

Quantum Physics Building From scratch

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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 we 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.

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

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}_{\parallel} and A_0 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,

$$j_\mu = 0 \quad (1.2)$$

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

$$\frac{1}{c} \frac{\partial \Lambda}{\partial t} = A_0 \quad (1.3)$$

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

$$\vec{\nabla} \cdot \vec{A} = 0 \quad (1.4)$$

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 $t = 0$

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

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

$$k_i = \frac{2\pi n_i}{L} \quad (1.6)$$

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

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

and

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

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

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

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

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

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

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

so that

$$k_p x_p = k \cdot x = \vec{k} \cdot \vec{x} - \omega t \quad (1.12)$$

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

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

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

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

Note again that we have made this a transverse field by construction. The unit vectors $\hat{\epsilon}^{(\alpha)}$ are transverse to the direction of propagation. Also note that we are working in a gauge 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 written very simply.

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

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.

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

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

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

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

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.

$$\mathcal{H} = F_{\mu 4} \frac{\partial A_\mu}{\partial x_4} + \frac{1}{4} F_{\mu\nu} F_{\mu\nu} \quad (1.15)$$

$$\begin{aligned} \mathcal{H} &= \left(\frac{\partial A_4}{\partial x_\mu} - \frac{\partial A_4}{\partial x_4} \right) \frac{\partial A_\mu}{\partial x_4} + \frac{1}{4} \left(\frac{\partial A_\nu}{\partial x_\mu} - \frac{\partial A_\mu}{\partial x_\nu} \right) \left(\frac{\partial A_\nu}{\partial x_\mu} - \frac{\partial A_\mu}{\partial x_\nu} \right) \\ \mathcal{H} &= - \frac{\partial A_4}{\partial x_\mu} \frac{\partial A_\mu}{\partial x_4} + \frac{1}{2} \left(\frac{\partial A_\nu}{\partial x_4} \frac{\partial A_\nu}{\partial x_4} - \frac{\partial A_\nu}{\partial x_\nu} \frac{\partial A_\mu}{\partial x_\nu} \right). \end{aligned}$$

Now let's 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 our 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.

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

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

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 $\mathcal{L} = \frac{1}{2} (E^2 - B^2)$ 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

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

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.

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

We can then simplify our notation a bit

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

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

We wish to 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 real coordinates is $c + c^*$. With a little effort we can identify the coordinate

$$Q_{k,\alpha} = \frac{1}{c} (c_{k,\alpha} + c_{k,\alpha}^*) \quad (1.21)$$

and its conjugate momentum for each oscillator,

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

The Hamiltonian can be written in terms of these

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

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

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

This one checks out OK.

The other equation of Hamiltonian is

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

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 momentum. The next step is to quantize the oscillators.

1.5 Quantization of the Oscillators

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

$\mathbf{H} = \sum_{k,\alpha} \left(\frac{\omega}{c}\right)^2 \left[c_{k,\alpha} c_{k,\alpha}^* + c_{k,\alpha}^* c_{k,\alpha} \right]$	(1.23)
$Q_{k,\alpha} = \frac{1}{c} (c_{k,\alpha} + c_{k,\alpha}^*)$	
$P_{k,\alpha} = -\frac{i\omega}{c} (c_{k,\alpha} - c_{k,\alpha}^*)$	
$H = \frac{1}{2} \sum_{k,\alpha} [P_{k,\alpha}^2 + \omega^2 Q_{k,\alpha}^2]$	

Soon after the development of non-relativistic quantum mechanics, Dirac proposed that the canonical variables of the radiation oscillators be treated 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 $[p_x, x] = \frac{\hbar}{i}$. Coordinates and momenta that do not correspond, do not commute. For example $[p_y, x] = 0$. Different coordinates commute with each other as do different momenta. We will impose the same rules here.

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

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 $H = A^\dagger A \hbar\omega$. Following the same idea, we get

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

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

(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 $[a_{k,\alpha}, a_{k,\alpha}^\dagger] = 1$, as we had for the 1D harmonic oscillator.

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

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

$$[a_{k,\alpha}, a_{k',\alpha'}^\dagger] = \delta_{kk'} \delta_{\alpha\alpha'} \quad (1.25)$$

(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.

$$a_{k,\alpha} |n_{k,\alpha}\rangle = \sqrt{n_{k,\alpha}} |n_{k,\alpha} - 1\rangle$$

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

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

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

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

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

$$a_{k,\alpha} = \frac{1}{\sqrt{2\hbar\omega}} (\omega Q_{k,\alpha} + iP_{k,\alpha})$$

$$Q_{k,\alpha} = \frac{1}{c} (c_{k,\alpha} + c_{k,\alpha}^*)$$

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

$$= \frac{1}{\sqrt{2\hbar\omega}} \frac{\omega}{c} ((c_{k,\alpha} + c_{k,\alpha}^*) + (c_{k,\alpha} - c_{k,\alpha}^*))$$

$$= \frac{1}{\sqrt{2\hbar\omega}} \frac{\omega}{c} (c_{k,\alpha} + c_{k,\alpha}^* + c_{k,\alpha} - c_{k,\alpha}^*)$$

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

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

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

(1.26)

Similarly we can compute that

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

(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.

$$|n_{k_1,\alpha_1}, n_{k_2,\alpha_2}, \dots, n_{k_i,\alpha_i}, \dots\rangle = |n_{k_1,\alpha_1}\rangle |n_{k_2,\alpha_2}\rangle \dots |n_{k_i,\alpha_i}\rangle \dots \quad (1.28)$$

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

$$|n_{k_1,\alpha_1}, n_{k_2,\alpha_2}, \dots, n_{k_i,\alpha_i}, \dots\rangle = \prod_i \frac{(a_{k_i,\alpha_i}^\dagger)^{n_{k_i,\alpha_i}}}{\sqrt{n_{k_i,\alpha_i}!}} \quad (1.29)$$

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 $[a_{k,\alpha}^\dagger, a_{k',\alpha'}^\dagger] = 0$, interchanging the photons gives the same state.

$$a_{k,\alpha}^\dagger, a_{k',\alpha'}^\dagger |0\rangle = a_{k',\alpha'}^\dagger, a_{k,\alpha}^\dagger |0\rangle \quad (1.30)$$

So the fact that the creation operators commute dictates that photon states are symmetric under 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 matrices), then we can show that fermion states are antisymmetric under interchange. Assume b_r^\dagger and b_r are the creation and annihilation operators for fermions and that they anti-commute.

$$\boxed{\{b_r^\dagger, b_{r'}^\dagger\} = 0} \quad (1.31)$$

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

$$b_r^\dagger b_{r'}^\dagger |0\rangle = -b_{r'}^\dagger b_r^\dagger |0\rangle \quad (1.32)$$

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.

$$\begin{aligned}
c_{k,\alpha} &\rightarrow \sqrt{\frac{\hbar c^2}{2\omega}} a_{k,\alpha} \\
c_{k,\alpha}^* &\rightarrow \sqrt{\frac{\hbar c^2}{2\omega}} a_{k,\alpha}^\dagger \\
A_\mu &= \frac{1}{\sqrt{V}} \sum_{k,\alpha} \sqrt{\frac{\hbar c^2}{2\omega}} \epsilon_\mu^{(\alpha)} (a_{k,\alpha}(t) e^{i\vec{k}\cdot\vec{x}} + a_{k,\alpha}^\dagger(t) e^{-i\vec{k}\cdot\vec{x}}).
\end{aligned}$$

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.

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

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

(1.33)

For our purposes, we may remove the (infinite) constant energy due to the ground state energy 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 do not expect electricity and magnetism to be completely valid up to infinite energy. Certainly by the gravitational or grand unified energy 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.

$$\mathbf{H} = \sum_{k,\alpha} \hbar\omega N_{k,\alpha} \quad (1.34)$$

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

$$\mathbf{H}|0\rangle = 0 \quad (1.35)$$

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.

$$\vec{P} = \sum_{k,\alpha} \hbar \vec{k} N_{k,\alpha} \quad (1.36)$$

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

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

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 $a_{k,\alpha}^\dagger |0\rangle$

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

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

$$P a_{k,\alpha}^\dagger |0\rangle = \left(a_{k,\alpha}^\dagger P + [P, a_{k,\alpha}^\dagger] \right) |0\rangle = 0 + \hbar \vec{k} a_{k,\alpha}^\dagger |0\rangle = \hbar \vec{k} a_{k,\alpha}^\dagger |0\rangle \quad (1.39)$$

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

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

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.

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

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

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.

$$\frac{d}{dt} B(t) = \frac{i}{\hbar} [H, B(t)]$$

$$\dot{a}_{k,\alpha} = \frac{i}{\hbar} [H, a_{k,\alpha}(t)] = \frac{i}{\hbar} (-\hbar\omega) a_{k,\alpha}(t) = -i\omega a_{k,\alpha}(t)$$

$$\dot{a}_{k,\alpha}^\dagger = \frac{i}{\hbar} [H, a_{k,\alpha}^\dagger(t)] = i\omega a_{k,\alpha}^\dagger(t).$$

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

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

$$a_{k,\alpha}^\dagger(t) = a_{k,\alpha}^\dagger(0) e^{i\omega t}.$$

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

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

(1.40)

Again, the 4-vector x_p is a parameter of this field, not the location of a photon. The field operator is Hermitian 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

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

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 $\langle |\vec{E} \cdot \vec{E}| 0 \rangle$.

$$\begin{aligned}
\vec{E} &= -\frac{1}{c} \frac{\partial \vec{A}}{\partial t} \\
A_\mu &= \frac{1}{\sqrt{V}} \sum_{k,\alpha} \sqrt{\frac{\hbar c^2}{2\omega}} \epsilon_\mu^{(\alpha)} \left(a_{k,\alpha}(0) e^{ik_p x_p} 0 a_{k,\alpha}^\dagger(0) e^{-ik_p x_p} \right) \\
\vec{A} &= \frac{1}{\sqrt{V}} \sum_{k,\alpha} \sqrt{\frac{\hbar c^2}{2\omega}} \hat{\epsilon}^{(\alpha)} \left(a_{k,\alpha}(0) e^{ik_p x_p} + a_{k,\alpha}^\dagger(0) e^{-ik_p x_p} \right) \\
\vec{E} &= -i \frac{1}{c} \frac{1}{\sqrt{V}} \sum_{k,\alpha} \sqrt{\frac{\hbar c^2}{2\omega}} \hat{\epsilon}^{(\alpha)} (-\omega a_{k,\alpha}(0)) e^{ik_p x_p} + \omega a_{k,\alpha}^\dagger(0) e^{-ik_p x_p} \\
\vec{E} &= \frac{i}{\sqrt{V}} \sum_{k,\alpha} \sqrt{\frac{\hbar\omega}{2}} \hat{\epsilon}^{(\alpha)} \left(a_{k,\alpha}(0) e^{ik_p x_p} - a_{k,\alpha}^\dagger(0) e^{-ik_p x_p} \right) \\
\vec{E}|0\rangle &= \frac{i}{\sqrt{V}} \sum_{k,\alpha} \sqrt{\frac{\hbar\omega}{2}} \hat{\epsilon}^{(\alpha)} \left(-a_{k,\alpha}^\dagger e^{-ik_p x_p} \right) |0\rangle \\
\langle 0 | \vec{E} \cdot \vec{E} | 0 \rangle &= \frac{1}{v} \sum_{k,\alpha} \frac{\hbar\omega}{2} 1 \\
\langle 0 | \vec{E} \cdot \vec{E} | 0 \rangle &= \frac{1}{V} \sum_k \hbar\omega \rightarrow \infty.
\end{aligned}$$

(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 proportional 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.

$$\langle 0 | \vec{E} \cdot \vec{e} | 0 \rangle \approx \frac{\hbar c}{\Delta l^4} \quad (1.42)$$

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

$$[E_x(x) B_y(x')] = i c \hbar \delta \left(ds = \sqrt{(x-x')_p (x-x')_p} \right) \quad (1.43)$$

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 commutator 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 of 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 $\mathbf{H} = -\vec{\mu} \cdot \vec{B}$

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

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 proportional 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

$$|i\rangle = |\psi_i; \vec{n}_{k,\alpha}\rangle \quad (1.45)$$

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 annihilation operators (only). This will just come from the linear term in A .

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

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

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

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

Chapter 2

Deriving the KG Equation

2.1 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 2.1.1: 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 2.1.2: 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:

$$\left(\frac{E}{c}\right)^2 \rightarrow \left(\frac{\hat{E}}{c}\right)^2 = \left(\frac{i\hbar}{c} \frac{\partial}{\partial t}\right)^2 = -\frac{\hbar^2}{c^2} \frac{\partial^2}{\partial t^2} \quad (2.1)$$

Momentum terms:

$$\hat{p}_x = -i\hbar \frac{\partial}{\partial x} \rightarrow -p_x^2 \rightarrow \hbar^2 \frac{\partial^2}{\partial x^2} \quad (2.2)$$

$$\text{Likewise: } -p_y^2 \rightarrow \hbar^2 \frac{\partial^2}{\partial y^2} \quad \text{and} \quad -p_z^2 \rightarrow \hbar^2 \frac{\partial^2}{\partial z^2} \quad (2.3)$$

2.2 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:

$$\frac{1}{c^2} \frac{\partial^2}{\partial t^2} - \frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial y^2} - \frac{\partial^2}{\partial z^2} + \left(\frac{mc}{\hbar}\right)^2 = 0 \quad (2.4)$$

2.3 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 :

$$\left[\frac{1}{c^2} \frac{\partial^2}{\partial t^2} - \frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial y^2} - \frac{\partial^2}{\partial z^2} + \left(\frac{mc}{\hbar}\right)^2 \right] \psi = 0 \quad (2.5)$$

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

2.4 Compact Notation: Laplacian

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

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \quad (2.6)$$

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

Substituting this into our equation:

$$\left[\frac{1}{c^2} \frac{\partial^2}{\partial t^2} - \nabla^2 + \left(\frac{mc}{\hbar} \right)^2 \right] \psi = 0 \quad (2.7)$$

This is cleaner and makes the equation look more symmetric.

2.5 Even More Compact: d'Alembertian Notation

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

The d'Alembertian operator (wave operator):

$$\square = \frac{1}{c^2} \frac{\partial^2}{\partial t^2} - \nabla^2 \quad (2.8)$$

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

The mass parameter:

$$\mu = \frac{mc}{\hbar} \quad (2.9)$$

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:

$$[\square + \mu^2] \psi = 0 \quad (2.10)$$

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

Chapter 3

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.

3.1 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 3.1.1: Klein-Gordon Plane Wave function

The general form using four-vector notation:

$$\psi = A \exp\left(-\frac{i}{\hbar} p \cdot x\right) \quad (3.1)$$

where:

$$p = [E/c, \vec{p}] \quad (\text{four-momentum})$$

$$x = [ct, \vec{x}] \quad (\text{four-position})$$

$$A \in \mathbb{C} \quad (\text{complex amplitude})$$

$$p^0 = \frac{E}{c} = \pm \sqrt{|\vec{p}|^2 + m^2 c^2} \quad (\text{energy, with } \pm \text{ solutions!})$$

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

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

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

3.2 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:

$$[\square + \mu^2] \psi = 0 \quad \Rightarrow \quad \square \psi = -\mu^2 \psi \quad (3.2)$$

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:

$$\square \left[\exp \left[\frac{i}{\hbar} (\vec{p} \cdot \vec{x} - Et) \right] \right] \quad (3.3)$$

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

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:

$$\square \psi = \left[-\frac{E^2}{c^2 \hbar^2} + \frac{|\vec{p}|^2}{\hbar^2} \right] \psi = -\frac{1}{\hbar^2} \left[\frac{E^2}{c^2} - |\vec{p}|^2 \right] \psi \quad (3.4)$$

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

$$\square \psi = -\frac{m^2 c^2}{\hbar^2} \psi = -\mu^2 \psi \quad \checkmark \quad (3.5)$$

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

Chapter 4

Superposition

4.1 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

$$[\square + \mu^2] \psi_1 = 0 \quad (4.1)$$

$$[\square + \mu^2] \psi_2 = 0 \quad (4.2)$$

Let's call their sum ψ_3 so

$$\psi_3 = \psi_1 + \psi_2 \quad (4.3)$$

The question then arises: does ψ_3 satisfy the Klein-Gordon Equation?

Well, yes it does. We can show this with:

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

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 $\{\psi_n\}$

$$\psi = \sum_n C_n \psi_n, \quad C_n \in \mathbb{C} \quad (4.4)$$

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

$$[\square + \mu^2] \psi_n = 0 \rightarrow [\square + \mu^2] \sum_n C_n \psi_n = 0 \quad (4.5)$$

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

Chapter 5

Group Velocity and the Speed of Light Limit

5.1 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.

5.2 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:

$$\psi = A \exp \left(i \left(\vec{k} \cdot \vec{x} - \omega t \right) \right) \quad (5.1)$$

Our Klein-Gordon plane wave:

$$\psi = A \exp \left(\frac{i}{\hbar} \left(\vec{p} \cdot \vec{x} - Et \right) \right) \quad (5.2)$$

Comparing these, we identify:

$$\begin{aligned} \vec{k} &= \frac{\vec{p}}{\hbar} && \text{(de Broglie relation)} \\ \omega &= \frac{E}{\hbar} && \text{(Planck relation)} \end{aligned}$$

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

$$\omega(k) = \sqrt{(kc)^2 + \left(\frac{mc^2}{\hbar} \right)^2} \quad (5.3)$$

This is the dispersion relation! Notice:

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

5.3 Step 2: Calculating the Group Velocity

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

$$v_g = \frac{d\omega}{dk} \quad (5.4)$$

$$v_g = \frac{d}{dk} \left[\sqrt{(kc)^2 + (mc^2/\hbar)^2} \right] \quad (5.5)$$

Using the chain rule:

$$v_g = \frac{kc^2}{\sqrt{(kc)^2 + (mc^2/\hbar)^2}} = \frac{kc^2}{\omega} \quad (5.6)$$

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

$$v_g = \frac{c|\vec{p}|}{\sqrt{|\vec{p}|^2 + (mc)^2}} \quad (5.7)$$

5.4 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 ($m = 0$):

$$v_g = \frac{c|\vec{p}|}{|\vec{p}|} = c \quad (5.8)$$

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 6

Fourier Transforms and Antimatter

6.1 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 $\phi(p)$.

6.2 The Fourier Transform

$$\psi(x) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \phi(p) \exp\left[-\frac{i}{\hbar} p \cdot x\right] dp \quad (6.1)$$

- 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!

6.3 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:

$$p^0 = \frac{E}{c} = \pm \sqrt{|\vec{p}|^2 + m^2 c^2} \quad (6.2)$$

This \pm sign gives us two branches:

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

6.3.1 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:

$$\hat{E} = i\hbar \frac{\partial}{\partial t} \quad (6.3)$$

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

$$-\hat{E} = -i\hbar \frac{\partial}{\partial t} \quad (6.4)$$

Negative energy?? \longrightarrow 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.

6.4 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.

6.4.1 Problem 1: Second-Order in Time

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

Compare the time derivatives:

$$\begin{aligned} \text{Schrödinger: } & i\hbar \frac{\partial \psi}{\partial t} = \hat{H}\psi \quad (\text{first-order in time}) \\ \text{Klein-Gordon: } & \frac{1}{c^2} \frac{\partial^2 \psi}{\partial t^2} - \nabla^2 \psi + \left(\frac{mc}{\hbar}\right)^2 \psi = 0 \quad (\text{second-order in time}) \end{aligned}$$

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.

6.4.2 Problem 2: Negative Probability Density

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

For Schrödinger, the probability density is simple:

$$\rho = |\psi|^2 = \psi^* \psi \geq 0 \quad (\text{always positive!}) \quad (6.5)$$

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

$$\rho = \frac{i\hbar}{2mc^2} \left(\psi^* \frac{\partial \psi}{\partial t} - \psi \frac{\partial \psi^*}{\partial t} \right) \quad (6.6)$$

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.

6.4.3 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** $\rho \geq 0$ 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 7

Dirac Equation

7.1 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.

$$H = \frac{1}{2m} \left(\vec{\sigma} \cdot \left[\vec{p} + \frac{e}{c} \vec{A}(\vec{r}, t) \right] \right)^2 - e\phi(\vec{r}, t) \quad (7.1)$$

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

$$H = \frac{1}{2m} \left[\vec{p} + \frac{e}{c} \vec{A}(\vec{r}, t) \right]^2 - e\psi(\vec{r}, t) + \frac{e\hbar}{2mc} \vec{\sigma} \cdot \vec{B}(\vec{r}, t) \quad (7.2)$$

This Hamiltonian acts on a two component spinor.

7.2 Deriving the Dirac Equation

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

$$\begin{aligned} \left(\frac{E^2}{c^2} - p^2 \right) - (mc)^2 &= (mc)^2 \\ \left(\frac{E}{c} - \vec{\sigma} \cdot \vec{p} \right) \left(\frac{E}{c} + \vec{\sigma} \cdot \vec{p} \right) &= (mc)^2 \\ \left(i\hbar \frac{\partial}{\partial x_0} + i\hbar \vec{\sigma} \cdot \vec{\nabla} \right) \left(i\hbar \frac{\partial}{\partial x_0} - i\hbar \vec{\sigma} \cdot \vec{\nabla} \right) \phi &= (mc)^2 \phi. \end{aligned}$$

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.

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

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.

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

7.3 Gamma Matrices and Their Properties

Define the 4 by 4 matrices γ_μ 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

$$\left(\gamma_\mu \frac{\partial}{\partial x_\mu} + \frac{mc}{\hbar} \right) \psi = 0 \quad (7.3)$$

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.

$$\{\gamma_\mu, \gamma_\nu\} = 2\delta_{\mu\nu} \quad (7.4)$$

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.

7.4 Conserved Current and Probability Density

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

$$j_\mu = i c \bar{\psi} \gamma_\mu \psi \quad (7.5)$$

satisfies the equation of a conserved 4-vector current

$$\frac{\partial}{\partial x_\mu} j_\mu = 0 \quad (7.6)$$

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

7.5 Non-Relativistic Limit

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

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

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

$$\left(\frac{p^2}{2m} - \frac{Ze^2}{4\pi r} - \frac{p^4}{8\pi m^2 c^2 r^3} + \frac{Ze^2 \vec{L} \cdot \vec{S}}{8m^2 c^2} \delta^3(\vec{r}) \right) \psi = E(N-R) \psi \quad (7.7)$$

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 Hamiltonian. 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.

7.6 Plane Wave Solutions

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

$$\psi_{\vec{p}} = u_{\vec{p}} e^{i(\vec{p} \cdot \vec{x} - Et)/\hbar} \quad (7.8)$$

This is consistent with the relativistic energy relation.

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

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

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.

7.6.1 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:

$$\psi_{\vec{p}}^{(r)} = \sqrt{\frac{mc^2}{|E| V}} u_{\vec{p}}^{(r)} e^{i(\vec{p} \cdot \vec{x} - Et)/\hbar} \quad (7.9)$$

where the four spinors are given by:

$$\begin{aligned}
u_{\vec{p}}^{(1)} &= \sqrt{\frac{E+mc^2}{2mc^2}} \begin{pmatrix} 1 \\ 0 \\ \frac{p_z c}{E+mc^2} \\ \frac{(p_x+ip_y)c}{E+mc^2} \end{pmatrix} & u_{\vec{p}}^{(2)} &= \sqrt{\frac{E+mc^2}{2mc^2}} \begin{pmatrix} 0 \\ 1 \\ \frac{(p_x-ip_y)c}{E+mc^2} \\ \frac{-p_z c}{E+mc^2} \end{pmatrix} \\
u_{\vec{p}}^{(3)} &= \sqrt{\frac{-E+mc^2}{2mc^2}} \begin{pmatrix} -\frac{E+mc^2}{-E+mc^2} \\ -\frac{(p_x+ip_y)c}{-E+mc^2} \\ 1 \\ 0 \end{pmatrix} & u_{\vec{p}}^{(4)} &= \sqrt{\frac{-E+mc^2}{2mc^2}} \begin{pmatrix} -\frac{E+mc^2}{-E+mc^2} \\ -\frac{p_z c}{-E+mc^2} \\ 0 \\ 1 \end{pmatrix}
\end{aligned} \quad (7.10)$$

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

$$u_{\vec{p}}^{(r)\dagger} u_{\vec{p}}^{(r')} = \frac{|E|}{mc^2} \delta_{rr'} \quad (7.11)$$

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.

7.7 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:

$$\begin{aligned}\vec{p} &\rightarrow -\vec{p} \\ E &\rightarrow -E.\end{aligned}$$

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

$$\begin{aligned}\psi_{\vec{p}}^{(1)} &= \sqrt{\frac{E + mc^2}{2EV}} \begin{pmatrix} 1 \\ 0 \\ \frac{p_z c}{E + mc^2} \\ \frac{(p_x + ip_y)c}{E + mc^2} \end{pmatrix} e^{i(\vec{p} \cdot \vec{x} - Et)/\hbar} \\ \psi_{\vec{p}}^{(2)} &= \sqrt{\frac{E + mc^2}{2EV}} \begin{pmatrix} 1 \\ 0 \\ \frac{(p_x - ip_y)c}{E + mc^2} \\ \frac{p_z c}{E + mc^2} \end{pmatrix} e^{i(\vec{p} \cdot \vec{x} - Et)/\hbar} \\ \psi_{\vec{p}}^{(3)} &= \sqrt{\frac{E + mc^2}{2EV}} \begin{pmatrix} \frac{p_z c}{E + mc^2} \\ \frac{(p_x + ip_y)c}{E + mc^2} \\ 1 \\ 0 \end{pmatrix} e^{-i(\vec{p} \cdot \vec{x} - Et)/\hbar} \\ \psi_{\vec{p}}^{(4)} &= \sqrt{\frac{|E| + mc^2}{2|E|V}} \begin{pmatrix} \frac{(p_x - ip_y)c}{E + mc^2} \\ \frac{E - p_z c}{E + mc^2} \\ 0 \\ 1 \end{pmatrix} e^{-i(\vec{p} \cdot \vec{x} - Et)/\hbar}.\end{aligned}$$

we have plane waves of the form

$$e^{\pm ip_\mu x_\mu / \hbar} \quad (7.12)$$

with the plus sign

With the plus sign or solutions 1 and 2 and the minus sign for solutions 3 and 4. These \pm 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 4 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.

7.8 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 to:

$$\begin{aligned}\psi' &= S_{boost}\psi \\ S_{boost} &= \cosh \frac{\chi}{2} + i\gamma_i\gamma_4 \sinh \frac{\chi}{2}.\end{aligned}$$

with $\tanh \chi = \beta$

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

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

with ijk is a cyclic permutation.

7.9 Parity and Discrete Symmetries

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

$$\psi' = S_P\psi = \gamma_4\psi \quad (7.13)$$

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.

$$\gamma_5 = \gamma_1\gamma_2\gamma_3\gamma_4 \quad (7.14)$$

which obviously anticommutes with all the gamma matrices.

$$\{\gamma_\mu, \gamma_5\} = 0 \quad (7.15)$$

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	$\bar{\psi}\psi$	1	
Pseudoscalar	$\bar{\psi}\gamma_5\psi$	1	
Vector	$\bar{\psi}\gamma_\mu\psi$	4	
Axial Vector	$\bar{\psi}\gamma_5\gamma_\mu\psi$	4	
Rank 2 antisymmetric tensor	$\bar{\psi}\sigma_{\mu\nu}\psi$	6	
Total		16	(7.16)

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

7.10 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.

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

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

Thus we can identify the operator below as the Hamiltonian.

$$H = ic\gamma_4\gamma_j p_j + mc^2\gamma_4 \quad (7.17)$$

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

7.10.1 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

$$[H, L_z] = ic\gamma_4 [\gamma_j p_j, xp_y - yp_x] = \hbar c\gamma_4 (\gamma_1 p_y - \gamma_2 p_x) \quad (7.18)$$

The components of spin also do not commute with H .

$$[H, S_z] = \hbar c\gamma_4 [\gamma_2 p_x - \gamma_1 p_y] \quad (7.19)$$

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

$$[H, J_z] = [H, L_z] + [H, S_z] = \hbar c\gamma_4 (\gamma_1 p_y - \gamma_2 p_x) + \hbar c\gamma_4 [\gamma_2 p_x - \gamma_1 p_y] = 0 \quad (7.20)$$

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.

$$[H, \vec{S} \cdot \vec{p}] = [H, \vec{S}] \cdot \vec{p} = 0 \quad (7.21)$$

7.10.2 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

$$H_{int} = \frac{1}{c} j_\mu A_\mu \quad (7.22)$$

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

$$H_{int} = ie\gamma_4\gamma_k A_k \quad (7.23)$$

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

7.11 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.

$$\langle v_k \rangle = \sum_{\vec{p}} \sum_{r=1}^4 |c_{\vec{p},r}|^2 \frac{p_k c^2}{E} + \sum_{\vec{p}} \sum_{r=1}^2 \sum_{r'=3}^4 \frac{mc^3}{|E|} \left[c_{\vec{p},r}^* c_{\vec{p},r} u_{\vec{p}}^{(r')\dagger} i\gamma_4 \gamma_k u_{\vec{p}}^{(r)} r^{-2i|E|t/\hbar} c_{\vec{p},r'}^* c_{\vec{p},r'} u_{\vec{p}}^{(r)\dagger} i\gamma_4 \gamma_k u_{\vec{p}}^{(r')} e^{-2i|E|t/\hbar} \right] \quad (7.24)$$

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.

7.12 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

$$E = \frac{mc^2}{\sqrt{1 + \frac{Z^2 \alpha^2}{\left(n_r + \sqrt{(j+\frac{1}{2})^2 - Z^2 \alpha^2}\right)}}} \quad (7.25)$$

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 our 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.

7.13 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 an 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.

7.14 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.

$$\psi' = \gamma_2 \psi^* \quad (7.26)$$

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

$$\begin{aligned} \psi_{\vec{p}}^{(1)} &= \sqrt{\frac{mc^2}{|E|V}} u_{\vec{p}}^{(1)} e^{i(\vec{p}\cdot\vec{x}-Et)/\hbar} \rightarrow -\sqrt{\frac{mc^2}{|E|V}} u_{\vec{p}}^{(4)} e^{i(-\vec{p}\cdot\vec{x}+Et)/\hbar} \equiv \sqrt{\frac{mc^2}{|E|V}} v_{\vec{p}}^{(1)} e^{i(-\vec{p}\cdot\vec{x}+Et)/\hbar} \\ \psi_{\vec{p}}^{(2)} &= \sqrt{\frac{mc^2}{|E|V}} u_{\vec{p}}^{(2)} e^{i(\vec{p}\cdot\vec{x}-Et)/\hbar} \rightarrow \sqrt{\frac{mc^2}{|E|V}} u_{-\vec{p}}^{(3)} e^{i(-\vec{p}\cdot\vec{x}+Et)/\hbar} \equiv \sqrt{\frac{mc^2}{|E|V}} u_{\vec{p}}^{(2)} e^{i(-\vec{p}\cdot\vec{x}+Et)/\hbar} \\ \psi_{\vec{p}}^{(3)} &= \sqrt{\frac{mc^2}{|E|V}} u_{\vec{p}}^{(3)} e^{i(\vec{p}\cdot\vec{x}+|E|t)/\hbar} \rightarrow \sqrt{\frac{mc^2}{|E|V}} u_{-\vec{p}}^{(2)} e^{i(-\vec{p}\cdot\vec{x}-|E|t)/\hbar} \\ \psi_{\vec{p}}^{(4)} &= \sqrt{\frac{mc^2}{|E|V}} u_{\vec{p}}^{(4)} e^{i(\vec{p}\cdot\vec{x}+|E|t)/\hbar} \rightarrow -\sqrt{\frac{mc^2}{|E|V}} u_{-\vec{p}}^{(1)} e^{i(-\vec{p}\cdot\vec{x}-|E|t)/\hbar}. \end{aligned}$$

The charge conjugate of an electron state is the "negative energy" electron state, 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 $\psi_{\vec{p}}^{(1)}$ 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.

$$\psi_{\vec{p}}^{(1)} = \sqrt{\frac{mc^2}{|E|V}} u_{\vec{p}}^{(1)} e^{i(\vec{p}\cdot\vec{x}-Et)/\hbar} \rightarrow -\sqrt{\frac{mc^2}{|E|V}} u_{-\vec{p}}^{(4)} e^{i(-\vec{p}\cdot\vec{x}+Et)/\hbar} \equiv \sqrt{\frac{mc^2}{|E|V}} v_{\vec{p}}^{(1)} e^{i(-\vec{p}\cdot\vec{x}+Et)/\hbar} \quad (7.27)$$

The charge conjugate of the electron solution is an electron with the same charge $-e$, opposite momentum $-\vec{p}$, 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 $e^{i(\vec{p}\cdot\vec{x}-Et)/\hbar}$. There is a symmetric set of solutions for the same particles moving "backwards in time" oscillating as $e^{i(-\vec{p}\cdot\vec{x}+Et)/\hbar}$. These solutions behave like antiparticles moving forward in time. Consider the following diagram (which contributes to Thomson scattering) from two points of view. From one point of view, an electron starts out at t_1 , lets say in the state $\psi_{\vec{p}}^{(1)}$. At time t_3 , the electron interacts with the field and makes a transition to the state $\psi_{\vec{p}'}^{(4)}$ which travels backwards in time to t_2 where it again interacts and makes a transition to $\psi_{\vec{p}'}^{(1)}$. 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 in 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.

7.15 Quantization of the Dirac Field

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

$$\mathcal{L} = -c\hbar\bar{\psi}\gamma_\mu \frac{\partial}{\partial x_\mu}\psi - mc^2\bar{\psi}\psi \quad (7.28)$$

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

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

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,

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

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 .

$$\Pi = \frac{\partial \mathcal{L}}{\partial \left(\frac{\partial \psi}{\partial t} \right)} = -c\hbar\bar{\psi}\gamma_4 \frac{1}{ic} = i\hbar\psi^\dagger\gamma_4\gamma_4 = i\hbar\psi^\dagger \quad (7.29)$$

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

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

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

$$\psi(\vec{x}, t) = \sum_{\vec{p}} \sum_{r=1}^4 \sqrt{\frac{mc^2}{|E|V}} c_{\vec{p},r} u_{\vec{p}}^{(r)} e^{i(\vec{p} \cdot \vec{x} - Et)/\hbar} \quad (7.30)$$

The conjugate can also be written out.

$$\psi^\dagger(\vec{x}, t) = \sum_{\vec{p}} \sum_{r=1}^4 \sqrt{\frac{mc^2}{|E|V}} c_{\vec{p},r} u_{\vec{p}}^{(r)} e^{i(\vec{p} \cdot \vec{x} - Et)/\hbar} \quad (7.31)$$

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

$$\begin{aligned}
\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 \mathbf{x} \\
\mathbf{H} &= \int \sum_{\vec{p}}^4 \sum_{r=1}^4 \sum_{\vec{p}}^4 \sum_{r'=1}^4 \sqrt{\frac{mc^2}{|E'| V}} c_{\vec{p}', r'}^* u_{\vec{p}'}^{(r')\dagger} e^{-i(\vec{p} \cdot \vec{x} - Et)/\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_{\vec{p}}^{(r)} e^{i(\vec{p} \cdot \vec{x} - Et)/\hbar} \mathbf{d}^3 \mathbf{x} \\
\mathbf{H} &= \int \sum_{\vec{p}}^4 \sum_{r=1}^4 \sum_{\vec{p}}^4 \sum_{r'=1}^4 \sqrt{\frac{mc^2}{|E'| V}} c_{\vec{p}', r'}^* u_{\vec{p}'}^{(r')\dagger} e^{-i(\vec{p} \cdot \vec{x} - Et)/\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_{\vec{p}}^{(r)} e^{i(\vec{p} \cdot \vec{x} - Et)/\hbar} \mathbf{d}^3 \mathbf{x} \\
\mathbf{H} &= \int \sum_{\vec{p}}^4 \sum_{r=1}^4 \sum_{\vec{p}}^4 \sum_{r'=1}^4 \sqrt{\frac{mc^2}{|E'| V}} c_{\vec{p}', r'}^* u_{\vec{p}'}^{(r')\dagger} e^{-i(\vec{p} \cdot \vec{x} - Et)/\hbar} (ic \gamma_4 \gamma_k p_k + mc^2 \gamma_4) \sqrt{\frac{mc^2}{|E| V}} c_{\vec{p}, r} u_{\vec{p}}^{(r)} e^{i(\vec{p} \cdot \vec{x} - Et)/\hbar} \mathbf{d}^3 \mathbf{x} \\
(ic \gamma_4 \gamma_k p_k + mc^2 \gamma_4) \psi &= E \psi \\
\mathbf{H} &= \int \sum_{\vec{p}}^4 \sum_{r=1}^4 \sum_{\vec{p}'}^4 \sum_{r'=1}^4 \sqrt{\frac{mc^2}{|E'| V}} c_{\vec{p}', r'}^* u_{\vec{p}'}^{(r')\dagger} e^{-i(\vec{p} \cdot \vec{x} - Et)/\hbar} (E) \sqrt{\frac{mc^2}{|E| V}} c_{\vec{p}, r} u_{\vec{p}}^{(r)} e^{i(\vec{p} \cdot \vec{x} - Et)/\hbar} \mathbf{d}^3 \mathbf{x} \\
\mathbf{H} &= \sum_{\vec{p}}^4 \sum_{r=1}^4 \sum_{\vec{p}'}^4 \sum_{r'=1}^4 \sqrt{\frac{mc^2}{|E'| V}} c_{\vec{p}', r'}^* u_{\vec{p}'}^{(r')\dagger} (E) \sqrt{\frac{mc^2}{|E| V}} c_{\vec{p}, r} u_{\vec{p}}^{(r)} \delta_{\vec{p} \vec{p}'} \\
\mathbf{H} &= \sum_{\vec{p}}^4 \sum_{r=1}^4 \sum_{r'=1}^4 \frac{mc^2}{|E|} c_{\vec{p}', r'}^* c_{\vec{p}, r} u_{\vec{p}}^{(r')\dagger} (E) u_{\vec{p}}^{(r)} \\
u_{\vec{p}}^{(r)\dagger} u_{\vec{p}}^{(r')} &= \frac{|E|}{mc^2} \delta_{rr'} \\
\mathbf{H} &= \sum_{\vec{p}}^4 \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}}^4 \sum_{r=1}^4 E c_{\vec{p}, r}^* c_{\vec{p}, r}.
\end{aligned}$$

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

$$\mathbf{H} = \sum_{k,\alpha} \left(\frac{\omega}{c} \right)^2 \left[c_{k,\alpha} c_{k,\alpha}^* + c_{k,\alpha}^* c_{k,\alpha} \right] \quad (7.32)$$

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

$$\begin{aligned}
c_{k,\alpha} &= \sqrt{\frac{\hbar c^2}{2\omega}} a_{k,\alpha} \\
c_{k,\alpha}^* &= \sqrt{\frac{\hbar c^2}{2\omega}} a_{k,\alpha}^\dagger.
\end{aligned}$$

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

$$\mathbf{H} = \frac{1}{2} \sum_{k,\alpha} \hbar \omega \left[a_{k,\alpha} a_{k,\alpha}^\dagger + a_{k,\alpha}^\dagger a_{k,\alpha} \right] \quad (7.33)$$

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.

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

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

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

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

$N_{\vec{p}}^{(r)}$ 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.

7.16 The Quantized Dirac Field with Positron Spinors

The basis states in our quantized Dirac field can be changed to 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 the electron spinors

$$S_C u_{\vec{p}}^{(s)*} = v_{\vec{p}}^{(s)} \quad s = 1, 2 \tag{7.34}$$

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

$$\left\{ d_{\vec{p}}^{(s)}, d_{\vec{p}'}^{(s')^\dagger} \right\} = \delta_{ss'}, \delta_{\vec{p}\vec{p}'} \quad (7.35)$$

The Dirac field and Hamiltonian can now be rewritten.

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

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 vacuum 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 particles satisfying the Dirac equation.

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

$$\{b_r^\dagger, b_{r'}^\dagger\} = 0 \quad (7.36)$$

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

$$b_r^\dagger b_{r'}^\dagger |0\rangle = -b_{r'}^\dagger b_r^\dagger |0\rangle \quad (7.37)$$

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.

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

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

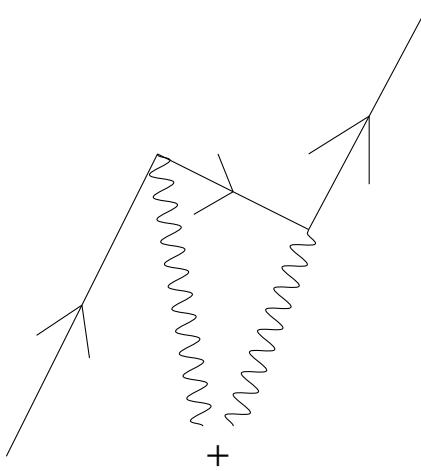
7.17 Vacuum Polarization

Vacuum polarization is an important effect in effectively reducing the charge on a particle. The reduction is dependent 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 analogous 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 referred 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 annihilates 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 $\Delta t = \frac{\hbar}{2mc^2}$ (which is approximately the reciprocal of the Zitterbewegung frequency). The distance the electron appears to jump then is of the order of $c\Delta t = \frac{\hbar c}{2mc^2} = 0.002 \text{ \AAngstrøms}$. This is the approximate size of the fast back and forth motion of Zitterbewegung.

7.18 The QED LaGrangian and Gauge Invariance

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

$$\mathcal{L} = -\hbar c \bar{\psi} \left(\gamma_\mu \frac{\partial}{\partial x_\mu} + \frac{mc}{\hbar} \right) \psi - \frac{1}{4} F_{\mu\nu} F_{\mu\nu} - ie \bar{\psi} \gamma_\mu A_\mu \psi \quad (7.38)$$

QED is our 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 particles 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.

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

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

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

Note that in the interaction term $-ie\bar{\psi}\gamma_\mu A_\mu\psi$ 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 deduce from the above transformation that

$$F_{\mu\nu} = \frac{\partial A_\nu}{\partial x_\mu} - \frac{\partial A_\mu}{\partial x_\nu} \rightarrow F_{\mu\nu} - \frac{\hbar c}{e} \left(\frac{\partial}{\partial x_\mu} \frac{\partial \lambda(x)}{\partial x_\nu} - \frac{\partial}{\partial x_\nu} \frac{\partial \lambda(x)}{\partial x_\mu} \right) = F_{\mu\nu} \quad (7.39)$$

The transformed LaGrangian then can be computed easily.

$$\mathcal{L} = -\hbar c \bar{\psi} \left(\gamma_\mu \frac{\partial}{\partial x_\mu} + \frac{mc}{\hbar} \right) \psi - \frac{1}{4} F_{\mu\nu} F_{\mu\nu} - ie\bar{\psi}\gamma_\mu A_\mu\psi \quad (7.40)$$

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

$$\mathcal{L} \rightarrow \mathcal{L} - i\hbar c \bar{\psi} \gamma_\mu \frac{\partial \lambda}{\partial x_\mu} \psi - ie\bar{\psi}\gamma_\mu \frac{-\hbar c}{e} \frac{\partial \lambda}{\partial x_\mu} \psi = \mathcal{L} \quad (7.41)$$

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 gauge invariant. Gauge invariance implies zero mass photons and even maintains the massless photon after radiative corrections. Gauge invariance also implies the existence of a conserved current. Remember that the electric current in 4D also includes the charge density. Gauge 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 gauge invariant. It turns out we need a triplet of bosons. (The weak interactions then get messy because of the Higgs mechanism but the underlying gauge 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 dimension 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 gauge invariant.

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

7.19 Interaction with a Scalar Field

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