\ 0 \\ \frac{p_z c}{E+mc^2} \\ \frac{(p_x+ip_y)c}{E+mc^2} \end{pmatrix} e^{i(\vec{p}\cdot\vec{x}-Et)/\hbar}$$

$$\psi^{(2}_{\vec{p}} = \sqrt{\frac{E+mc^2}{2EV}} \begin{pmatrix} 1 \\ 0 \\ \frac{(p_x-ip_y)c}{E+mc^2} \\ \frac{-p_z c}{E+mc^2} \end{pmatrix} e^{i(\vec{p}\cdot\vec{x}-Et)/\hbar}$$

$$\psi^{(3)} = \sqrt{\frac{E+mc^2}{2EV}} \begin{pmatrix} \frac{p_z c}{E+mc^2} \\ \frac{(p_x+ip_y)c}{E+mc^2} \\ 1 \\ 0 \end{pmatrix} e^{-i(\vec{p}\cdot\vec{x}-Et)/\hbar}$$

$$\psi^{(4)}_{\vec{p}} = \sqrt{\frac{|E|+mc^2}{2|E|V}} \begin{pmatrix} \frac{(p_x-ip_y)c}{E+mc^2} \\ \frac{-p_z c}{E+mc^2} \\ 0 \\ 1 \end{pmatrix} e^{-i(\vec{p}\cdot\vec{x}-Et)/\hbar}.$$

we have plane waves of the form

$$e^{\pm ip_\mu x_\mu/\hbar} \tag{10.12}$$

with the plus sign

With the plus sign or solutions 1 and 2 and the minus sign for solutions 3 and 4. These ± sign in the exponential is not very surprising from the point of view of possible solutions to a differential equation. The problem now is that for solutions 3 and for the momentum and energy operators must have a minus sign added to them and the phase of the wave function at a fixed position behaves in the opposite way as a function of time than what we expect and from solutions 1 and 2. It is as if solutions 3 and 4 are moving backward in time

if we change the charge of the electron from $-e$ to $+e$ and change the sign of the exponent, the Dirac equation remains invariant. Thus, we can turn the negative exponent solution (going backwards in time) into the

conventional positive exponent solution if we change the charge to $+e$. We can interpret solutions 3 and 4 as positrons. We will make this switch more carefully when we study the charge conjugation operator.

10.8 Lorentz Invariance

The Dirac equation should be the invariant under Lorentz boosts and under rotation, both of which are just changes in the definition of an inertial coordinate system. Under Lorentz boosts, $\frac{\partial}{\partial x_\mu}$ transforms like a 4-vector but the γ_μ matrices are constant. The Dirac equation is shown to be invariant under boosts along the x_i direction if we transform the Dirac spinor according yo:

$$\psi' = S_{boost}\psi$$
$$S_{boost} = \cosh\frac{\chi}{2} + i_{\gamma_i\gamma_4}\sinh\frac{\chi}{2}.$$

with $\tanh_\chi = \beta$

the Dirac equation is invariant under rotations about the k axis if we transform the Dirac equation spinor according to

$$\psi' = S_{rot}\psi$$
$$S_{rot} = \cos\frac{\theta}{2} + \gamma_i\gamma_j\sin\frac{\theta}{2}.$$

with ijk is a cyclic permutation.

10.9 Parity and Discrete Symmetries

Another symmetry related to the choice of coordinates system s parity. Under a parity inversion equation the Dirac equation remains invariant if

$$\psi' = S_P\psi = \gamma_4\psi \tag{10.13}$$

since $\gamma_4 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$, the third and fourth components of the spinor change sign while the first two don't. Since we could have chosen $-\gamma_4$, all we know is that components 3 and 4 have the opposite parity of components 1 and 2. From 4 by 4 matrices, we may derive 16 independent components of covariant objects. We define the product of all gamma matrices.

$$\gamma_5 = \gamma_1\gamma_2\gamma_3\gamma_4 \tag{10.14}$$

which obviously anticommutes with all the gamma matrices.

$$\{\gamma_\mu, \gamma_5\} = 0 \tag{10.15}$$

For rotations and boosts, γ_5 commutes with S since it commutes with the pair of gamma matrices. For a parity inversion, it anticommutes with $S_P = \gamma_4$. The simplest set of covariants we can make from Dirac spinors and γ matrices are tabulated below.

Classification	Covariant Form	no. of Components
Scalar	$\overline{\psi}\psi$	1
Pseudoscalar	$\overline{\psi}\gamma_5\psi$	1
Vector	$\overline{\psi}\gamma_\mu\psi$	4
Axial Vector	$\overline{\psi}\gamma_5\gamma_\mu\psi$	4
Rank 2 antisymmetric tensor	$\overline{\psi}\sigma_{\mu v}\psi$	6
Total		16

(10.16)

Products of more γ matrices turn out to repeat the same quantities because the square of any γ matrix is 1.

10.10 Hamiltonian Formulation

For many purposes, it is useful to write the Dirac equation in the traditional form $H\psi = E\psi$. To do this, we must separate the space and time derivatives, making the equation less covariant looking.

$$\left(\gamma_\mu \frac{\partial}{\partial x_\mu} + \frac{mc}{\hbar}\right)\psi = 0$$

$$\left(ic\gamma_4\gamma_j p_j + mc^2\gamma_4\right)\psi = -\hbar\frac{\partial}{\partial t}\psi.$$

Thus we can identify the operator below as the Hamiltonian.

$$H = ic\gamma_4\gamma_j p_j + mc^2\gamma_4 \tag{10.17}$$

The Hamiltonian helps us identify constants of the motion. If an operator commutes with H, it represents a conversed quantity.

10.10.1 Conservation Laws

It's easy to see the p_k commutes with the Hamiltonian for a free particle so that momentum will be conserved. The components of orbital angular momentum do not commute with H

$$[H, L_z] = ic\gamma_4\left[\gamma_j p_j, xp_y - yp_x\right] = \hbar c\gamma_4\left(\gamma_1 p_y - \gamma_2 p_x\right) \tag{10.18}$$

The components of spin also do not commute with H.

$$[H, S_z] = \hbar c\gamma_4\left[\gamma_2 p_x - \gamma_1 p_y\right] \tag{10.19}$$

But, from the above, the components of total angular momentum do commute with H.

$$[H, J_z] = [H, L_z] + [H, S_z] = \hbar c\gamma_4\left(\gamma_1 p_y - \gamma_2 p_x\right) + \hbar c\gamma_4\left[\gamma_2 p_x - \gamma_1 p_y\right] = 0 \tag{10.20}$$

The Dirac equation naturally conserves total angular momentum but not the orbital spin parts of it. We can also see that helicity, or spin along the direction of motion does commute.

$$\left[H, \vec{S}\cdot\vec{p}\right] = \left[H, \vec{S}\right]]\cdot\vec{p} = 0 \tag{10.21}$$

10.10.2 Electromagnetic Interactions

For any calculation, we need to know the interaction term with the Electromagnetic field. Based on the interaction of field with a current

$$H_{int} = \frac{1}{c} j_\mu A_\mu \tag{10.22}$$

and the current we have found for the Dirac equation, the interaction Hamiltonian is.

$$H_{int} = ie\gamma_4\gamma_k A_k \tag{10.23}$$

This is simpler than the non-relativistic case, with no A^2 term and only one power of e.

10.11 Zitterbewegung

The Dirac equation has some unexpected phenomena we can derive. Velocity eigenvalues for electrons are always $\pm c$ along any direction. Thus the only values of velocity that we could measure are $\pm c$

Localized states, expanded in place waves, contain all four components of the plane wave solutions. Mixing components 1 and 2 with components 3 and 4 gives rise to Zitterbewegung, the very rapid oscillation of an electrons velocity and position.

$$\langle v_k \rangle = \sum_{\vec{p}} \sum_{r=1}^{4} \left| c_{\vec{p},r} \right|^2 \frac{p_k c^2}{E} + \sum_{\vec{p}} \sum_{r=1}^{2} \sum_{r'=3}^{4} \frac{mc^3}{|E|} \left[c^*_{\vec{p},r'} c_{\vec{p},r} u^{(r')^\dagger}_{\vec{p}} i\gamma_4 \gamma_k u^{(r)}_{\vec{p}} r^{-2i|E|t/\hbar} c_{\vec{p},r'} c^*_{\vec{p},r} u^{(r)^\dagger}_{\vec{p}} i\gamma_4 \gamma_k u^{(r')}_{\vec{p}} e^{-2i|E|t/\hbar} \right] \tag{10.24}$$

The last sum which contains the cross terms between negative and positive energy represents extremely high frequency oscillations in the expected value of the velocity, known as Zitterbewegung. The expected value of the position has similar rapid oscillations.

10.12 Hydrogen Atom Solution

It is possible to solve the Dirac equation exactly for Hydrogen in a way very similar to the non-relativistic solution. One difference is that it is clear from the beginning that the total angular momentum is a constant of the motion and is used as a basic quantum number. There is another conserved quantum number related to the component of spin along the direction of $\vec{J}$. With these quantum numbers, the radial equation can be solved in a similar way as for the non-relativistic case yielding the energy relation

$$E = \frac{mc^2}{\sqrt{1 + \frac{Z^2\alpha^2}{\left(n_r + \sqrt{\left(j+\frac{1}{2}\right)^2 - Z^2\alpha^2}\right)}}} \tag{10.25}$$

We can identify the standard principle quantum number in this case as $n = n_r + j + \frac{1}{2}$. This result gives the same answer as out non-relativistic calculation to order α^4 but is also correct to higher order. It is an exact solution to the quantum mechanics problem posed but does not include the effects of field theory, such as the Lamb shift and the anomalous magnetic moment of the electron.

10.13 Thomson Scattering and the Role of Positron States

A calculation of Thomson scattering shows that even simple low energy photon relies on the "negative energy" or positron states to get a non-zero answer. If the calculation is done with the two diagrams in which a photon is absorbed then emitted by an electron (and vice-versa) the result is zero at low energy because the interaction Hamiltonian connects the first and second plane wave states with the third and fourth at zero momentum. This is in contradiction to the classical and non-relativistic calculations as well as measurement. There are additional diagrams if we consider the possibility that the photon can create and electron positron pair which annihilates with the initial electron emitting a photon (or with the initial and final photons swapped). These two terms give the right answer. The calculation of Thomson scattering makes it clear that we cannot ignore the new "negative energy" or positron states.

10.14 Charge Conjugation

The Dirac equation is invariant under charge conjugation, defined as changing electron states into the opposite charged positron states with the same momentum and spin (and changing the sign of external fields). To do this the Dirac spinor is transformed according to.

$$\psi' = \gamma_2 \psi^* \tag{10.26}$$

Of course a second charge conjugation operation takes the state back to the original ψ. Applying this to the place wave function gives

$$\begin{aligned}
\psi^{(1)}_{\vec{p}} &= \sqrt{\frac{mc^2}{|E|\,V}}\, u^{(1)}_{\vec{p}}\, e^{i\left(\vec{p}\cdot\vec{x}-Et\right)/\hbar} \rightarrow -\sqrt{\frac{mc^2}{|E|\,V}}\, u^{(4)}_{\vec{p}}\, e^{i\left(-\vec{p}\cdot\vec{x}+Et\right)/\hbar} \equiv \sqrt{\frac{mc^2}{|E|\,V}}\, v^{(1)}_{\vec{p}}\, e^{i\left(-\vec{p}\cdot\vec{x}+Et\right)/\hbar} \\
\psi^{(2)}_{\vec{p}} &= \sqrt{\frac{mc^2}{|E|\,V}}\, u^{(2)}_{\vec{p}}\, e^{i\left(\vec{p}\cdot\vec{x}-Et\right)/\hbar} \rightarrow \sqrt{\frac{mc^2}{|E|\,V}}\, u^{(3)}_{-\vec{p}}\, e^{i\left(-\vec{p}\cdot\vec{x}+Et\right)/\hbar} \equiv \sqrt{\frac{mc^2}{|E|\,V}}\, u^{(2)}_{\vec{p}}\, e^{i\left(-\vec{p}\cdot\vec{x}+Et\right)/\hbar} \\
\psi^{(3)}_{\vec{p}} &= \sqrt{\frac{mc^2}{|E|\,V}}\, u^{(3)}_{\vec{p}}\, e^{i\left(\vec{p}\cdot\vec{x}+|E|t\right)/\hbar} \rightarrow \sqrt{\frac{mc^2}{|E|\,V}}\, u^{(2)}_{-\vec{p}}\, e^{i\left(-\vec{p}\cdot\vec{x}-|E|t\right)/\hbar} \\
\psi^{(4)}_{\vec{p}} &= \sqrt{\frac{mc^2}{|E|\,V}}\, u^{(4)}_{\vec{p}}\, e^{i\left(\vec{p}\cdot\vec{x}+|E|t\right)/\hbar} \rightarrow -\sqrt{\frac{mc^2}{|E|\,V}}\, u^{(1)}_{-\vec{p}}\, e^{i\left(-\vec{p}\cdot\vec{x}-|E|t\right)/\hbar}.
\end{aligned}$$

The charge conjugate of an electron state is the "negative energe" electron tate, the absence of which would produce a positron of the same energy, momentum, spin and velocity as the electron. That is, the conjugate is the hole needed to make a positron with the same properties as the electron except that it has the opposite charge.

Let us take one more look at a plane wave solution to the Dirac equation, for example $\psi^{(1)}_{\vec{p}}$ and its charge conjugate, from the point of view that a positron is an electron moving backwards in time. Discard the idea of the "negative energy" sea. Assume that we have found a new solution to the field equations that moves backwards in time rather than forward.

$$\psi^{(1)}_{\vec{p}} = \sqrt{\frac{mc^2}{|E|\,V}}\, u^{(1)}_{\vec{p}}\, e^{i\left(\vec{p}\cdot\vec{x}-Et\right)/\hbar} \rightarrow -\sqrt{\frac{mc^2}{|E|\,V}}\, u^{(4)}_{-\vec{p}}\, e^{i\left(-\vec{p}\cdot\vec{x}+Et\right)/\hbar} \equiv \sqrt{\frac{mc^2}{|E|\,V}}\, v^{(1)}_{\vec{p}}\, e^{i\left(-\vec{p}\cdot\vec{x}+Et\right)/\hbar} \tag{10.27}$$

The charge conjugate of the electron solution is an electron with the same charge $-\mathbf{e}$, opposite momentum $-\mathbf{p}$, and spin opposite to the original state. It satisfies the equation with the signs of the EM fields reversed and, because the sign of the **Et** term in the exponential is reversed, it behaves as a positive energy solution moving backward in time, with the right momentum and spin.

Our opinion of the "negative energy" solutions has been biased by living in a world of matter. We know about matter waves oscillating as $e^{i\left(\vec{p}\cdot\vec{x}-Et\right)/\hbar}$. There is a symmetric set of solutions for the same particles moving "backwards in time" oscillating as $e^{i\left(-\vec{p}\cdot\vec{x}+Et\right)/\hbar}$. These solutions behave like antiparticles moving forward in time. Consider the following diagram (which contributes to Thomson scattering) from two points of view. Fron one point of view, an electron starts out at t_1, lets say in the state $\psi^{(1)}_{\vec{p}}$. At time t_3, the electron interacts with the field and make s a transition to the state $\psi^{(4)}_{\vec{p''}}$ which travels backwards in time to t_2 where it again interacts and makes a transition to $\psi^{(1)}_{\vec{p'}}$. From the other point of view, the electron starts out at t_1, then, at time t_2, the field causes the creation of an electron positron pair both of which propagate forwards n time. At time t_3, the positron and initial annihilate interacting with the field. The electron produced at t_2 propagates on into the future.

10.15 Quantization of the Dirac Field

The classical free field Lagrangian density for the Dirac electron field is

$$\mathcal{L} = -c\hbar\overline{\psi}\gamma_\mu\frac{\partial}{\partial x_\mu}\psi - mc^2\overline{\psi}\psi \tag{10.28}$$

The independent fields are considered to be the 4 components of ψ and the four components of $\overline{\psi}$. This Lagrange density is a Lorents scalar that depends only on the fields. The Euler-Lagrange equation using the $\overline{\psi}$ independent fields is simple since there is no derivative of $\overline{\psi}$ in the Lagrangian.

$$\begin{aligned}
\frac{\partial}{\partial x_\mu}\left(\frac{\partial\mathcal{L}}{\partial(\partial\overline{\psi}/\partial x_\mu)}\right) - \frac{\partial\mathcal{L}}{\partial\overline{\psi}} &= 0 \\
\frac{\partial\mathcal{L}}{\partial\overline{\psi}} &= 0 \\
-c\hbar\gamma_\mu\frac{\partial}{\partial x_\mu}\psi - mc^2\psi &= 0 \\
\left(\gamma_\mu\frac{\partial}{\partial x_\mu} + \frac{mc}{\hbar}\right) &= 0
\end{aligned}$$

This gives us the Dirac equation indicating that this Lagrangian is the right one. The Euler-Lagrange equation derived using the fields ψ is the Dirac adjoint equation,

$$\begin{aligned}
\frac{\partial}{\partial x_\mu}\left(\frac{\partial\mathcal{L}}{\partial\left(\partial\psi/\partial x_\mu\right)}\right) - \frac{\partial\mathcal{L}}{\partial\psi} &= 0 \\
\frac{\partial}{\partial x_\mu}\left(-c\hbar\overline{\psi}\gamma_\mu\right) + mc^2\overline{\psi} &= 0 \\
-\frac{\partial}{\partial x_\mu}\overline{\psi}\gamma_\mu + \frac{mc}{\hbar}\overline{\psi} &= 0.
\end{aligned}$$

again indicating that this is the correct Lagrangian if the Dirac equation is assumed to be correct.

To compute the Hamiltonian density, we start by finding the momenta conjugate to the fields ψ.

$$\Pi = \frac{\partial\mathcal{L}}{\partial\left(\frac{\partial\psi}{\partial t}\right)} = -c\hbar\overline{\psi}\gamma_4\frac{1}{ic} = i\hbar\psi^\dagger\gamma_4\gamma_4 = i\hbar\psi^\dagger \tag{10.29}$$

There is no time derivation of $\overline{\psi}$ so those momenta are zero. The Hamiltonian can then be computed.

$$\begin{aligned}
\mathcal{H} &= \frac{\partial \psi}{\partial t}\Pi - \mathcal{L} \\
&= i\hbar\psi^\dagger \frac{\partial \psi}{\partial t} + c\hbar\overline{\psi}\gamma_\mu \frac{\partial}{\partial x_\mu} + mc^2\overline{\psi}\psi \\
&= -c\hbar\psi^\dagger \frac{\partial \psi}{\partial x_4} + c\hbar\psi^\dagger\gamma_4\gamma_4 \frac{\partial \psi}{\partial x_4} + c\hbar\overline{\psi}\gamma_k \frac{\partial}{\partial x_k} + mc^2\overline{\psi}\psi \\
&= \hbar c\psi^\dagger\gamma_4\gamma_k \frac{\partial}{\partial x_k}\psi + mc^2\psi^\dagger\gamma_4\psi \\
&= \psi^\dagger\left(\hbar c\gamma_4\gamma_k \frac{\partial}{\partial x_k}\psi + mc^2\gamma_4\right)\psi \\
\mathbf{H} &= \int \psi^\dagger\left(\hbar c\gamma_4\gamma_k \frac{\partial}{\partial x_k} + mc^2\gamma_4\right)\psi\, \mathbf{d^3x}.
\end{aligned}$$

We may expand the field ψ in the complete set of plane waves either using the four spinors $u_{\vec{p}}^{(r)}$ for $\mathbf{r = 1, 2, 3, 4}$ or using the electron and positron spinors $u_{\vec{p}}^{(4)}$ and $u_{\vec{p}}^{(r)}$ for $\mathbf{r = 1, 2}$. For economy of notation, we chose the former with a plan to change to the later once the quantization is completed.

$$\psi\left(\vec{x}, t\right) = \sum_{\vec{p}}\sum_{r=1}^{4}\sqrt{\frac{mc^2}{|E|\,V}}c_{\vec{p},r}u_{\vec{p}}^{(r)}e^{i\left(\vec{p}\cdot\vec{x}-Et\right)/\hbar} \tag{10.30}$$

The conjugate can also be written out.

$$\psi^\dagger\left(\vec{x}, t\right) = \sum_{\vec{p}}\sum_{r=1}^{4}\sqrt{\frac{mc^2}{|E|\,V}}c_{\vec{p},r}u_{\vec{p}}^{(r)}e^{i\left(\vec{p}\cdot\vec{x}-Et\right)/\hbar} \tag{10.31}$$

Writing the Hamiltonian in terms of these fields, the formula can be simplified ad follows

$$\mathbf{H} = \int \psi^\dagger \left(\hbar c \gamma_4 \gamma_k \frac{\partial}{\partial x_k} + mc^2 \gamma_4 \right) \psi \mathbf{d^3 x}$$

$$\mathbf{H} = \int \sum_{\vec{p}} \sum_{r=1}^{4} \sum_{\vec{p}} \sum_{r'=1}^{4} \sqrt{\frac{mc^2}{|E'|\,V}} c^*_{\vec{p}',r'} u^{(r')\dagger}_{\vec{p}'} e^{-i\left(\vec{p}\cdot\vec{x}-Et\right)/\hbar} \left(\hbar c \gamma_4 \gamma_k \frac{\partial}{\partial x_\mu} + mc^2 \gamma_4 \right) \sqrt{\frac{mc^2}{|E|\,V}} c_{\vec{p},r} u^{(r)}_{\vec{p}} e^{i\left(\vec{p}\cdot\vec{x}-Et\right)/\hbar}$$

$$\mathbf{H} = \int \sum_{\vec{p}} \sum_{r=1}^{4} \sum_{\vec{p}} \sum_{r'=1}^{4} \sqrt{\frac{mc^2}{|E'|\,V}} c^*_{\vec{p}',r'} u^{(r')\dagger}_{\vec{p}'} e^{-i\left(\vec{p}\cdot\vec{x}-Et\right)/\hbar} \left(\hbar c \gamma_4 \gamma_k \frac{ip_k}{\hbar} + mc^2 \gamma_4 \right) \sqrt{\frac{mc^2}{|E|\,V}} c_{\vec{p},r} u^{(r)}_{\vec{p}} e^{i\left(\vec{p}\cdot\vec{x}-Et\right)/\hbar} \mathbf{d}$$

$$\mathbf{H} = \int \sum_{\vec{p}} \sum_{r=1}^{4} \sum_{\vec{p}} \sum_{r'=1}^{4} \sqrt{\frac{mc^2}{|E'|\,V}} c^*_{\vec{p}',r'} u^{(r')\dagger}_{\vec{p}'} e^{-i\left(\vec{p}\cdot\vec{x}-Et\right)/\hbar} \left(ic \gamma_4 \gamma_k p_k + mc^2 \gamma_4 \right) \sqrt{\frac{mc^2}{|E|\,V}} c_{\vec{p},r} u^{(r)}_{\vec{p}} e^{i\left(\vec{p}\cdot\vec{x}-Et\right)/\hbar} \mathbf{d^3 x}$$

$\left(ic \gamma_4 \gamma_k p_k + mc^2 \gamma_4 \right) \psi = E\psi$

$$\mathbf{H} = \int \sum_{\vec{p}} \sum_{r=1}^{4} \sum_{\vec{p}'} \sum_{r'=1}^{4} \sqrt{\frac{mc^2}{|E'|\,V}} c^*_{\vec{p}',r'} u^{(r')^\dagger}_{\vec{p}'} e^{-i\left(\vec{p}\cdot\vec{x}-Et\right)/\hbar} (E) \sqrt{\frac{mc^2}{|E|\,V}} c_{\vec{p},r} u^{(r)}_{\vec{p}} e^{i\left(\vec{p}\cdot\vec{x}-Et\right)/\hbar} \mathbf{d^3 x}$$

$$\mathbf{H} = \sum_{\vec{p}} \sum_{r=1}^{4} \sum_{\vec{p}'} \sum_{r'=1}^{4} \sqrt{\frac{mc^2}{|E'|}} c^*_{\vec{p},r'} u^{(r')^\dagger}_{\vec{p}} (E) \sqrt{\frac{mc^2}{|E|}} c_{\vec{p},r} u^{(r)}_{\vec{p}} \delta_{\vec{p}\vec{p}'}$$

$$\mathbf{H} = \sum_{\vec{p}} \sum_{r=1}^{4} \sum_{r'=1}^{4} \frac{mc^2}{|E|} c^*_{\vec{p},r'} c_{\vec{p},r} u^{(r')^\dagger}_{\vec{p}} (E)\, u^{(r)}_{\vec{p}}$$

$u^{(r)^\dagger}_{\vec{p}} u^{(r')}_{\vec{p}} = \frac{|E|}{mc^2} \delta_{rr'}$

$$\mathbf{H} = \sum_{\vec{p}} \sum_{r=1}^{4} \sum_{r'=1}^{4} \frac{mc^2 E}{|E|} c^*_{\vec{p},r'} c_{\vec{p}r} \frac{|E|}{mc^2} \delta_{rr'}$$

$$\mathbf{H} = \sum_{\vec{p}} \sum_{r=1}^{4} E c^*_{\vec{p},r} c_{\vec{p},r}.$$

where the previous results from the Hamiltonian form of the Dirac equation and the normalization of the Dirac spinors have been used to simplify the formula greatly. Compare this Hamiltonian to the one used to quantize the Electromagnetic field

$$\mathbf{H} = \sum_{k,\alpha} \left(\frac{\omega}{c} \right)^2 \left[c_{k,\alpha} c^*_{k,\alpha} + c^*_{k,\alpha} c_{k,\alpha} \right] \tag{10.32}$$

for which the Fourier coefficients were replaced by operators as follows.

$$c_{k,\alpha} = \sqrt{\frac{\hbar c^2}{2\omega}} a_{k,\alpha}$$

$$c^*_{k,\alpha} = \sqrt{\frac{\hbar c^2}{2\omega}} a^\dagger_{k,\alpha}.$$

The Hamiltonian written in the terms of the creation and annihilation operators is.

$$\mathbf{H} = \frac{1}{2} \sum_{k,\alpha} \hbar\omega \left[a_{k,\alpha} a^\dagger_{k,\alpha} + a^\dagger_{k,\alpha} a_{k,\alpha} \right] \tag{10.33}$$

By analogy, we can skip the steps of making coordinates and momenta for the individual oscillators, and just replace the Fourier coefficients for the Dirac plane waves by operators.

$$\mathbf{H} = \sum_{\vec{p}} \sum_{r=1}^{4} E b_{\vec{p}}^{(r)^\dagger} b_{\vec{p}}^{(r)}$$

$$\psi\left(\vec{x}, t\right) = \sum_{\vec{p}} \sum_{r=1}^{4} \sqrt{\frac{mc^2}{|E|\, V}} b_{\vec{p}}^{(r)} u_{\vec{p}}^{(r)} e^{i\left(\vec{p}\cdot\vec{x} - Et\right)/\hbar}$$

$$\psi^\dagger\left(\vec{x}, t\right) = \sum_{\vec{p}} \sum_{r=1}^{4} \sqrt{\frac{mc^2}{|E|\, V}} b_{\vec{p}}^{(r)^\dagger} u_{\vec{p}}^{(r)\dagger} e^{i\left(\vec{p}\cdot\vec{x} - Et\right)/\hbar}.$$

(Since the Fermi-Dirac operators will anti-commute, the analogy is imperfect.)

The creation an annihilation operators $b_{\vec{p}}^{(r)^\dagger}$ and $b_{\vec{p}}^{(r)}$ satisfy anti-commutation relations.

$$\begin{aligned}
\left\{b_{\vec{p}}^{(r)}, b^{(r')^\dagger}\right\} &= \delta_{\vec{p}\vec{p}'} \\
\left\{b_{\vec{p}}^{(r)}, b_{\vec{p}}^{(r)}\right\} &= 0 \\
\left\{b_{\vec{p}}^{(r)\dagger}, b_{\vec{p}}^{(r)^\dagger}\right\} &= 0 \\
N_{\vec{p}}^{(r)} &= b_{\vec{p}}^{(r)^\dagger} b_{\vec{p}}^{(r)}.
\end{aligned}$$

$N_{\vec{p}}^{(r)}$ is the occupation number operator. The anti-commutation relations constrain the occupation number to be 1 or 0.

A state of the electrons in a system can be described by the occupation numbers (0 or 1 for each plane wave). The state can be generated by operation on the vacuum state with the appropriate set of creation operators.

10.16 The Quantized Dirac Field with Positron Spinors

The basis states in out quantized Dirac field can be changed eliminate the "negative energy" states and replace them with positron states. Recall that we can replace $-u_{-\vec{p}}^{(4)}$

positron spinor $v_{\vec{p}}^{(1)}$ and $u_{-\vec{p}}^{(3)}$ with $v_{\vec{p}}^{(2)}$ such that the new spinors are charge conjugates of th electron spinors

$$S_C u_{\vec{p}}^{(s)*} = v_{\vec{p}}^{(s)} \qquad s = 1, 2 \tag{10.34}$$

The positron spinor is actually just the same as the negative energy spinor when the momentum is reversed.

We name the creation and annihilation operators for the positron states to be $d_{\vec{p}}^{(s)^\dagger}$ and $d_{\vec{p}}^{(s)}$ and identify the to be.

$$\begin{aligned}
d_{\vec{p}}^{(1)} &= -b_{\vec{p}}^{(4)^\dagger} \\
d_{\vec{p}}^{(2)} &= b_{\vec{p}}^{(3)^\dagger}.
\end{aligned}$$

These anti-commute with everything else with the exception that

$$\left\{d_{\vec{p}}^{(s)}, d_{\vec{p'}}^{(s')^\dagger}\right\} = \delta_{ss'}, \delta_{\vec{p}\vec{p'}} \tag{10.35}$$

The Dirac field and Hamiltonian can now be rewritten.

$$\begin{aligned}
\psi\left(\vec{x}, t\right) &= \sum_{\vec{p}} \sum_{x=1}^{2} \sqrt{\frac{mc^2}{EV}} \left(b_{\vec{p}}^{(s)} u_{\vec{p}}^{(s)} e^{i\left(\vec{p}\cdot\vec{x}-Et\right)/\hbar} + d_{\vec{p}}^{(s)\dagger} v_{\vec{p}}^{(s)} e^{-i\left(\vec{p}\cdot\vec{x}-Et\right)/\hbar}\right) \\
\psi^\dagger\left(\vec{x}, \vec{t}\right) &= \sum_{\vec{p}} \sum_{s=1}^{2} \sqrt{\frac{mc^2}{EV}} \left(b_{\vec{p}}^{(s)\dagger} u_{\vec{p}}^{(s)\dagger} e^{-i\left(\vec{p}\cdot\vec{x}-Et\right)/\hbar} + d_{\vec{p}}^{(s)} e^{i\left(\vec{p}\cdot\vec{x}-Et\right)/\hbar}\right) \\
\mathbf{H} &= \sum_{\vec{p}} \sum_{s=1}^{2} E\left(b_{\vec{p}}^{(s)^\dagger} b_{\vec{p}}^{(s)} - d_{\vec{p}}^{(s)} d_{\vec{p}}^{(s)^\dagger}\right) \\
&= \sum_{\vec{p}} \sum_{s=1}^{2} \left(b_{\vec{p}}^{(s)^\dagger} b_{\vec{p}}^{(s)} + d_{\vec{p}}^{(s)^\dagger} d_{\vec{p}}^{(s)} - 1\right).
\end{aligned}$$

All the energies of these states are positive.
There is an (infinite) constant energy, similar but opposite sign to the one for the quantized EM field, which we must add to make the bacuum state have zero energy. Note that, had we used commuting operators (Bose-Einstein) instead of anti-commuting, there would have been no lowest energy ground state so this Energy subtraction would not have been possible. Fermi-Dirac statistics are required for particled satisfying the Dirac equation.

Since the operators creating fermion states anti-commute, fermion states must be antisymmetric under interchange. Assume $\mathbf{b}^\dagger{}_r$ and $\mathbf{b_r}$ re the creation and annihilation operators for fermions and that they anti-commute.

$$\left\{b_r^\dagger, b_{r'}^\dagger\right\} = 0 \tag{10.36}$$

The states are then antisymmetric under interchange of pairs of fermions.

$$b_r^\dagger b_{r'}^\dagger \left|0\right\rangle = -b_{r'}^\dagger b_r^\dagger \left|0\right\rangle \tag{10.37}$$

It's not hard to show that the occupation number for fermion states is either zero or one.
Note that the spinors satisfy the following equations.

$$\begin{aligned}
\left(i\gamma_\mu p_\mu\right) u_{\vec{p}}^{(s)} &= 0 \\
\left(-i\gamma_\mu p_\mu + mc\right) v_{\vec{p}}^{(s)} &= 0.
\end{aligned}$$

Since we changed the sign of the momentum in out definition of $v_{\vec{p}}^{(s)}$, the momentum term in the diract equation had to change sign

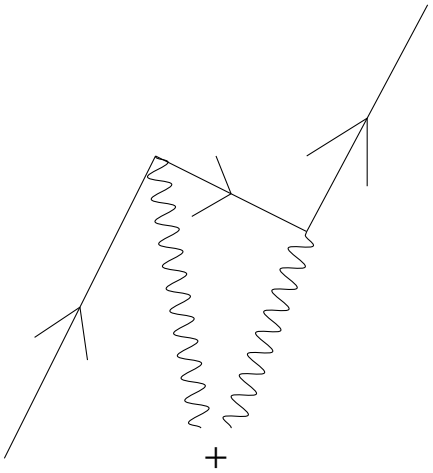
10.17 Vacuum Polarization

Vacuum polarization is an important effect in effectively reducing the charge on a particle. The reduction is depentent on distance and hence on the energy scale.

The term Vacuum Polarization is descriptive of the effect. A charged particle will polarize the vacuum in a way analagous to the way a dielectric is polarized. A virtual electron positron pair in the vacuum will be affected by the charge. If the original charged source is nucleus for example, the virtual electron will be attracted and the virtual positron repelled, causing a net polarization of the vacuum which screens the nuclear charge. At very short distances from the nucleus, the bare charge is seen, while at long distances the screening is important. This causes the basic coupling α to vary a bit with distance and therefore with energy. This polarization of the vacuum is similar to the polarization of a dielectric material. In this case, what is being polarized are the virtual electrons and positrons in the vacuum. Of course other particles than the electron can be polarized in the vacuum so the energy variation of the coupling "constant" is an interesting subject for research.

The effect of vacuum polarization on Hydrogen would be to lower the energy of **S** states relative to others since they are close to the nucleus and therefore see an unscreened charge. This effect is actually rather small even compared to the Lamb shift and of opposite sign. Vacuum Polarization has larger effects at higher energies at which shorter distances are probed. In fact we can say that the electromagnetic coupling varies slowly with the energy scale, increasing (logarithmically) at higher energies. This is reffered to as the running of the coupling constant.

We can get some qualitative understanding of the origin of Zitterbewegung from the idea of virtual pair production in the field of the nucleus. The diagram below shows a photon from the Coulomb field of the nucleus producing an electron positron pair. The original real electron from the atom then anihillates with the positron, coupling to another field photon. The electron from the pair is left over and becomes the new atomic electron, however, it need not be in the same place as the original electron.



We can estimate the distance an electron might jump as it undergoes the process. First the time for which the virtual pair exists can be estimated from the uncertainty principle. Energy conservation is violated by $2mc^2$ at least so $\Delta t = \dfrac{\hbar}{2mc^2}$ (which is approximately the reciprocal of the Zitterbewegung frequency). The distance the electron appears to jump then is of the order of $c\Delta t = \frac{\hbar c}{2mc^2} = 0.002$ angstroms. This is the approximate size of the fast back and forth motion of Zitterbewegung.

10.18 The QED LaGrangian and Gauge Invariance

The LaGrangian for electrons, photons, and the interaction between the two is the LaGrangian of Quantum ElectroDynamics.

$$\mathcal{L} = -\hbar c\overline{\psi}\left(\gamma_\mu \frac{\partial}{\partial x_\mu} + \frac{mc}{\hbar}\right)\psi - \frac{1}{4}F_{\mu v}F_{\mu v} - ie\overline{\psi}\gamma_\mu A_\mu \psi \tag{10.38}$$

QED is out first complete example on an interacting Quantum Field Theory. It taught us a great deal about the laws of physics.

The primary difference between Quantum Mechanics and Quantum Field Theory is that particled can be created

and destroyed. The probability to find an electron or a photon integrated over space does not have to be done. It can change with time. We have written the field of the photon and the electron in terms of creation and annihilation operators.

$$A_\mu = \frac{1}{\sqrt{V}} \sum_{k\alpha} \sqrt{\frac{\hbar c^2}{2\omega}} \epsilon_\mu^{(\alpha)} \left(a_{k,\alpha}(t)\, e^{i\vec{k}\cdot\vec{x}} + a_{k,\alpha}^\dagger(t)\, e^{-i\vec{k}\cdot\vec{x}} \right)$$

$$\psi(\vec{x},t) = \sum_{\vec{p}} \sum_{s=1}^{2} \sqrt{\frac{mc^2}{EV}} \left(b_{\vec{p}}^{(s)} u_{\vec{p}}^{(s)} e^{i(\vec{p}\cdot\vec{x}-Et)/\hbar} + d_{\vec{p}}^{(s)\dagger} v_{\vec{p}}^{(s)} e^{-i(\vec{p}\cdot\vec{x}-Et)/\hbar} \right)$$

$$\psi^\dagger(\vec{x},t) = \sum_{\vec{p}} \sum_{s=1}^{2} \sqrt{\frac{mc^2}{EV}} \left(b_{\vec{p}}^{(s)\dagger} u_{\vec{p}}^{(s)\dagger} e^{-i(\vec{p}\cdot\vec{x}-Et)/\hbar} + d_{\vec{p}}^{(s)} v_{\vec{p}}^{(s)\dagger} e^{i(\vec{p}\cdot\vec{x}-Et)/\hbar} \right).$$

Note that in the interaction term $-ie\overline{\psi}\gamma_\mu A_\mu \psi$ photons can be created or destroyed singly but that electrons must be created and destroyed along with a positron.
Phase (or Gauge) symmetry can be studied very simply from this LaGrangian. We have shown that the phase transformation

$$\psi \rightarrow e^{i\lambda(x)}\psi$$
$$A_\mu \rightarrow A_\mu - \frac{\hbar c}{e}\frac{\partial \lambda(x)}{\partial x_\mu}.$$

leaves the Schrodinger equation invariant. This can be most directly studied using the LaGrangian. We can deduve from the above transformation that

$$F_{\mu v} = \frac{\partial A_v}{\partial x_\mu} - \frac{\partial A_\mu}{\partial x_v} \rightarrow F_{\mu v} - \frac{\hbar c}{e}\left(\frac{\partial}{\partial x_\mu}\frac{\partial \lambda(x)}{\partial x_v} - \frac{\partial}{\partial x_v}\frac{\partial \lambda(x)}{\partial x_\mu} \right) = F_{\mu v} \tag{10.39}$$

The transformed LaGrangian then can be computed easily.

$$\mathcal{L} = -\hbar c\overline{\psi}\left(\gamma_\mu \frac{\partial}{\partial x_\mu} + \frac{mc}{\hbar} \right)\psi - \frac{1}{4}F_{\mu v}F_{\mu v} - ie\overline{\psi}\gamma_\mu A_\mu \psi \tag{10.40}$$

The exponentials from $\overline{\psi}$ and ψ cancel except for the term in which ψ is differentiated.

$$\mathcal{L} \rightarrow \mathcal{L} - i\hbar c\overline{\psi}\gamma_\mu \frac{\partial \lambda}{\partial x_\mu}\psi - ie\overline{\psi}\gamma_\mu \frac{-\hbar c}{e}\frac{\partial \lambda}{\partial x_\mu}\psi = \mathcal{L} \tag{10.41}$$

This all may seem fairly simple but imagine that we add a mass term for the EM field, $-m^2 A_\mu a_\mu$. The LaGrangian is no longer guage invariant. Guage invariance implies zero mass photons and even maintains the massless photon after radiative corrections. Guage invariance also implies the existance of a conserved current. Remember that the electric current in 4D also includes the charge density. Guage invariance implies conservation of charge, another important result.

This simple transformation $\psi \rightarrow e^{i\lambda(x)}$ is called a local U(1) symmetry where the U stands for unitary.

The Weak interactions are based on an SU(2) symmetry. This is just a local phase symmetry times arbitrary local rotation in SU(2) space. The SU(2) group is familiar to us since angular momentum is based on SU(2). In the weak interactions, there are two particles that are symmetric (much like a spin up and a spin down electron but NOT a spin up and spin down electron). We can rotate our states into different linear combinations of the symmetric particles and the LaGrangian remains invariant. Given this local SU(2) symmetry of the fermion wave functions, we can easily deduce what boson fields are required to make the LaGrangian guage invariant. It turns out we need a triplet of bosons. (The weak interactions then get messy because of the Higgs mechanism but the underlying guage theory is still correct.)

The strong interactions are based on the SU(3) group. Instead of having 3 sigma matrices to do rotations in the lowest dimention representation of the group, SU(3) has eight (8) lambda matrices. The SU(3) symmetry for the quark wavefunctions require an octet of massless vector boson called gluons to make the LaGrangian guage invariant.

So the standard Model is as simple as 1 2 3 in Quantum Field Theories.

10.19 Interaction with a Scalar Field

Yukawa couplings to a scalar field would be of the form $G\overline{\psi}\psi$ while couplings to a pseudoscalar field would be of the form $iG\overline{\psi}\gamma_5\psi$.