Quantum Mechanics Part 2

Chapter 15

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Chapter 15 **Relativistic Wave Equations, Electromagnetic Radiation in Matter**

15.1 **Spin 0 particles: Klein-Gordon Equation**

A classical nonrelativistic free particle has an energy-momentum relation $E = p^2/2m$. Under a Galilean transformation to a new coordinate system traveling with $-\vec{v}$ with respect to the first system, we have

$$\vec{r}\,' = \vec{r} + \vec{v}t \quad , \quad t' = t \tag{15.1}$$

which gives

$$\begin{aligned}
\vec{u}\,' &= \frac{d\vec{r}\,'}{dt'} = \frac{d\vec{r}}{dt} + \vec{v} = \vec{u} + \vec{v} \\
m' &= m \\
\vec{p}\,' &= \vec{p} + m\vec{v}
\end{aligned}$$

We then have

$$\vec{F}\,' = \frac{d\vec{p}\,'}{dt'} = \frac{d\vec{p}}{dt} = \vec{F} \tag{15.2}$$

which implies the invariance of the form $E = p^2/2m$, i.e.,

$$E\,' = \int \vec{F}\,' \cdot d\vec{r}\,' = \frac{1}{m'} \int \vec{p}\,' \cdot d\vec{p}\,' = \frac{\vec{p}\,'^2}{2m'}$$

$$E = \int \vec{F} \cdot d\vec{r} = \frac{1}{m} \int \vec{p} \cdot d\vec{p} = \frac{\vec{p}^2}{2m}$$

and

$$E\,' = \frac{\vec{p}\,'^2}{2m'} = \frac{(\vec{p} + m\vec{v})^2}{2m} = E + \vec{p} \cdot \vec{v} + \frac{1}{2} m v^2 \tag{15.3}$$

Thus, the final Galilean transformation relations are

$$E\,' = E + \vec{p} \cdot \vec{v} + \frac{1}{2} m v^2 \quad , \quad \vec{p}\,' = \vec{p} + m\vec{v} \tag{15.4}$$

which, as shown, leaves the quadratic form $E = p^2/2m$ invariant, i.e., if $E = \vec{p}^2/2m$, then $E\,' = \vec{p}\,'^2/2m'$ and we derive the transformation rules for E and $\vec{p}$ from that condition.

The non-relativistic Schrodinger equation for the free particle then follows from the standard identifications

$$E \to i\hbar\frac{\partial}{\partial t} \quad , \quad \vec{p} \to \frac{\hbar}{i}\nabla$$

$$H\psi = E\psi \quad , \quad H = \frac{p^2}{2m}$$

which gives

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi \tag{15.5}$$

It is clear from the form of the Schrodinger equation for a free particle that the equation cannot be invariant under Lorentz transformation (Lorentz covariant), i.e., the time derivative is first order and the space derivatives are second order.

15.1.1 How to find correct form of relativistic wave equation?

Before proceeding let us recall some results from special relativity.

Components of spacetime four-vectors will be labeled by Greek indices and the components of spatial three-vectors will be labeled by Latin indices and we will use Einstein summation convention.

Starting from $x^\mu(s) = (ct, \vec{x}) = (x^0, \vec{x})$, the contravariant 4-vector representation of the worldline as a function of the proper time s, we first obtain the 4-velocity, i.e.,

$$\dot{x}^\mu(s) = \frac{dx^\mu(s)}{ds} = \frac{dx^\mu(s)}{\frac{1}{\gamma}dx^0} = \gamma\left(\frac{dx^0}{dx^0}, \frac{d\vec{x}}{dx^0}\right) = \gamma\,(1, \vec{v}/c) \quad (15.6)$$

where

$$\gamma = \frac{1}{\sqrt{1-\frac{v^2}{c^2}}} \quad , \quad \vec{v} = \frac{d\vec{x}}{dt} = c\frac{d\vec{x}}{dx^0} \quad (15.7)$$

The 4-momentum vector is then given by

$$p^\mu = mc\dot{x}^\mu(s) = \gamma m\,(c, \vec{v}) = (E/c, \vec{p}) \quad (15.8)$$

where we have used the fact that

$$p^0 = \frac{E}{c} = \gamma mc \quad , \quad m = \text{ rest mass} \tag{15.9}$$

This says that the energy E and momentum $\vec{p}$ transform as the components of a contravariant 4-vector and we know that the *square* of any 4-vector is invariant.

The metric tensor defined by

$$g_{\mu\nu} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \tag{15.10}$$

allows the construction of the covariant components(using Einstein summation convention)

$$p_\mu = g_{\mu\nu} p^\nu = \left(\frac{E}{c}, -\vec{p}\right) \tag{15.11}$$

We can then calculate the invariant *square* or the invariant scalar product of the 4-momentum with itself as

$$p_\mu p^\mu = g_{\mu\nu} p^\nu p^\mu = \frac{E^2}{c^2} - \vec{p}^2 = m^2 c^2 \tag{15.12}$$

We therefore have the relativistic energy momentum relation

$$E = \left(\vec{p}^2 c^2 + m^2 c^4\right)^{1/2} \tag{15.13}$$

If we use this expression to construct a new wave equation by operator substitution we would have

$$i\hbar \frac{\partial \psi}{\partial t} = \left(-\hbar^2 c^2 \nabla^2 + m^2 c^4\right)^{1/2} \psi \tag{15.14}$$

Although the energy formula is now relativistically correct, the time and space derivatives still do not appear symmetrically. In fact, a Taylor expansion of the square root gives infinitely high-order derivatives leading to a very difficult mathematical equation to deal with.

This fact, in itself, is not a valid reason for rejecting the equation.

There are, however, strong physical reasons for rejecting this equation. The equation says that the momentum space amplitude

$$\psi_{\vec{p}}(t) = \int d^3r\, e^{-i\vec{p}\cdot\vec{r}/\hbar}\psi(\vec{r},t) \tag{15.15}$$

obeys the equation

$$i\hbar\frac{\partial\psi_{\vec{p}}(t)}{\partial t} = \left(p^2c^2 + m^2c^4\right)^{1/2}\psi_{\vec{p}}(t) \tag{15.16}$$

If we Fourier transform both sides back to position space we get

$$i\hbar\frac{\partial\psi(\vec{r},t)}{\partial t} = \int d^3r'\, K(\vec{r}-\vec{r}')\psi(\vec{r}',t) \tag{15.17}$$

where

$$K(\vec{r}-\vec{r}\,') = \int \frac{d^3p}{(2\pi\hbar)^3} e^{i\vec{p}\cdot(\vec{r}-\vec{r}\,')/h} \left(p^2c^2 + m^2c^4\right)^{1/2} \tag{15.18}$$

This equation for $\psi(\vec{r},t)$ is *nonlocal*, which means that the value of the integral at $vecr$ depends on the value of ψ at the other points $vecr\,'$. The function $K(\vec{r}-\vec{r}\,')$ is large as long as $vecr\,'$ is within a distance

$$\approx \frac{\hbar}{mc} = \text{ Compton wavelength} \tag{15.19}$$

from $vecr$. As a consequence of the nonlocality, the rate of change in time of ψ at the spacetime point $(\vec{r},t)$ depends on the values of ψ at points $(\vec{r}\,',t)$ *outside the light cone* centered on $(\vec{r},t)$.

If we construct a wave packet localized well within a Compton wavelength of the origin, then the packet will be nonzero an arbitrarily short time later at points as distant as the Compton wavelength.

Thus, this equation leads to violations of relativistic causality when used to describe particles localized to within more than a Compton wavelength, which is unacceptable.

Instead, we will start from an equation involving E^2, i.e., we have

$$E^2\psi = \left(i\hbar\frac{\partial}{\partial t}\right)^2 \psi = \left(\vec{p}^2 c^2 + m^2 c^4\right)\psi = \left(-\hbar^2 c^2 \nabla^2 + m^2 c^4\right)\psi$$

$$\left(\nabla^2 - \left(\frac{mc}{\hbar}\right)^2\right)\psi = \frac{1}{c^2}\frac{\partial^2\psi}{\partial^2 t} \tag{15.20}$$

which looks like a classical wave equation with an extra term of the form

$$\left(\frac{mc}{\hbar}\right)^2 \tag{15.21}$$

It is called the *Klein-Gordon* equation. In 4-vector notation it looks like

$$\left(\partial_\mu \partial^\mu + \left(\frac{mc}{\hbar}\right)^2\right)\psi = 0 \quad , \quad \partial_\mu = \frac{\partial}{\partial x^\mu} \tag{15.22}$$

The equation can be generalized in a relativistically invariant way to include the coupling of charged particles to the electromagnetic field by the substitutions (corresponding to minimal coupling we discussed earlier in Chapter 6)

$$i\hbar\frac{\partial}{\partial t} \to i\hbar\frac{\partial}{\partial t} - e\Phi \quad , \quad \frac{\hbar}{i}\nabla \to \frac{\hbar}{i}\nabla - \frac{e}{c}\vec{A} \tag{15.23}$$

to obtain

$$\frac{1}{c^2}\left(i\hbar\frac{\partial}{\partial t} - e\Phi(\vec{r},t)\right)^2 \psi(\vec{r},t) = \left(\left(\frac{\hbar}{i}\nabla - \frac{e}{c}\vec{A}(\vec{r},t)\right)^2 + m^2c^2\right)\psi(\vec{r},t) \tag{15.24}$$

The Klein-Gordon equation has several unusual features.

First, it is second-order in time (space and time derivatives are now the same order). This means we need to specify twice as much initial information (the function and its derivative) at one time to specify the relativistic solution as compared to the nonrelativistic solution which only required specification of the function at one time.

This will mean that the equation has an extra degree of freedom. We will see shortly that this extra degree of freedom corresponds to specifying the *charge* of the particle and that the Klein-Gordon equation actually describes both a particle and its *antiparticle* together. .

Second, since the equation is second order in time, the functions

$$\psi = e^{i(\vec{p}\cdot\vec{r}-Et)/\hbar} \tag{15.25}$$

satisfy the free particle equation with either sign of E, i.e.,

$$E = \pm\left(\vec{p}^2c^2 + m^2c^4\right)^{1/2} \tag{15.26}$$

The Klein-Gordon equation has negative energy solutions for a free particle! For these solutions when we *increase* the magnitude of the momentum $\vec{p}$, then the energy of the particle *decreases*! As we will see later, these negative energy solutions are real and will correspond to antiparticles, while the positive energy solutions will be particles.

In nonrelativistic Schrodinger theory we were able to interpret $\psi^*\psi$ as a positive probability density that was conserved in time (no sinks or sources of probability in nonrelativistic Schrodinger theory). Let us see what happens in the case of the Klein-Gordon equation.

For the Klein-Gordon equation

$$\int \psi^* \psi d^3 r \tag{15.27}$$

changes in time and thus, we cannot interpret $\psi^*(\vec{r},t)\psi(\vec{r},t)$ as being the probability of finding a particle at $\vec{r}$ at time t.

We can, however, construct a different conserved density as follows. We write

$$\psi^* \left(\partial_\mu \partial^\mu + \left(\frac{mc}{\hbar} \right)^2 \right) \psi = 0 \tag{15.28}$$

and

$$\psi \left(\partial_\mu \partial^\mu + \left(\frac{mc}{\hbar} \right)^2 \right) \psi^* = 0 \tag{15.29}$$

which give(subtracting)

$$\psi^* \partial_\mu \partial^\mu \psi - \psi \partial_\mu \partial^\mu \psi^* = 0 \tag{15.30}$$

$$\partial_\mu \left(\psi^* \partial^\mu \psi - \psi \partial^\mu \psi^* \right) = 0 \tag{15.31}$$

Expanding these expressions, we have the continuity equation

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \vec{j} = 0 \tag{15.32}$$

where

$$\rho(\vec{r}, t) = \frac{i\hbar}{2mc^2} \left(\psi^* \frac{\partial \psi}{\partial t} - \psi \frac{\partial \psi^*}{\partial t} \right) \tag{15.33}$$

$$\vec{j}(\vec{r}, t) = \frac{\hbar}{im} \left(\psi^* \nabla \psi - \psi \nabla \psi^* \right) \tag{15.34}$$

We have inserted a multiplicative constant so that the current density vector $\vec{j}(\vec{r}, t)$ is identical to the nonrelativistic case.

Because this density $\rho(\vec{r}, t)$ satisfies a continuity equation, its integral over all space does not change in time. Clearly, however, it is not necessarily positive. In particular, $\rho < 0$ for a negative energy free particle eigenstate.

This means that we cannot interpret this new $\rho(\vec{r})$ as being the particle (probability) density at $\vec{r}$ and we cannot interpret $\vec{j}(\vec{r})$ as a particle current.

The interpretation that will eventually emerge is that for charged particles $e\rho(\vec{r})$ represents the charge density at $\vec{r}$, which can have either sign and $e\vec{j}(\vec{r})$ represents the electric current at $\vec{r}$.

15.1.2 **Negative Energy States and Antiparticles**

How do we interpret the Klein-Gordon equation and its solutions?

Consider a free particle at rest, i.e., $\vec{p} = 0$.

The wave function for the positive energy solution is

$$\psi(\vec{r}, t) = e^{-imc^2 t/\hbar} \tag{15.35}$$

where the energy of a particle at rest is $E = mc^2$. The density for this state is $\rho(\vec{r}, t) = +1$.

Now make a Lorentz transformation to a new frame moving with velocity $-\vec{v}$ with respect to the particle at rest. The particle now appears to have a velocity $\vec{v}$ in this new frame. It, therefore, has

$$\text{momentum } = \vec{p} = \gamma m\vec{v} \text{ and energy } = E = \gamma mc^2 \tag{15.36}$$

where

$$\gamma = \frac{1}{\sqrt{1 - v^2/c^2}} \tag{15.37}$$

This result follows because

$$\begin{aligned} p_\mu x'^\mu &= \text{ Lorentz scalar} \\ &= -mc^2 t \text{ in the rest frame} \\ &= \vec{p}\cdot\vec{r}\,' - Et\,' \text{ in the moving frame} \end{aligned}$$

The new wave function

$$\psi(\vec{r}\,', t') = e^{i(\vec{p}\cdot\vec{r}\,' - Et')/\hbar} = e^{i(\vec{p}\cdot\vec{r}\,' - E_{\vec{p}}t')/\hbar} \tag{15.38}$$

is the result we expect for a particle of momentum $\vec{p}$ and energy $E_{\vec{p}}$. If we calculate the density ρ for this wave function we get

$$\rho(\vec{r}\,', t') = \frac{E_{\vec{p}}}{mc^2} \tag{15.39}$$

and the current is

$$\vec{j}(\vec{r}\,', t') = \frac{\vec{p}}{m} = \frac{\vec{p}c^2}{E_{\vec{p}}}\rho(\vec{r}\,', t') = \vec{v}\rho(\vec{r}\,', t') \text{ (as expected)} \tag{15.40}$$

where

$$\vec{v} = \frac{\vec{p}c^2}{E_{\vec{p}}} \tag{15.41}$$

We see that $\rho(\vec{r}, t)$ transforms like $E_{\vec{p}}$ or as the time component of a 4-vector, which makes physical sense. Since a unit volume in the rest frame appears smaller by a factor

$$1/\gamma = \sqrt{1 - v^2/c^2} \tag{15.42}$$

when observed from the moving frame, a unit density in the rest frame will appear as a density

$$\frac{1}{\gamma} = \frac{E_{\vec{p}}}{mc^2} \tag{15.43}$$

in a frame in which the particle is moving.

What about the negative energy solutions?

For a particle at rest we have, in this case,

$$\psi(\vec{r}, t) = e^{imc^2 t/\hbar} \tag{15.44}$$

where the energy of this particle at rest is $E = -mc^2$.

The density for this state is $\rho(\vec{r}, t) = -1$.

It turns out that one way to interpret a state with a negative particle density is to say that it is a state with a positive density of antiparticles.

We will make the interpretation that a particle at rest with energy $E = -mc^2$ is actually an antiparticle with positive energy $E = mc^2$. As we shall see, this interpretation of negative energy states will lead to a consistent theoretical picture that is confirmed experimentally.

In a Lorentz frame traveling with velocity $-\vec{v}$ with respect to the antiparticle, the wave function is

$$\psi(\vec{r}', t') = e^{-i(\vec{p}\cdot\vec{r}' - Et')/\hbar} = e^{imc^2 t/\hbar} \tag{15.45}$$

where

$$\text{momentum } = \vec{p} = \gamma m\vec{v} \text{ and energy } = E = \gamma mc^2 \tag{15.46}$$

In this new frame the particle has velocity $\vec{v}$, momentum $\vec{p}$ and energy $E_{\vec{p}}$. The wave function, however, describes a particle of energy $-E_{\vec{p}}$ and momentum $-\vec{p}$.

The density in the moving frame is

$$\rho(\vec{r}', t') = -\frac{E_{\vec{p}}}{mc^2} \tag{15.47}$$

and the current is

$$\vec{j}(\vec{r}', t') = -\frac{\vec{p}}{m}\rho(\vec{r}', t') = \frac{\vec{p}c^2}{E_{\vec{p}}}\rho(\vec{r}', t') \tag{15.48}$$

Thus, an antiparticle moving with velocity $\vec{v}$ has associated with it a current moving in the opposite direction, i.e., a flow of antiparticles in one direction is equivalent to a flow of particles in the opposite direction.

For a charged particle $e\rho(\vec{r}, t)$ is the charge density. It is positive for a free particle with $e > 0$ and negative for a free antiparticle, which has opposite charge to the particle.

The quantity $e\vec{j}(\vec{r}, t)$ is the electric current of the state ψ. For a particle the electric current is in the direction of the particle velocity. For the antiparticle with $e < 0$, the electric current is opposite to the velocity.

This says that the interpretation of the negative energy solutions as antiparticles is consistent with the interpretation of the density ρ as a charge density and $\vec{j}$ as an electric current.

Is this interpretation consistent with the way charged particles interact with the electromagnetic field?

The Klein-Gordon equation with an electromagnetic field present is given by

$$\frac{1}{c^2}\left(i\hbar\frac{\partial}{\partial t} - e\Phi(\vec{r},t)\right)^2 \psi(\vec{r},t) = \left(\left(\frac{\hbar}{i}\nabla - \frac{e}{c}\vec{A}(\vec{r},t)\right)^2 + m^2c^2\right)\psi(\vec{r},t) \tag{15.49}$$

Taking the complex conjugate we have

$$\frac{1}{c^2}\left(i\hbar\frac{\partial}{\partial t} + e\Phi(\vec{r},t)\right)^2 \psi^*(\vec{r},t) = \left(\left(\frac{\hbar}{i}\nabla + \frac{e}{c}\vec{A}(\vec{r},t)\right)^2 + m^2c^2\right)\psi^*(\vec{r},t) \tag{15.50}$$

These equations say that if $\psi(\vec{r},t)$ is a solution to the Klein-Gordon equation with a certain sign of the charge, then $\psi^*(\vec{r},t)$ is a solution of the Klein-Gordon equation with the *opposite* sign of the charge and the *same* mass.

Thus, the relativistic theory of a spin zero particle predicts the existence of its antiparticle with the opposite charge and same mass, i.e., the theory contains solutions for both particles and antiparticles.

Relativistic invariance requires the existence of antiparticles

The complex conjugate of a negative energy solution is a positive energy solution with the opposite sign of the charge. The operation of taking the complex conjugate of the wave function will be called *charge conjugation.* Charge conjugation changes particles into antiparticles and vice versa. If we label quantities calculated with the complex conjugate wave function by a subscript **c** , we find

$$\rho(\vec{r},t) = -\rho_c(\vec{r},t) \quad , \quad \vec{j}(\vec{r},t) = -\vec{j}_c(\vec{r},t) \tag{15.51}$$

as expected.

The solutions are normalized by the requirement that the total associated charge equals ± 1 unit, i.e.,

$$\int d^3r \rho(\vec{r},t) = +1 = -\int d^3r \rho_c(\vec{r},t) \tag{15.52}$$

This normalization is conserved in time and invariant under a Lorentz transformation.

15.2 **Physics of the Klein-Gordon Equation**

We first transform the Klein-Gordon equation into two equations, each first order in time.

We define

$$\psi^0(\vec{r},t) = \left(\frac{\partial}{\partial t} + \frac{ie}{\hbar}\Phi(\vec{r},t)\right)\psi(\vec{r},t) \qquad (1^{st}\text{ - order equation \#1}) \tag{15.53}$$

We then have

$$\left(\frac{\partial}{\partial t} + \frac{ie}{\hbar}\Phi(\vec{r},t)\right)\psi^0(\vec{r},t) = \left(\frac{\partial}{\partial t} + \frac{ie}{\hbar}\Phi(\vec{r},t)\right)^2\psi(\vec{r},t) \tag{15.54}$$

Now using the Klein-Gordon equation we have

$$\left(\frac{\partial}{\partial t} + \frac{ie}{\hbar}\Phi(\vec{r},t)\right)^2\psi(\vec{r},t) = c^2\left(\left(\nabla + \frac{ie}{\hbar c}\vec{A}(\vec{r},t)\right)^2 - \frac{m^2c^4}{\hbar^2}\right)\psi(\vec{r},t) \tag{15.55}$$

so we get

$$\left(\frac{\partial}{\partial t} + \frac{ie}{\hbar}\Phi(\vec{r},t)\right)\psi^0(\vec{r},t) \tag{15.56}$$

$$= c^2\left(\left(\nabla + \frac{ie}{\hbar c}\vec{A}(\vec{r},t)\right)^2 - \frac{m^2c^4}{\hbar^2}\right)\psi(\vec{r},t) \qquad (1^{st}\text{ -order equation}$$

These two new first-order equations involve the two functions $\psi^0(\vec{r},t)$ and $\psi(\vec{r},t)$.

Now define the linear combinations

$$\phi = \frac{1}{2}\left[\psi + \frac{i\hbar}{mc^2}\psi^0\right] \quad , \quad \chi = \frac{1}{2}\left[\psi - \frac{i\hbar}{mc^2}\psi^0\right] \tag{15.57}$$

Substitution then gives the more symmetric equations

$$\left(i\hbar\frac{\partial}{\partial t} - e\Phi\right)\phi = \frac{1}{2m}\left[\frac{\hbar}{i}\nabla - \frac{e}{c}\vec{A}\right]^2(\phi+\chi) + mc^2\phi \tag{15.58}$$

$$\left(i\hbar\frac{\partial}{\partial t} - e\Phi\right)\chi = -\frac{1}{2m}\left[\frac{\hbar}{i}\nabla - \frac{e}{c}\vec{A}\right]^2(\phi+\chi) + mc^2\chi \tag{15.59}$$

Now define a two-component wave function

$$\Psi(\vec{r},t) = \begin{pmatrix} \phi(\vec{r},t) \\ \chi(\vec{r},t) \end{pmatrix} \tag{15.60}$$

and three 2×2 matrices

$$\tau_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad , \quad \tau_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad , \quad \tau_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{15.61}$$

The two symmetric equations can then be combined into the single equation

$$i\hbar\frac{\partial\Psi}{\partial t} = \left[\left[\frac{\hbar}{i}\nabla - \frac{e}{c}\vec{A}\right]^2(\tau_3 + i\tau_2) + mc^2\tau_3 + e\Phi\right]\Psi \tag{15.62}$$

This equation is completely equivalent to the original Klein-Gordon equation where

$$\psi = \phi + \chi \quad , \quad \psi^0 = \frac{mc^2}{i\hbar}(\phi - \chi) \tag{15.63}$$

The internal degree of freedom represented by these two components is the charge of the particle(one component represents the particle and the other the antiparticle).

Using the two component equation, we can write the density as

$$\rho(\vec{r},t) = |\phi|^2 - |\chi|^2 = \Psi^+ \tau_3 \Psi \tag{15.64}$$

where $\Psi^+ = (\phi^*, \chi^*)$. A very simple expression. The current density, however, becomes less transparent

$$\vec{j}(\vec{r},t) = \frac{\hbar}{2im}\left[\Psi^+\tau_3(\tau_3 + i\tau_2)\nabla\Psi - (\nabla\Psi^+)\tau_3(\tau_3 + i\tau_2)\Psi\right] - \frac{e\vec{A}}{mc}\Psi^+\tau_3(\tau_3 + i\tau_2)\Psi \tag{15.65}$$

The normalization condition becomes

$$\int d^3r\, \Psi^+\tau_3\Psi = \pm 1 \tag{15.66}$$

The scalar product between two such wave functions Ψ and $|Psi'$ is defined by

$$\langle \Psi \mid \Psi' \rangle = \int d^3r\, \Psi^+(\vec{r},t)\tau_3\Psi'(\vec{r},t) \tag{15.67}$$

Finally, the wave equation is of the form

$$i\hbar\frac{\partial\Psi}{\partial t} = \hat{H}\Psi \tag{15.68}$$

where the Hamiltonian is

$$\hat{H} = \left[\frac{\hbar}{i}\nabla - \frac{e}{c}\vec{A}\right]^2 (\tau_3 + i\tau_2) + mc^2\tau_3 + e\Phi \tag{15.69}$$

Since $(\tau_3 + i\tau_2)^+ = \tau_3 - i\tau_2$, we find that $\hat{H}^+ \neq \hat{H}$, which seems to indicate that $\hat{H}$ is not Hermitian. It is Hermitian, however, when we use the proper scalar product definition of hermiticity, i.e.,

$$\langle\Psi|\left(\hat{H}\left|\Psi'\right\rangle\right) = \left[\left\langle\Psi'\right|\left(\hat{H}\left|\Psi\right\rangle\right)\right]^* \tag{15.70}$$

This relation requires that

$$\tau_3\hat{H}^+\tau_3 = \hat{H} \tag{15.71}$$

All required properties of Hermitian operators, i.e., real eigenvalues and so on, follow from the scalar product definition so that is all that is actually required.

Under the charge conjugation operation

$$\left.\begin{array}{l} \phi \rightarrow \chi^* \\ \chi \rightarrow \phi^* \end{array}\right\} \rightarrow \Psi_c = \tau_1 \Psi^* \tag{15.72}$$

which is the form of the charge conjugation operation in two-component language.

We can now see the physical meaning of charge conjugation. Using

$$\vec{p}^* = \left(\frac{\hbar}{i}\nabla\right)^* = -\frac{\hbar}{i}\nabla = -\vec{p} \tag{15.73}$$

and $\tau_3 + i\tau_2 =$ real matrix, we find that

$$\hat{H}^*(e) = \left[-\vec{p} - \frac{e}{c}\vec{A}\right]^2 (\tau_3 + i\tau_2) + mc^2\tau_3 + e\Phi \tag{15.74}$$

We then have

$$\tau_1 \hat{H}^*(e)\tau_1 = -\left[\vec{p} + \frac{e}{c}\vec{A}\right]^2 (\tau_3 + i\tau_2) - mc^2\tau_3 + e\Phi = -\hat{H}(-e) \tag{15.75}$$

This means that, if Ψ solves the equation

$$i\hbar \frac{\partial \Psi}{\partial t} = \hat{H}(e)\Psi \tag{15.76}$$

we have

$$-i\hbar \frac{\partial \Psi^*}{\partial t} = \hat{H}^*(e)\Psi^* = -\tau_1 \hat{H}(-e)\tau_1 \Psi^* \tag{15.77}$$

Multiplying by τ_1 we get

$$i\hbar \frac{\partial \Psi_c}{\partial t} = \hat{H}(-e)\Psi_c \tag{15.78}$$

which is the two-component statement of the fact that Ψ_c solves the Klein-Gordon equation with the opposite sign of the charge.

What can we say about the two-component solutions for free particles and antiparticles?

The wave function of a free particle (positive energy solution) of momentum $\vec{p}$ (normalized to 1) is given by

$$\psi_{\vec{p}}^{(+)}(\vec{r},t) = \sqrt{\frac{mc^2}{E_{\vec{p}}}} e^{i(\vec{p}\cdot\vec{r} - E_{\vec{p}}t)/\hbar} \tag{15.79}$$

where

$$E_{\vec{p}} = \sqrt{p^2c^2 + m^2c^4} \tag{15.80}$$

Using

$$\psi^0(\vec{r},t) = \left(\frac{\partial}{\partial t} + \frac{ie}{\hbar}\Phi(\vec{r},t)\right)\psi(\vec{r},t) \tag{15.81}$$

and

$$\phi = \frac{1}{2}\left[\psi + \frac{i\hbar}{mc^2}\psi^0\right] \quad , \quad \chi = \frac{1}{2}\left[\psi - \frac{i\hbar}{mc^2}\psi^0\right] \tag{15.82}$$

we find (in two-component language)

$$\Psi^{(+)}_{\vec{p}}(\vec{r},t) = \Psi^{(+)}_{\vec{p}} e^{i(\vec{p}\cdot\vec{r}-E_{\vec{p}}t)/\hbar} \tag{15.83}$$

where the two-component vector $\Psi^{(+)}_{\vec{p}}$ is given by

$$\Psi^{(+)}_{\vec{p}} = \frac{1}{2\sqrt{E_{\vec{p}}mc^2}} \begin{pmatrix} mc^2 + E_{\vec{p}} \\ mc^2 - E_{\vec{p}} \end{pmatrix} \tag{15.84}$$

In a similar manner, we can write for the negative energy solutions (free antiparticles)

$$\psi^{(-)}_{\vec{p}}(\vec{r},t) = \sqrt{\frac{mc^2}{E_{\vec{p}}}} e^{-i(\vec{p}\cdot\vec{r}-E_{\vec{p}}t)/\hbar} \tag{15.85}$$

$$\Psi^{(-)}_{\vec{p}}(\vec{r},t) = \Psi^{(-)}_{\vec{p}} e^{-i(\vec{p}\cdot\vec{r}-E_{\vec{p}}t)/\hbar} \tag{15.86}$$

$$\Psi^{(-)}_{\vec{p}} = \frac{1}{2\sqrt{E_{\vec{p}}mc^2}} \begin{pmatrix} mc^2 - E_{\vec{p}} \\ mc^2 + E_{\vec{p}} \end{pmatrix} = \tau_1 \Psi^{(+)}_{\vec{p}} \tag{15.87}$$

We note that in the nonrelativistic limit

$$E_{\vec{p}} = \sqrt{p^2c^2 + m^2c^4} = mc^2\left(1 + \frac{p^2}{m^2c^2}\right)^{1/2} \approx mc^2\left(1 + \frac{p^2}{2m^2c^2}\right) \tag{15.88}$$

$$mc^2 \pm E_{\vec{p}} \approx \begin{cases} 2mc^2 \\ -p^2/2m \end{cases} \tag{15.89}$$

so that

$$\Psi_{\vec{p}}^{(+)} = \begin{pmatrix} 1 \\ -v^2/4c^2 \end{pmatrix} \quad , \quad \Psi_{\vec{p}}^{(-)} = \begin{pmatrix} -v^2/4c^2 \\ 1 \end{pmatrix} \tag{15.90}$$

This shows that in the nonrelativistic limit

$$\chi \text{ is } \approx v^2/c^2 \text{ times } \phi \text{ for a particle} \tag{15.91}$$

If we drop χ, then ϕ satisfies the nonrelativistic Schrodinger equation with the constant mc^2 included in the energy.

Similarly, dropping ϕ in the antiparticle solution shows that χ satisfies the nonrelativistic Schrodinger equation for the opposite charge with the constant mc^2 included in the energy.

The particle and antiparticle solutions are orthogonal in the sense that

$$\Psi_{\vec{p}}^{(+)}\tau_3\Psi_{\vec{p}}^{(-)} = 0 = \Psi_{\vec{p}}^{(-)}\tau_3\Psi_{\vec{p}}^{(+)} \tag{15.92}$$

which should be the case since they represent different energy eigenstates of the same Hamiltonian.

The free particle solutions form a complete set since any wave function Ψ can be expanded as a linear combination of the free particle and antiparticle solutions.

We first write Ψ as a Fourier transform

$$\Psi(\vec{r},t) = \int \frac{d^3p}{(2\pi\hbar)^3} e^{i\vec{p}\cdot\vec{r}/\hbar} \begin{pmatrix} \phi_{\vec{p}} \\ \chi_{\vec{p}} \end{pmatrix} \tag{15.93}$$

Since the two vectors $\Psi_{\vec{p}}^{(+)}$ and $\Psi_{\vec{p}}^{(-)}$ are linearly independent, we can write

$$\Psi_{\vec{p}}(t) = \begin{pmatrix} \phi_{\vec{p}} \\ \chi_{\vec{p}} \end{pmatrix} = u_{\vec{p}}(t)\Psi_{\vec{p}}^{(+)} + v_{-\vec{p}}^{*}(t)\Psi_{-\vec{p}}^{(-)} \tag{15.94}$$

Good reasons for the choice of $-\vec{p}$ and $*$ will appear shortly.

Substituting we get

$$\begin{aligned}\Psi(\vec{r},t) &= \int \frac{d^3p}{(2\pi\hbar)^3} e^{i\vec{p}\cdot\vec{r}/\hbar}\left[u_{\vec{p}}(t)\Psi_{\vec{p}}^{(+)} + v_{-\vec{p}}^{*}(t)\Psi_{-\vec{p}}^{(-)}\right] \\ &= \int \frac{d^3p}{(2\pi\hbar)^3}\left[u_{\vec{p}}(t)\Psi_{\vec{p}}^{(+)}e^{i\vec{p}\cdot\vec{r}/\hbar} + v_{\vec{p}}^{*}(t)\Psi_{\vec{p}}^{(-)}e^{-i\vec{p}\cdot\vec{r}/\hbar}\right]\end{aligned} \tag{15.95}$$

where a change of variables was made in the second term.

From the form of this result, $u_{\vec{p}}(t)$ is the amplitude for a particle in the state Ψ to have momentum $\vec{p}$ and positive charge and $v_{\vec{p}}(t)$ is the amplitude for a particle in the state Ψ to have momentum $\vec{p}$ and negative charge.

Using the orthonormality of $\Psi_{\vec{p}}^{(\pm)}$ we get

$$u_{\vec{p}}(t) = \int d^3r \Psi_{\vec{p}}^{(+)+} e^{-i\vec{p}\cdot\vec{r}/\hbar} \tau_3 \Psi(\vec{r}, t) \tag{15.96}$$

$$v_{\vec{p}}^*(t) = -\int d^3r \Psi_{\vec{p}}^{(-)+} e^{i\vec{p}\cdot\vec{r}/\hbar} \tau_3 \Psi(\vec{r}, t) \tag{15.97}$$

The normalization integral for Ψ then becomes

$$\int \frac{d^3p}{(2\pi\hbar)^3} \left(\left|u_{\vec{p}}\right|^2 - \left|v_{\vec{p}}\right|^2 \right) = \pm 1 \tag{15.98}$$

This says that there is no restriction on the magnitude of either $u_{\vec{p}}$ or $v_{\vec{p}}$. Only the integral of the difference(above) is fixed.

Physically, we can then say that one can have a state with an arbitrarily large amplitude for finding a particle with a certain momentum, which is the first indication that we are dealing with *bosons* or that spin zero particles must be bosons.

We can write some expectation values in this formalism, i.e.,

$$\hat{H}_0 = \frac{p^2}{2m}(\tau_3 + i\tau_2)^2 + mc^2\tau_3 = \text{Kineticenergy} \tag{15.99}$$

$$\int \Psi^+(\vec{r})\tau_3\hat{H}_0\Psi(\vec{r})d^3r = \int \frac{d^3p}{(2\pi\hbar)^3}E_{\vec{p}}\left(\left|u_{\vec{p}}\right|^2 + \left|v_{\vec{p}}\right|^2\right) \tag{15.100}$$

and

$$\vec{p} = \frac{\hbar}{i}\nabla = \text{ momentum} \tag{15.101}$$

$$\int \Psi^+(\vec{r})\tau_3\left(\frac{\hbar}{i}\nabla\right)\Psi(\vec{r})d^3r = \int \frac{d^3p}{(2\pi\hbar)^3}\vec{p}\left(\left|u_{\vec{p}}\right|^2 + \left|v_{\vec{p}}\right|^2\right) \tag{15.102}$$

15.3 **Free Particles as Wave Packets**

A wave packet formed from the positive energy solutions is given by

$$\Psi^{(+)}(\vec{r}, t) = \int \frac{d^3p}{(2\pi\hbar)^3}\, u_{\vec{p}} e^{i(\vec{p}\cdot\vec{r} - E_{\vec{p}}t)/\hbar} \Psi^{(+)}_{\vec{p}} \tag{15.103}$$

Let us assume that $u_{\vec{p}}$ is peaked about $\vec{p} = \vec{p}\,'$. Then, using arguments similar to our earlier discussions on stationary phase, the center of the wave packet moves with a group velocity

$$\vec{v}_g = \left(\nabla_{\vec{p}} E_{\vec{p}}\right)_{\vec{p}=\vec{p}\,'} = \frac{\vec{p}\,' c^2}{E_{\vec{p}\,'}} \tag{15.104}$$

and similarly for a free wave packet made of the negative energy solutions for antiparticles.

Can we construct a free particle wave packet perfectly localized at the origin? It would have the form

$$\Psi(\vec{r}) = \begin{pmatrix} a \\ b \end{pmatrix} \delta(\vec{r}) \tag{15.105}$$

We then have

$$\begin{aligned} u_{\vec{p}} &= \int d^3r \Psi_{\vec{p}}^{(+)+} e^{-i\vec{p}\cdot\vec{r}/\hbar} \tau_3 \Psi(\vec{r}) \\ &= \int d^3r \Psi_{\vec{p}}^{(+)+} e^{-i\vec{p}\cdot\vec{r}/\hbar} \tau_3 \begin{pmatrix} a \\ b \end{pmatrix} \delta(\vec{r}) = \Psi_{\vec{p}}^{(+)+} \tau_3 \begin{pmatrix} a \\ b \end{pmatrix} \\ &= \frac{1}{2\sqrt{E_{\vec{p}} mc^2}} \begin{pmatrix} mc^2 + E_{\vec{p}} \\ mc^2 - E_{\vec{p}} \end{pmatrix}^+ \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} \\ &= \frac{E_{\vec{p}}(a+b) + mc^2(a-b)}{2\sqrt{E_{\vec{p}} mc^2}} \end{aligned} \tag{15.106}$$

and similarly

$$v_{\vec{p}}^* = -\Psi_{\vec{p}}^{(-)+} \tau_3 \begin{pmatrix} a \\ b \end{pmatrix} = \frac{E_{\vec{p}}(a+b) - mc^2(a-b)}{2\sqrt{E_{\vec{p}} mc^2}} \tag{15.107}$$

Looking at these results we can see that independent of the choice of a and b, the wave packet will always have both particle and antiparticle components. This means that it is impossible to construct a perfectly localized wave packet from positive energy solutions alone.

Suppose that we take a general wave packet made up of positive energy solutions and try to squeeze it(make it more localized) with real-world devices such as collimators. To see what might happen we multiply the wave packet by the position operator $\vec{r}$. We then have

$$\begin{aligned} \vec{r}\Psi^{(+)}(\vec{r},t) &= \int \frac{d^3p}{(2\pi\hbar)^3} u_{\vec{p}}(t)\Psi^{(+)}_{\vec{p}}\vec{r}e^{i\vec{p}\cdot\vec{r}/\hbar} \\ &= \int \frac{d^3p}{(2\pi\hbar)^3} u_{\vec{p}}(t)\Psi^{(+)}_{\vec{p}}\frac{\hbar}{i}\nabla_{\vec{p}}e^{i\vec{p}\cdot\vec{r}/\hbar} \end{aligned} \tag{15.108}$$

Integrating by parts we have

$$\vec{r}\Psi^{(+)}(\vec{r},t) = \int \frac{d^3p}{(2\pi\hbar)^3}(i\hbar\nabla_{\vec{p}}u_{\vec{p}}(t))\Psi^{(+)}_{\vec{p}}e^{i\vec{p}\cdot\vec{r}/\hbar} + \int \frac{d^3p}{(2\pi\hbar)^3}u_{\vec{p}}(t)(i\hbar\nabla_{\vec{p}}\Psi^{(+)}_{\vec{p}})e^{i\vec{p}\cdot\vec{r}/\hbar} \quad (15.109)$$

Using

$$\nabla_{\vec{p}}\Psi^{(\pm)}_{\vec{p}} = -\frac{\vec{p}c^2}{2E^2_{\vec{p}}}\Psi^{(\mp)}_{\vec{p}} \quad (15.110)$$

we get

$$\vec{r}\Psi^{(+)}(\vec{r},t) = \vec{r}_+\Psi^{(+)}(\vec{r},t) + \vec{r}_-\Psi^{(+)}(\vec{r},t) \quad (15.111)$$

where

$$\vec{r}_+\Psi^{(+)}(\vec{r},t) = \int \frac{d^3p}{(2\pi\hbar)^3}(i\hbar\nabla_{\vec{p}}u_{\vec{p}}(t))\Psi^{(+)}_{\vec{p}}e^{i\vec{p}\cdot\vec{r}/\hbar} \quad (15.112)$$

$$\vec{r}_-\Psi^{(+)}(\vec{r},t) = -\int \frac{d^3p}{(2\pi\hbar)^3}u_{\vec{p}}(t)\frac{i\hbar\vec{p}c^2}{2E^2_{\vec{p}}}\Psi^{(-)}_{\vec{p}}e^{i\vec{p}\cdot\vec{r}/\hbar} \quad (15.113)$$

This says that multiplying a wave packet of positive energy states by the position operator mixes in negative energy solutions, i.e.,

> $\vec{r}_+$ generates positive energy solutions while $\vec{r}_-$
> generates negative energy solutions
> or changes free particles in free antiparticles and vices versa

The same result occurs for any function of the position operator.

Suppose that $\vec{r}\Psi^{(+)}(\vec{r}) = \vec{r}_0\Psi^{(+)}(\vec{r})$, i.e., it is an eigenstate of $\vec{r}$ with eigenvalue $\vec{r}_0$. This says that

$$i\hbar\nabla_{\vec{p}}u_{\vec{p}} = \vec{r}_0 u_{\vec{p}} \rightarrow u_{\vec{p}} = e^{-i\vec{p}\cdot\vec{r}_0/\hbar} \tag{15.114}$$

and the state

$$\Psi^{+}_{\vec{r}_0}(\vec{r}) = \int \frac{d^3p}{(2\pi\hbar)^3} e^{i\vec{p}\cdot(\vec{r}-\vec{r}_0)/\hbar}\Psi^{(+)}_{\vec{p}} \tag{15.115}$$

is an eigenstate of $\vec{r}_+$.

This eigenstate is not normalizable. It is large over a region of space within $\hbar/mc$ (a Compton wavelength) of $\vec{r}_0$ or, in other words, the theory with positive energy solutions cannot describe particles localized to a region smaller than a Compton wavelength.

The presence of the $\vec{r}_-$ part in the position operator says that putting a wave packet made from positive energy solutions (a particle) through a potential $\Phi(\vec{r})$ (which multiplies by functions of r) causes the creation of antiparticles and because charge must be conserved, creates new particles also.

Thus, the relativistic spin-zero theory of the Klein-Gordon equation has built into it the mechanism of particle-antiparticle production by external potentials.

An example of this phenomenon is *Klein's paradox*. Suppose we have a beam of positively charged particles with momentum p hitting an electrostatic potential barrier of height $e\varphi$ from the left as shown in the figure below.

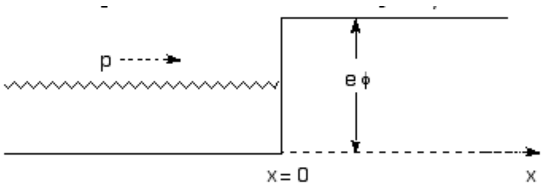

Figure: Electrostatic Potential Barrier - Klein Paradox

The solution follows the same lines as the nonrelativistic problem. For $x < 0$ we have

$$\psi(x) = ae^{ipx/\hbar} + be^{-ipx/\hbar} \quad , \text{ Energy } = E_p \tag{15.116}$$

This corresponds to incident and reflected waves. For $x > 0$, the Klein-Gordon equation is

$$(E_p - V)^2\psi(x) = -\hbar^2 c^2 \frac{\partial^2\psi(x)}{\partial x^2} + mc^2\psi(x) \quad , \quad V = e\varphi \tag{15.117}$$

The solution takes the form $\psi(x) = de^{ikx}$ where substitution gives

$$(E_p - V)^2 = \hbar^2 c^2 k^2 + m^2 c^4 \tag{15.118}$$

We have the boundary conditions at $x = 0$ (since potential only has a finite discontinuity)

$$\psi(x) \ , \ \frac{\partial \psi}{\partial x} \text{ continuous} \tag{15.119}$$

Note that ψ^0 is given by

$$\psi^0(\vec{r}, t) = \left(\frac{\partial}{\partial t} + \frac{ie}{\hbar} \Phi(\vec{r}, t) \right) \psi(\vec{r}, t) \tag{15.120}$$

is not continuous at $x = 0$.

We obtain

$$b = \frac{p - \hbar k}{p + \hbar k} a \quad , \quad d = \frac{2p}{p + \hbar k} a \tag{15.121}$$

We consider three cases:

1. If $E_p > V + mc^2$, then the particle can pass the over the barrier and the results are identical to the nonrelativistic case, i.e., part of the wave is reflected and part is transmitted.

2. If we have a stronger potential such that $E_p + mc^2 > V > E_p - mc^2$, then k must be imaginary so that the wave function goes to zero as $x \to \infty$. We then have

$$k = i\kappa \to \kappa = \frac{\sqrt{m^2c^4 - (E_p - V)^2}}{\hbar c} \tag{15.122}$$

and the wave is totally reflected at the barrier. The charge density on the right $(x > 0)$ is given by

$$\rho(x) = \frac{E_p - V}{2mc^2} \left|d\right|^2 e^{-2\kappa x} \tag{15.123}$$

For $E_p > V$, there exists a positive, exponentially decaying charge density to the right of the barrier.

For $E_p < V$, however, the density is *negative* (remember it is a beam of positive particles). We reflect positively charged particles from the barrier and find negative particles inside the barrier.

3. We make the potential even stronger so that $V > E_p + mc^2$. Nonrelativistically it would be even more impossible for the particles to pass over the barrier. In the relativistic case, however, k is real again, This says that once again there is a particle current to the right of the barrier. The group velocity of the waves for $x > 0$ is

$$v_g = \frac{\partial E_p}{\partial(\hbar k)} \tag{15.124}$$

Using $(E_p - V)^2 = \hbar^2 c^2 k^2 + m^2 c^4$ we get

$$(E_p - V)\frac{\partial E_p}{\partial k} = \hbar c^2 k \rightarrow v_g = \frac{\hbar c^2 k}{E_p - V} \tag{15.125}$$

Since $E_p - V < 0$, we must have $k < 0$ (negative!) in order to have a wave(packet) traveling from the barrier towards positive x.

This says that the reflection coefficient b/a is greater than one, i.e., more wave is reflected than is incident! In addition, the charge density on the right is

$$\rho(x) = \frac{E_p - V}{2mc^2} |d|^2 < 0 \tag{15.126}$$

and the current on the right is negative.

One possible explanation is to say that the incident particle induces the creation of particle-antiparticle pairs at the barrier. The created antiparticles, having the opposite charge, find $x > 0$ a region of attractive potential and thus travel towards the right, which explains the negative current on the right. The created particles travel to the left and together with the incident particles (wave) which are(is) totally reflected, they add up to an outgoing current on the left that is larger than the incident current.

The total outgoing current on the left and right equals the incident current since total charge must be conserved.

This pair creation solution does not violate conservation of energy. The energy of a created particle on the left is E_p. The energy of a created antiparticle on the right is $\sqrt{\hbar^2 c^2 k^2 + m^2 c^4} - V$ since the electrostatic potential energy has the opposite sign for a particle of opposite charge.

Adding the two energies we get $E_p + \sqrt{\hbar^2 c^2 k^2 + m^2 c^4} - V = 0$, i.e., it takes zero energy to create a particle-antiparticle pair. This happens because the potential V is so large that the energy of the antiparticle on the right is not only less than mc^2 but is negative.

15.4 **Bound State Problems**

We now study the bound states of spin zero relativistic particles in a static potential $\Phi(\vec{r})$. For a positively charged particle with energy E the bound state wave function is

$$\psi(\vec{r}, t) = e^{-iEt/\hbar}\psi(\vec{r}) \tag{15.127}$$

and the charge density of the bound state particle is

$$e\rho(\vec{r}) = \frac{e\left[E - e\Phi(\vec{r})\right]}{mc^2} \left|\psi(\vec{r})\right|^2 \tag{15.128}$$

This says that in regions where $E > e\Phi(\vec{r})$, which includes classically accessible regions, the charge density is positive. But, in regions where $E < e\Phi(\vec{r})$, the charge density is negative. The way to think about this is to say the particle in the potential is a linear combination of free particle and free antiparticle states.

Because we are considering an electrostatic potential, the positively charged parts will be found mainly in regions of smaller $e\Phi(\vec{r})$ while the negatively charged parts will be found in regions of larger $e\Phi(\vec{r})$. A relativistic particle seems to have an internal structure that can be polarized by and electric field.

Alternatively, we might say that the potential produces particle-antiparticle pairs in the vacuum, The positively charged particles are attracted to regions of smaller $e\Phi(\vec{r})$ while the negatively charged particles are attracted to regions of larger $e\Phi(\vec{r})$. We say that the electric potential has *polarized* the vacuum. This polarization modifies the effective potential felt by the bound particle.

This interaction cannot be taken into account in the present one-particle relativistic theory(requires quantum field theory).

We now turn to the problem of a spin zero particle bound in a Coulomb potential. An example is a π^- bound to a nucleus. We have

$$e\Phi(\vec{r}) = -\frac{Ze^2}{r} \tag{15.129}$$

which leads to the Klein-Gordon equation

$$\left[\left(E + \frac{Ze^2}{r}\right)^2 + \hbar^2 c^2 \nabla^2 - mc^2\right] \psi(\vec{r}) = 0 \tag{15.130}$$

Since this is a central potential, we can assume that the eigenstates have definite values of total orbital angular momentum. We then have

$$\left[\left(\frac{E^2}{c^2} - m^2 c^2\right) + \hbar^2 \left(\frac{1}{r}\frac{\partial^2}{\partial r^2} r - \frac{\ell(\ell+1) - (Z\alpha)^2}{r^2}\right) + \frac{2Ze^2}{r}\frac{E}{c}\right] \psi(r) = \tag{15.131}$$

or

$$\left[-\frac{1}{r}\frac{\partial^2}{\partial r^2} r + \frac{\ell(\ell+1) - (Z\alpha)^2}{r^2} - \frac{2Z\alpha E}{\hbar c r} - \left(\frac{E^2 - m^2 c^4}{\hbar^2 c^2}\right)\right] \psi(r) = 0 \tag{15.132}$$

where

$$\alpha = \frac{e^2}{\hbar c} = \text{ fine structure constant} \tag{15.133}$$

Now we define

$$\gamma = Z\alpha \quad , \quad \ell'(\ell'+1) = \ell(\ell+1) - \gamma^2$$
$$\lambda = \frac{2E\gamma}{\hbar c\sigma} \quad , \quad \frac{4(m^2c^4 - E^2)}{\hbar^2 c^2} = \sigma^2 \quad , \quad \rho = \sigma r$$

and we get

$$\left[\frac{d^2}{d(\rho/2)^2} + \frac{2\lambda}{\rho/2} - 1 + \frac{\ell'(\ell'+1)}{(\rho/2)^2}\right]\rho\psi(\rho) = 0 \qquad (15.134)$$

which is identical to the radial equation for the nonrelativistic Coulomb problem for the function $u = \rho\psi(\rho)$. The difference is that ℓ' is not necessarily an integer (remember that it is an integer in the nonrelativistic problem), which causes the orbits of the relativistic Coulomb (Kepler) problem to no longer be closed, i.e., the orbits precess.

This also means that the extra degeneracy of the nonrelativistic problem which causes the energy to be independent of ℓ is broken in the relativistic problem. We now solve this equation in the standard way. For

$$\rho \to 0 \qquad \psi(\rho) \to \rho^{\ell'}$$
$$\rho \to \infty \qquad \psi(\rho) \to e^{-\rho/2}$$

Therefore, we guess a solution of the form

$$u = \rho\psi(\rho) = \left(\frac{\rho}{2}\right)^{\ell'+1} e^{-\rho/2} w(\rho/2) \tag{15.135}$$

The solution method is identical to the nonrelativistic hydrogen atom. We get a power series which must terminate (so that the solution is normalizable) when

$$\lambda = N + \ell' + 1 \quad , \quad N = 0, 1, 2, 3, ...$$

$$E = mc^2 \left(1 + \frac{\gamma^2}{\lambda^2}\right)^{-1/2} \rightarrow E = \frac{mc^2}{\sqrt{1 + \frac{\gamma^2}{\left[N + \frac{1}{2} + \sqrt{(\ell + \frac{1}{2})^2 - \gamma^2}\right]^2}}} \tag{15.136}$$

If we define the principal quantum number $n = N + \ell + 1 =$ integer, then we have

$$E_{n\ell} = \frac{mc^2}{\sqrt{1 + \frac{\gamma^2}{\left[n - (\ell + \frac{1}{2}) + \sqrt{(\ell + \frac{1}{2})^2 - \gamma^2}\right]^2}}} \tag{15.137}$$

The principal quantum number has the possible values $n = 1, 2, 3, ...$ For a given n the possible values of the total orbital angular momentum are $\ell = 0, 1, 2, 3, ..., n - 1$.

The degeneracy that was present in the nonrelativistic theory with respect to orbital angular momentum ℓ is clearly removed.

If we expand the energy in a power series in the fine structure constant α (or γ) we get

$$E_{n\ell} = mc^2 - Ry\frac{1}{n^2} - Ry\frac{\gamma^2}{n^3}\left(\frac{1}{\ell+\frac{1}{2}} - \frac{3}{4n}\right) + O(Ry\gamma^4) \quad (15.138)$$

The first term is the rest energy. The second term is the nonrelativistic Rydberg formula. The third term is the relativistic correction due to using the relativistic form of the kinetic energy, which as we saw earlier in Chapter 10 took the form

$$\hat{H}_{rel} = -\frac{p^4}{8m^3c^2} \quad (15.139)$$

It is this correction that removes the degeneracy in ℓ, i.e.,

$$E_{n,\ell=0} - E_{n,\ell=n-1} = Ry\frac{4\gamma^2}{n^3}\frac{n-1}{2n-1} \quad (15.140)$$

As we shall see later when we derive the Dirac equation, there are more corrections to this formula due to the fact that the electron has spin = 1/2.

15.4.1 **Nonrelativistic Limit**

The Klein-Gordon equation in the presence of an electromagnetic field is

$$\frac{1}{c^2}\left(i\hbar\frac{\partial}{\partial t}-e\Phi(\vec{r},t)\right)^2\psi(\vec{r},t)=\left(\left(\frac{\hbar}{i}\nabla-\frac{e}{c}\vec{A}(\vec{r},t)\right)^2+m^2c^2\right)\psi(\vec{r},t) \tag{15.141}$$

and using

$$\psi(\vec{r},t)=\begin{pmatrix}\phi(\vec{r},t)\\ \chi(\vec{r},t)\end{pmatrix} \tag{15.142}$$

we have as earlier

$$\left(i\hbar\frac{\partial}{\partial t}-e\Phi\right)\phi=\frac{1}{2m}\left[\frac{\hbar}{i}\nabla-\frac{e}{c}\vec{A}\right]^2\phi+mc^2\phi+\frac{1}{2m}\left[\frac{\hbar}{i}\nabla-\frac{e}{c}\vec{A}\right]^2\chi \tag{15.143}$$

$$\left(i\hbar\frac{\partial}{\partial t} - e\Phi\right)\chi = -\frac{1}{2m}\left[\frac{\hbar}{i}\nabla - \frac{e}{c}\vec{A}\right]^2(\phi+\chi) - mc^2\chi \quad (15.144)$$

Remember that in the nonrelativistic limit the dominant term in the energy will be mc^2 so that we expect the zeroth order equation for χ to be

$$i\hbar\frac{\partial\chi}{\partial t} = mc^2\chi \quad (15.145)$$

which then implies in the next approximation that

$$\chi = -\frac{1}{4m^2c^2}\left[\frac{\hbar}{i}\nabla - \frac{e}{c}\vec{A}\right]^2\phi \quad (15.146)$$

and that ϕ satisfies the equation

$$\left(i\hbar\frac{\partial}{\partial t} - e\Phi\right)\phi = \frac{1}{2m}\left[\frac{\hbar}{i}\nabla - \frac{e}{c}\vec{A}\right]^2\phi + mc^2\phi - \frac{1}{8m^3c^2}\left[\frac{\hbar}{i}\nabla - \frac{e}{c}\vec{A}\right]^4\phi \quad (15.147)$$

The operator on the right-hand side is just the kinetic energy operator

$$\sqrt{m^2c^4 + c^2\left(\frac{\hbar}{i}\nabla - \frac{e}{c}\vec{A}\right)^2} \tag{15.148}$$

expanded to second order in $1/mc^2$. This agrees with our earlier result that the first relativistic correction for a spinless particle is entirely due to the relativistic modification of the kinetic energy.

For a weak magnetic field $\vec{B}$ this becomes (to order $(v/c)^3$) after much algebra

$$i\hbar\frac{\partial\phi}{\partial t} = -\frac{\hbar^2\nabla^2}{2m}\left[1 + \frac{\hbar^2\nabla^2}{2m^2c^2}\right]\phi + (mc^2 + e\Phi)\phi - \frac{e}{2mc}\vec{B}\cdot\vec{L}\left[1 + \frac{\hbar^2\nabla^2}{2m^2c^2}\right]\phi \tag{15.149}$$

where $\vec{L}$ is the orbital angular momentum of the particle. The term

$$\left[1 + \frac{\hbar^2\nabla^2}{2m^2c^2}\right] \rightarrow \left[1 - \frac{p^2}{2m^2c^2}\right] \tag{15.150}$$

represents the relativistic correction to the magnetic moment.

15.5 Relativistic Spin 1/2 Particles - The Dirac Equation

15.5.1 Lorentz Transformation of Spin

The contravariant and covariant components of the position 4-vector in spacetime are:

$$x^\mu: \quad x^0 = ct \quad , \quad x^1 = x \quad , \quad x^2 = y \quad , \quad x^3 = z$$
$$x_\mu: \quad x^0 = ct \quad , \quad x_1 = -x \quad , \quad x_2 = -y \quad , \quad x_3 = -z$$

The flat spacetime metric tensor is defined by

$$g = (g_{\mu\nu}) = (g^{\mu\nu}) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \tag{15.151}$$

The metric tensor relates covariant and contravariant components by

$$x_\mu = g_{\mu\nu} x^\nu \quad , \quad x^\mu = g^{\mu\nu} x_\nu \tag{15.152}$$

We also have

$$g^\mu_\nu = g^{\mu\alpha} g_{\alpha\nu} \equiv \delta^\mu_\nu \quad , \quad (\delta^\mu_\nu) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \tag{15.153}$$

Under the action of a Lorentz transformation along the z-axis with velocity $v = \beta c$, a 4-vector (any type) since it is a first-rank tensor, transforms as

$$V'^\mu = \Lambda^\mu_\nu V^\nu \tag{15.154}$$

where

$$(\Lambda^\mu_\nu) = \begin{pmatrix} \gamma & 0 & 0 & -\beta\gamma \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ -\beta\gamma & 0 & 0 & \gamma \end{pmatrix} \quad , \quad \gamma = \frac{1}{\sqrt{1-\beta^2}} \quad , \quad \beta = \frac{v}{c} \tag{15.155}$$

This corresponds to the standard transformation relations for the position and momentum 4-vectors

$$ct' = \gamma(ct - \beta z)\ ,\ x' = x\ ,\ y' = y\ ,\ z' = \gamma(z - \beta ct)$$
$$\frac{E'}{c} = \gamma\left(\frac{E}{c} - \beta p_z\right)\ ,\ p'_x = p_x\ ,\ p'_y = p_y\ ,\ p'_z = \gamma\left(p_z - \beta\frac{E}{c}\right)$$

Spin is an angular momentum corresponding to internal degrees of freedom of the system. This means, as we showed earlier, that spin must have the same transformation properties as any other angular momentum.

Nonrelativistically, we think of angular momentum as a vector and, in fact, under a simple spatial rotation it does transform as a vector (as we saw earlier). Consider, however, the behavior of an orbital angular momentum

$$\vec{L} = \vec{r} \times \vec{p} \rightarrow L_i = \varepsilon_{ijk} x_j p_k \tag{15.156}$$

under the action of a Lorentz transformation along the $z-$direction. We find that

$$L'_z = x'p'_y - y'p'_x = xp_y - yp_x = L_z \tag{15.157}$$

since the components of vectors orthogonal to the $z-$axis are unchanged. This is clearly not the transformation property of a vector.

In fact, $\vec{L}$ is the product of two vectors and therefore should have the transformation properties of a second-rank tensor, i.e., as

$$Q'^{\,\mu\nu} = \Lambda^\mu_\alpha \Lambda^\nu_\beta Q^{\alpha\beta} \tag{15.158}$$

Relativistic electrodynamics can be written in terms of a second-rank field tensor

$$(\, F^{\mu\nu}) = \begin{pmatrix} 0 & \varepsilon_1 & \varepsilon_2 & \varepsilon_3 \\ -\varepsilon_1 & 0 & B_3 & -B_2 \\ -\varepsilon_2 & -B_3 & 0 & B_1 \\ -\varepsilon_3 & B_2 & -B_1 & 0 \end{pmatrix} \tag{15.159}$$

as Maxwell's equations

$$\frac{\partial F^{\mu\nu}}{\partial x^\mu} = \frac{4\pi}{c} J^\nu$$
$$\frac{\partial F^{\mu\nu}}{\partial x^\alpha} + \frac{\partial F^{\nu\alpha}}{\partial x^\mu} + \frac{\partial F^{\alpha\mu}}{\partial x^\nu} = 0$$

where the current density 4-vector is

$$J^\mu = (c\rho, J_x, J_y, J_z) \tag{15.160}$$

and the Lorentz force law is

$$\frac{dp^\mu}{d\tau} = \frac{q}{m} p_\nu F^{\mu\nu} \tag{15.161}$$

The transformation rule then says that the fields transform according to the relations

$$F'^{\,01} = \varepsilon_1' = \Lambda^\mu_\alpha \Lambda^\nu_\beta F^{\alpha\beta} = \Lambda^0_\alpha \Lambda^1_\beta F^{\alpha\beta} = \Lambda^0_\alpha \Lambda^1_1 F^{\alpha 1} = \Lambda^0_\alpha F^{\alpha 1}$$
$$= \Lambda^0_0 F^{01} + \Lambda^0_3 F^{31} = \gamma\varepsilon_1 - \beta\gamma B_2 = \gamma(\varepsilon_1 - ((\vec{v}/c) \times \vec{B})_1)$$

or

$$\varepsilon_1' = \gamma(\varepsilon_1 + ((\vec{v}/c) \times \vec{B})_1) \text{ where } \vec{v} = v\hat{e}_z \tag{15.162}$$

Similarly, we find

$$\varepsilon_2' = \gamma(\varepsilon_2 + ((\vec{v}/c) \times \vec{B})_2) \ , \ \varepsilon_3' = \varepsilon_3$$
$$B_1' = \gamma(B_1 - ((\vec{v}/c) \times \vec{\varepsilon})_1) \ , \ B_2' = \gamma(B_2 - ((\vec{v}/c) \times \vec{\varepsilon})_2) \ , \ B_3' = B_3$$

We can summarize these results for an arbitrary (direction) Lorentz transformation applied to a second-rank tensor by

$$B_{||}' = B_{||} \quad , \quad \varepsilon_{||}' = \varepsilon_{||} \ \ || = \text{ component parallel to } \vec{v}$$
$$\vec{B}_\perp' = \gamma\left(\vec{B}_\perp - (\vec{v}/c) \times \vec{\varepsilon}\right)$$
$$\vec{\varepsilon}_\perp' = \gamma\left(\vec{\varepsilon}_\perp + (\vec{v}/c) \times \vec{B}\right) \ \ \perp = \text{ component perpendicular to } \vec{v}$$

Thus, a pure magnetic field in one frame is a mixture of magnetic and electric fields in the new frame.

Now, under a spatial inversion transformation, we have

$$\vec{\varepsilon} \to -\vec{\varepsilon} \quad , \quad \vec{B} \to \vec{B}$$
$$\vec{r} \to -\vec{r} \quad , \quad \vec{p} \to -\vec{p} \Rightarrow \vec{L} \to \vec{L}$$

Therefore, an angular momentum(including spin) has the same transformation properties as the magnetic field.

Since spin,

$$\bar{S} = \frac{1}{2}\vec{\sigma} \tag{15.163}$$

must transform as an angular momentum, which transforms like a magnetic field and the magnetic field is part of second-rank tensor with the electric field, we must conclude that there exists another set of dynamical variables generated by the internal degrees of freedom of the particle that will be analogous to the electric field. Do not think of the operator $\vec{\sigma}$ as the standard 2×2 Pauli matrices; we shall see later that $\vec{\sigma}$ will need to be represented by 4×4 matrices relativistically.

We define these new variables as $i\vec{\alpha}/2$ where the $i/2$ factor is chosen for later convenience. We then have that $\vec{S}$ and $i\vec{\alpha}/2$ or $\vec{\sigma}$ and $i\vec{\alpha}$ transform as $\vec{B}$ and $\vec{\varepsilon}$, i.e.,

$$\sigma'_{||} = \sigma_{||} \quad , \quad \vec{\sigma}'_{\perp} = \gamma\left(\vec{\sigma}_{\perp} - (\vec{v}/c) \times i\vec{\alpha}\right)$$
$$i\alpha'_{||} = i\alpha_{||} \quad , \quad i\vec{\alpha}'_{\perp} = \gamma\left(i\vec{\alpha}_{\perp} + (\vec{v}/c) \times \vec{\sigma}\right)$$

and they form a second-rank tensor $\sigma^{\mu\nu}$ analogous to $F^{\mu\nu}$, i.e.,

$$(\sigma^{\mu\nu}) = \begin{pmatrix} 0 & i\alpha_1 & i\alpha_2 & i\alpha_3 \\ -i\alpha_1 & 0 & \sigma_3 & -\sigma_2 \\ -i\alpha_2 & -\sigma_3 & 0 & \sigma_1 \\ -i\alpha_3 & \sigma_2 & -\sigma_1 & 0 \end{pmatrix} \qquad (15.164)$$

We must now investigate the dynamical properties of the new variables $\vec{\alpha}$ and also ask this question - where have these objects been hiding in all of previous discussions?

Since spin is an angular momentum, we know its algebraic properties (commutators). In addition, spin generates rotations of the internal degrees of freedom. Spin commutes with spatial degrees of freedom like $\vec{r}$ and $\vec{p}$ and, thus, so does $\vec{\alpha}$.

Since $\vec{\alpha}$ behaves like a vector under spatial rotations (it is like the electric field vector), it must have the standard commutation relations with $\vec{S}$

$$[\alpha_i, S_j] = i\varepsilon_{ijk}\alpha_k \to [\alpha_i, \sigma_j] = 2i\varepsilon_{ijk}\alpha_k \tag{15.165}$$

Since $\vec{\sigma}$ is angular momentum, it satisfies the relations

$$\sigma_i\sigma_j = i\varepsilon_{ijk}\sigma_k + \delta_{ij} \tag{15.166}$$

which must be true in all Lorentz frames, i.e., since $\sigma_1^2 = 1$, we must have $\sigma_1'^2 = 1$.

Let us now determine all the properties of $\vec{\alpha}$.

For a Lorentz transformation along the $z-$direction we have

$$\begin{aligned}\sigma_x' &= \gamma\,(\sigma_x + iv\alpha_y/c)\\ \sigma_y' &= \gamma\,(\sigma_y - iv\alpha_x/c)\end{aligned}$$

Squaring σ'_x we get

$$\sigma_x'^2 = 1 = \gamma^2 \left(\sigma_x^2 + iv(\sigma_x\alpha_y + \alpha_y\sigma_x)/c - \left(v/c\right)^2\right) \alpha_y^2\right)$$
$$= \gamma^2 \left(1 - \left(v/c\right)^2\right) \alpha_y^2\right) + \gamma^2 \left(iv(\sigma_x\alpha_y + \alpha_y\sigma_x)/c\right)$$

Since this must be true for all v, the coefficient of v/c must vanish. Thus,

$$\sigma_x\alpha_y + \alpha_y\sigma_x = 0 \tag{15.167}$$

We then have

$$1 = \gamma^2 \left(1 - \left(v/c\right)^2\right) \alpha_y^2\right) \tag{15.168}$$

Since

$$1 = \gamma^2 \left(1 - \left(v/c\right)^2\right) \alpha_y^2\right) \tag{15.169}$$

we must also have

$$\alpha_y^2 = 1 \tag{15.170}$$

These results generalize to the following:

$$i \neq j \qquad \sigma_i\alpha_j = -\alpha_j\sigma_i \tag{15.171}$$
$$i = j \qquad [\sigma_i, \alpha_i] = 0 \tag{15.172}$$

Multiplying σ'_y by σ'_x we get

$$\sigma'_x\sigma'_y = i\sigma'_z = i\sigma_z = \gamma^2\left(\sigma_x + iv\alpha_y/c\right)\left(\sigma_y - iv\alpha_x/c\right)$$
$$i\sigma_z = \gamma^2\left(\sigma_x\sigma_y + (v/c)^2\alpha_y\alpha_x + i(v/c)(\alpha_y\sigma_y - \sigma_x\alpha_x\right)$$

Multiplying σ'_x by σ'_y we get

$$\sigma'_y\sigma'_x = -i\sigma'_z = -i\sigma_z = \gamma^2\left(\sigma_y - iv\alpha_x/c\right)\left(\sigma_x + iv\alpha_y/c\right)$$
$$-i\sigma_z = \gamma^2\left(\sigma_y\sigma_x + (v/c)^2\alpha_x\alpha_y + i(v/c)(\sigma_y\alpha_y - \alpha_x\sigma_x\right)$$

Adding, we have

$$(\sigma_y\sigma_x + \sigma_x\sigma_y) + (v/c)^2(\alpha_x\alpha_y + \alpha_y\alpha_x) = 0$$
$$(\alpha_x\alpha_y + \alpha_y\alpha_x) = 0 \to (\alpha_i\alpha_j + \alpha_j\alpha_i) = 0 \quad i \neq j$$

Continuing, we find these other relations

$$\alpha_y\alpha_x = -i\sigma_z = -\alpha_x\alpha_y \to \alpha_i\alpha_j - \alpha_j\alpha_i = 2i\varepsilon_{ijk}\sigma_k \tag{15.173}$$

or summarizing we have

$$\{\alpha_i, \alpha_j\} = 2\delta_{ij} \quad , \quad [\alpha_i, \alpha_j] = 2i\varepsilon_{ijk}\sigma_k \tag{15.174}$$
$$[\alpha_i, \sigma_j] = 2i\varepsilon_{ijk}\alpha_k \quad , \quad \{\alpha_i, \sigma_j\} = 0 \quad , \quad i \neq j \tag{15.175}$$

So α obeys exactly the same algebraic relations as σ. How do we know that α is not equal to σ? If we apply a parity transformation, we find that $\vec{\sigma} \rightarrow \vec{\sigma}$ since angular momentum is unchanged by spatial inversion, i.e., the space-space components of a second-rank tensor do not change sign under parity. On the other hand, the time-space components such as the electric field or $i\vec{\alpha}$ do change sign, i.e., $\vec{\alpha} \rightarrow -\vec{\alpha}$. So they cannot be the same operator!

Let β be the operator that corresponds to the parity transformation in spin space. Now two successive inversions brings us back to the starting configuration. Remember, however, that the spin representation of rotations is doubled valued, i.e., a rotation by 2π produces a minus sign. We have a choice of letting the square of the parity operation include a 2π rotation(about any axis) or not. This means that we can have $\beta^2 = +1 \; or \; -1$.

In the first case, the eigenvalues of β are ± 1 and in the second case $\pm i$. We choose $\beta^2 = +1 \to \beta^{-1} = \beta$. The properties under parity become

$$\beta^{-1}\vec{\sigma}\beta = \vec{\sigma} \to \beta\vec{\sigma} = \vec{\sigma}\beta \tag{15.176}$$

$$\beta^{-1}\vec{\alpha}\beta = -\vec{\alpha} \to \beta\vec{\alpha} = -\vec{\alpha}\beta \tag{15.177}$$

We can now construct an explicit matrix representation for the operators $\vec{\alpha}$, β and $\vec{\sigma}$ similar to the two-dimensional Pauli matrix representation in the nonrelativistic case.

Consider the determinant of the matrix for $\beta^{-1}\alpha_i\beta$. Using $\beta\vec{\alpha} = -\vec{\alpha}\beta$ we have

$$\det(\beta^{-1}\alpha_i\beta) = \det(-\beta^{-1}\beta\alpha_i) = \det(-\alpha_i) = (-1)^N \det(\alpha_i) \tag{15.178}$$

where N is the dimension of the matrix representation. However, using the cyclic property of determinants, i.e.,

$$\det ABC = \det BCA = \det CAB \tag{15.179}$$

we get

$$\det(\beta^{-1}\alpha_i\beta) = \det(\beta\beta^{-1}\alpha_i) = \det(\alpha_i) \tag{15.180}$$

Putting these results together we get

$$(-1)^N \det(\alpha_i) = \det(\alpha_i) \to (-1)^N = 1 \to N = 2, 4, 6, ... \tag{15.181}$$

We have used the fact that $\det(\alpha_i) \neq 0$, since $\alpha_i^2 = 1$.

Now, $N = 2$ is not possible as we show below.

All 2×2 matrices can be constructed from the set $\{I, \vec{\sigma}\}$ and $[\beta, \vec{\sigma}] = 0$. This means that β would have to commute with all 2×2 matrices. Since $\vec{\alpha}$ would then have to commute with β, we would then violate the relation $\beta\vec{\alpha} = -\vec{\alpha}\beta$.

This means N must be at least as large as 4. This says that a relativistic spin 1/2 particle would have 4 internal states (the nonrelativistic case has 2). This is similar to the Klein-Gordon case and it will turn out here also that this doubling signals the appearance of antiparticles.

An explicit representation(not unique) using the 2×2 matrices

$$I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} , \tau_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} , \tau_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} , \tau_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

where the the last three matrices are the standard Pauli matrices. It is given by

$$\vec{\sigma} = \begin{pmatrix} \vec{\tau} & 0 \\ 0 & \vec{\tau} \end{pmatrix} , \vec{\alpha} = \begin{pmatrix} 0 & \vec{\tau} \\ \vec{\tau} & 0 \end{pmatrix} , \beta = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix} \qquad (15.182)$$

Note that the trace of each of these matrices is zero, which is a general property of matrices that obey anticommutation relations.

We can make the following physical interpretations of the components of the tensor $\sigma^{\mu\nu}$.

It follows from earlier discussions that the space-space components, i.e., the spin operators σ_j, generate (in the spin degrees of freedom) a rotation of the coordinate system.

This implies that the operators $\vec{\sigma}\,'$, $\vec{\alpha}\,'$, β' in a spatially rotated frame are given by the operator relations

$$\vec{\sigma}\,' = R_\varphi \vec{\sigma} R_\varphi^{-1} \ , \qquad \vec{\alpha}\,' = R_\varphi \vec{\alpha} R_\varphi^{-1} \ , \qquad \beta' = R_\varphi \beta R_\varphi^{-1} \tag{15.183}$$

where

$$R_\varphi = e^{-i\vec{\sigma}\cdot\hat{n}\varphi/2} \tag{15.184}$$

and

$$\hat{n} = \text{ unit vector in direction of axis of rotation}$$
$$\varphi = \text{ angle of rotation}$$

We then assume that time-space components generate a rotation of the space axes with the time axis, which is a Lorentz transformation and that the operators in the new frame are given by

$$\vec{\sigma}\,' = L_v \vec{\sigma} L_v^{-1} \ , \ \vec{\alpha}\,' = L_v \vec{\alpha} L_v^{-1} \ , \ \beta' = L_v \beta L_v^{-1} \tag{15.185}$$

where

$$L_v = e^{-i(i\vec{\alpha})\cdot\vec{\omega}/2} = e^{\vec{\alpha}\cdot\vec{\omega}/2} \to L_v^{-1} = e^{-\vec{\alpha}\cdot\vec{\omega}/2} \tag{15.186}$$

and

$$\begin{aligned}\vec{\omega} = & \text{ vector in direction of velocity of primed frame} \\ & \text{ with respect to unprimed frame and of magnitude} \\ \tanh(\omega) = & \frac{v}{c}\end{aligned}$$

Proof: First,

$$\sigma'_{||} = L\sigma_{||}L^{-1} = e^{\alpha_{||}\omega/2}\sigma_{||}e^{-\alpha_{||}\omega/2} = e^{\alpha_{||}\omega/2}e^{-\alpha_{||}\omega/2}\sigma_{||} = \sigma_{||} \tag{15.187}$$

where we have used

$$[\alpha_i, \sigma_j] = 2i\varepsilon_{ijk}\alpha_k \to \left[\alpha_{||}, \sigma_{||}\right] = 0 \tag{15.188}$$

This agrees with our earlier result.

Second,

$$\begin{aligned} \sigma'_\perp = L\sigma_\perp L^{-1} = e^{\alpha_{||}\omega/2}\sigma_\perp e^{-\alpha_{||}\omega/2} = e^{\alpha_{||}\omega/2}e^{\alpha_{||}\omega/2}\sigma_\perp \\ = e^{\alpha_{||}\omega}\sigma_\perp = e^{\vec{\alpha}\cdot\vec{\omega}}\sigma_\perp \end{aligned} \tag{15.189}$$

where we have used

$$\{\alpha_i, \sigma_j\} = 0 \quad , \quad i \neq j \to \{\alpha_{||}, \sigma_\perp\} = 0 \tag{15.190}$$

Now using $\vec{\omega} = \omega\hat{\omega}$, $\hat{\omega}\cdot\hat{\omega} = 1$ and $(\vec{\alpha}\cdot\hat{\omega})^2 = 1$ we get

$$e^{\vec{\alpha}\cdot\vec{\omega}} = \cosh\omega + \vec{\alpha}\cdot\hat{\omega}\sinh\omega \tag{15.191}$$

This derivation is the analog of

$$e^{i\vec{\sigma}\cdot\hat{n}\theta} = \cos\theta + i\vec{\sigma}\cdot\hat{n}\sin\theta \tag{15.192}$$

Therefore,

$$\sigma'_\perp = e^{\vec{\alpha}\cdot\vec{\omega}}\sigma_\perp = \cosh\omega\,[1 + \vec{\alpha}\cdot\hat{\omega}\tanh\omega]\,\sigma_\perp = \gamma\,[1 + \vec{\alpha}\cdot\hat{\omega}\tanh\omega]\,\sigma_\perp \tag{15.193}$$

where we have used

$$\cosh^2\omega = \frac{1}{1-\tanh^2\omega} = \frac{1}{1-(v/c)^2} = \gamma^2 \tag{15.194}$$

Using $\hat{\omega}\tanh\omega = \vec{v}/c$ we then get

$$\sigma'_\perp = \gamma\left[1+\vec{\alpha}\cdot\hat{\omega}\tanh\omega\right]\sigma_\perp = \gamma\left[1+\vec{\alpha}\cdot\vec{v}/c\right]\sigma_\perp \tag{15.195}$$

Finally, assuming $\vec{v} = v\hat{e}_z$ and using $\alpha_i\sigma_j = i\varepsilon_{ijk}\alpha_k,\ \ i\neq j$ we get

$$(\vec{\alpha}\cdot\vec{v}/c)\sigma_\perp = i\frac{\vec{v}}{c}\times\vec{\alpha} \tag{15.196}$$

so that

$$\sigma'_\perp = \gamma\left[\sigma_\perp + i\frac{\vec{v}}{c}\times\vec{\alpha}\right] \tag{15.197}$$

which agrees with our earlier result. Thus, $\vec{\sigma}$ transforms correctly. A similar calculation shows that $\vec{\alpha}$ transforms correctly also and, thus, our interpretation is correct.

What about the operator β? In a new Lorentz frame we get

$$\beta' = L_v \beta L_v^{-1} = e^{\vec{\alpha}\cdot\vec{\omega}} \beta \tag{15.198}$$

since β anticommutes with $\vec{\alpha}$. We then get (as above)

$$\beta' = \gamma \left[\beta - (\vec{v}/c) \cdot \beta \vec{\alpha}\right] \tag{15.199}$$

where we have used $\beta\,\vec{\alpha} = -\,\vec{\alpha}\beta$. From the form of this transformation relation, it looks like β transforms as the time-component of a 4-vector of which $\beta\vec{\alpha}$ is the space part.

Some algebra shows that

$$\beta' \alpha'_{\perp} = L \beta \alpha_{\perp} L^{-1} = \beta \alpha_{\perp} \tag{15.200}$$

since both β and $\alpha_{\perp}$ anticommute with L and therefore $\beta\alpha_{\perp}$ commutes with L. In addition, we can show that

$$\beta' \alpha'_{||} = \gamma \left[\beta \alpha_{||} - (v/c)\beta\right] \tag{15.201}$$

Therefore, $(\beta, \beta\,\vec{\alpha})$ does transform like a 4-vector.

This 4-vector is called $\gamma^\mu = (\beta, \beta\,\vec{\alpha})$. In our earlier notation the space part is

$$\vec{\gamma} = \beta\vec{\alpha} = \begin{pmatrix} I & \vec{\tau} \\ -\vec{\tau} & I \end{pmatrix} \tag{15.202}$$

$\vec{\gamma}$ is anti-Hermitian and γ^0 is Hermitian.

Some properties

$$(\gamma^0)^2 = 1 \quad , \quad (\gamma^i)^2 = -1 \quad , \quad i = 1, 2, 3 \tag{15.203}$$

$$\{\gamma^\mu, \gamma^\nu\} = 0 \quad , \quad \mu \neq \nu \tag{15.204}$$

which are summarized by the relation

$$\{\gamma^\mu, \gamma^\nu\} = 2g^{\mu\nu} \tag{15.205}$$

We also have

$$\sigma^{\mu\nu} = \frac{i}{2}\left[\gamma^\mu, \gamma^\nu\right] \tag{15.206}$$

In fact, any 4×4 matrix can be written as a unique linear combination of the γ^μ. The set of 16 matrices

$$I\ ,\ \gamma^\mu\ ,\ \sigma^{\mu\nu}\ ,\ \gamma_5\gamma^\mu\ ,\ \gamma_5 \quad , \qquad \text{where } \gamma_5 = \gamma^0\gamma^1\gamma^2\gamma^3 \tag{15.207}$$

are linearly independent and complete. All are traceless except for the identity matrix.

The new operator γ_5 commutes with the γ^μ. This implies that it commutes with $\alpha_i = \gamma^0\gamma^i$ and is invariant under a Lorentz transformation. It is not a scalar, however, since under parity

$$\beta\gamma_5\beta = -\gamma_5 \tag{15.208}$$

This means that it is a *pseudoscalar*.

Similarly, $\gamma_5\gamma^\mu$ is a *pseudovector* (or *axial vector*), which is a 4-vector whose space part does not change sign under parity and whose time component does.

We see that the set I , γ^μ , $\sigma^{\mu\nu}$, $\gamma_5\gamma^\mu$, γ_5 transforms as a scalar or zeroth-rank tensor, a vector or first-rank tensor, a second-rank tensor, a pseudovector or axial vector or a first-rank pseudotensor and a pseudoscalar or a zeroth-rank pseudotensor.

This is a clear indication that they are linearly independent.

15.6 **The Dirac Equation**

The scalar product of two 4-vectors is a Lorentz invariant. We have identified two 4-vectors, namely,

$$\gamma^\mu = (\beta, \beta\vec{\alpha}) \quad , \quad p^\mu = (E/c, \vec{p}) \tag{15.209}$$

Their scalar product is

$$\beta\frac{E}{c} - \beta\vec{\alpha}\cdot\vec{p} \tag{15.210}$$

Since it is an invariant, it has the same value in all frames. What is that value? We can find out by looking at its square

$$\begin{aligned}\left(\beta\frac{E}{c} - \beta\vec{\alpha}\cdot\vec{p}\right)^2 &= \beta^2\left(\frac{E}{c}\right)^2 + (\beta\vec{\alpha}\cdot\vec{p})^2 - \beta\left(\beta\vec{\alpha} + \vec{\alpha}\beta\right)\cdot\frac{\vec{p}E}{c} \\ &= (1)\left(\frac{E}{c}\right)^2 + \sum_i\left(\beta\alpha_i p_i\right)^2 - \beta\,(0)\cdot\frac{\vec{p}E}{c} = \left(\frac{E}{c}\right)^2 - \sum_i\left(\beta\alpha_i\right)^2 p_i^2 \\ &= \left(\frac{E}{c}\right)^2 - \sum_i (1)^2 p_i^2 = \left(\frac{E}{c}\right)^2 - p^2\end{aligned} \tag{15.211}$$

This says that

$$\beta\frac{E}{c} - \beta\vec{\alpha}\cdot\vec{p} = \sqrt{\left(\frac{E}{c}\right)^2 - p^2} = \pm mc \tag{15.212}$$

The sign depends on the sign we choose for β. If we had interpreted $\beta^2 = 1$ to mean $\beta = -1$ instead of $+1$, which is equivalent to choosing the parity operator as $-\beta$, no physics would have changed. This means we are free to choose the sign. We choose

$$\beta \frac{E}{c} - \beta \vec{\alpha} \cdot \vec{p} = +mc \tag{15.213}$$

or

$$\beta E - \beta c \vec{\alpha} \cdot \vec{p} = mc^2 \tag{15.214}$$

This operator equation involves 4×4 matrices which implies that any physical state vectors must be 4-component spinors.

We make the standard operator correspondence

$$E \rightarrow i\hbar \frac{\partial}{\partial t} \quad , \quad \vec{p} \rightarrow i\hbar \nabla \tag{15.215}$$

and obtain a wave equation

$$i\hbar\beta \frac{\partial \psi}{\partial t} = \beta c \vec{\alpha} \cdot \frac{\hbar}{i} \nabla \psi + mc^2 \psi \tag{15.216}$$

or multiplying by β we get

$$i\hbar\frac{\partial\psi}{\partial t} = \left[c\vec{\alpha}\cdot\frac{\hbar}{i}\nabla + \beta mc^2\right]\psi \tag{15.217}$$

which is the *Dirac equation* for a relativistic spin 1/2 particle.

The form of the result says that the Hamiltonian of a relativistic spin 1/2 particle is

$$\hat{H} = c\vec{\alpha}\cdot\vec{p} + \beta mc^2 \tag{15.218}$$

In the presence of an electromagnetic field we use minimal coupling to get

$$\left(i\hbar\frac{\partial}{\partial t} - e\Phi\right)\psi(\vec{r},t) = \left[c\vec{\alpha}\cdot\left(\frac{\hbar}{i}\nabla - \frac{e}{c}\vec{A}\right) + \beta mc^2\right]\psi(\vec{r},t) \tag{15.219}$$

We note that the vector potential $\vec{A}$ (corresponding to spatial degrees of freedom) is directly coupled to $\vec{\alpha}$ corresponding to internal degrees of freedom).

15.6.1 **Nonrelativistic Limit**

First, we separate time using

$$\psi(t) = \psi e^{-iEt/\hbar} \tag{15.220}$$

to get

$$(E - e\Phi)\,\psi = \left[c\vec{\alpha}\cdot\left(\frac{\hbar}{i}\nabla - \frac{e}{c}\vec{A}\right) + \beta mc^2\right]\psi \tag{15.221}$$

We then write

$$\psi = \begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix} \tag{15.222}$$

where ψ_A and ψ_B are still two-component functions and use the explicit Dirac matrices to obtain

$$(E - e\Phi)\begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix} = \left[\begin{pmatrix} 0 & \vec{\tau} \\ \vec{\tau} & 0 \end{pmatrix}\cdot\left(c\vec{p} - e\vec{A}\right) + \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix} mc^2\right]\begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix} \tag{15.223}$$

This is equivalent to two coupled equations

$$\vec{\tau} \cdot \left(c\vec{p} - e\vec{A} \right) \psi_B + mc^2 \psi_A = (E - e\Phi)\, \psi_A \tag{15.224}$$

$$\vec{\tau} \cdot \left(c\vec{p} - e\vec{A} \right) \psi_A - mc^2 \psi_B = (E - e\Phi)\, \psi_B \tag{15.225}$$

Letting $E = E' + mc^2$ the second equation of the pair becomes

$$\psi_B = \frac{1}{E' - e\Phi + 2mc^2} \vec{\tau} \cdot \left(c\vec{p} - e\vec{A} \right) \psi_A \tag{15.226}$$

Inserting this result into the first equation of the pair we get

$$\frac{1}{2mc^2} \vec{\tau} \cdot \left(c\vec{p} - e\vec{A} \right) \frac{1}{1 + \frac{E' - e\Phi}{2mc^2}} \vec{\tau} \cdot \left(c\vec{p} - e\vec{A} \right) \psi_A = \left(E' - e\Phi \right) \psi_A \tag{15.227}$$

These last two equations are exact and very useful substitutes for the Dirac equation.

We now make some approximations relevant to the nonrelativistic case. We assume that

$$E' << mc^2 \quad , \quad e\Phi << mc^2$$
$$\text{eigenvalues of } \vec{p} \text{ are of order } mv << mc$$

This says that the components satisfy

$$\psi_B \approx \frac{v}{c}\psi_A \tag{15.228}$$

Or that the 4-component wavefunction ψ has two large components ψ_A and two small components ψ_B.

If we ignore terms of order $(v/c)^2$ the equation for ψ_A becomes

$$\frac{1}{2mc^2}\left(\vec{\tau}\cdot\left(c\vec{p}-e\vec{A}\right)\right)^2\psi_A + e\Phi\psi_A = E'\psi_A \tag{15.229}$$

Now, earlier we derived the identity

$$(\vec{\tau} \cdot \vec{a})(\vec{\tau} \cdot \vec{b}) = \vec{a} \cdot \vec{b} + i\vec{\tau} \cdot \left(\vec{a} \times \vec{b}\right) \tag{15.230}$$

We then have

$$\left(\vec{\tau} \cdot \left(c\vec{p} - e\vec{A}\right)\right)^2 = \left(c\vec{p} - e\vec{A}\right)^2 + i\vec{\tau} \cdot \left(\left(c\vec{p} - e\vec{A}\right) \times \left(c\vec{p} - e\vec{A}\right)\right) \tag{15.231}$$

Now

$$\left(\vec{\tau} \cdot \left(c\vec{p} - e\vec{A}\right)\right)^2 = \left(c\vec{p} - e\vec{A}\right)^2 \tag{15.232}$$

and

$$\left(c\vec{p} - e\vec{A}\right) \times \left(c\vec{p} - e\vec{A}\right) = -ec\left(\vec{p} \times \vec{A} + \vec{A} \times \vec{p}\right) = +ie\hbar c\left(\nabla \times \vec{A} + \vec{A} \times \tag{15.233}$$

Now

$$\begin{aligned}(\nabla \times \vec{A} + \vec{A} \times \nabla)^i \psi_A &= \varepsilon^{ijk}\left(\partial_j A^k - A^k \partial_j\right)\psi_A \\ &= \varepsilon^{ijk}\left((\partial_j A^k)\psi_A + A^k(\partial_j \psi_A) - A^k(\partial_j \psi_A)\right) \\ &= \varepsilon^{ijk}(\partial_j A^k)\psi_A = (\nabla \times \vec{A})\psi_A = \vec{B}\psi_A\end{aligned} \tag{15.234}$$

Putting everything together we get

$$\frac{1}{2m}\left(\vec{p}-\frac{e}{c}\vec{A}\right)^2\psi_A-\frac{e}{mc}\frac{\hbar}{2}\vec{\tau}\cdot\vec{B}+e\Phi\psi_A=E'\psi_A \tag{15.235}$$

This the *Pauli equation*. The term involving the magnetic field has the form of a magnetic dipole interaction energy

$$-\frac{e}{mc}\vec{S}\cdot\vec{B} \tag{15.236}$$

with a gyromagnetic ratio

$$2\times\frac{e}{mc}\rightarrow g=2 \tag{15.237}$$

The full time-dependent form of the nonrelativistic limit is given by

$$\frac{1}{2m}\left(\frac{\hbar}{i}\nabla-\frac{e}{c}\vec{A}\right)^2\psi_A-\frac{e}{mc}\frac{\hbar}{2}\vec{\tau}\cdot\vec{B}+(e\Phi+mc^2)\psi_A=i\hbar\frac{\partial\psi_A}{\partial t} \tag{15.238}$$

15.6.2 **Currents and Continuity Equations**

Going back to the full equation

$$\left(i\hbar\frac{\partial}{\partial t} - e\Phi\right)\psi(\vec{r},t) = \left[c\vec{\alpha}\cdot\left(\frac{\hbar}{i}\nabla - \frac{e}{c}\vec{A}\right) + \beta mc^2\right]\psi(\vec{r},t) \tag{15.239}$$

we take the Hermitian conjugate to get

$$\left(-i\hbar\frac{\partial}{\partial t} - e\Phi\right)\psi^+(\vec{r},t) = c\left(-\frac{\hbar}{i}\nabla - \frac{e}{c}\vec{A}\right)\psi^+(\vec{r},t)\cdot\vec{\alpha}+\beta mc^2\psi^+(\vec{r},t) \tag{15.240}$$

Note that the Hermitian conjugate operation reverses matrix order. Now multiply the first equation by $\psi^+(\vec{r},t)$ on the left and the second equation by $\psi(\vec{r},t)$ on the right and subtracting we get the continuity-type equation

$$\frac{\partial\left(\psi^+\psi\right)}{\partial t} + \nabla\cdot\left(\psi^+ c\vec{\alpha}\psi\right) = 0 \tag{15.241}$$

This says that the quantity $\psi^+\psi$ is a positive conserved quantity that can be interpreted as a probability density and then

$$\vec{j} = \psi^+ c\vec{\alpha}\psi \tag{15.242}$$

is the corresponding probability current. The operator $c\vec{\alpha}$ corresponds to the velocity operator, which is the derivative of the Hamiltonian with respect to $\vec{p}$.

What happens to the Dirac equation under a Lorentz transformation?

In one frame we have

$$i\hbar\beta\frac{\partial\psi}{\partial t} = \beta c\vec{\alpha}\cdot\frac{\hbar}{i}\nabla\psi + mc^2\psi \tag{15.243}$$

and in a new frame we have

$$i\hbar\beta'\frac{\partial\hat{\psi}(\vec{r}\,',t')}{\partial t'} = \beta' c\vec{\alpha}\,'\cdot\frac{\hbar}{i}\nabla'\hat{\psi}(\vec{r}\,',t') + mc^2\hat{\psi}(\vec{r}\,',t') \tag{15.244}$$

where $\hat{\psi}(\vec{r}\,', t')$ is the wave function in the new frame.

We already determined, however, that

$$i\hbar\beta'\frac{\partial}{\partial t'} - \beta' c\vec{\alpha}\,' \cdot \frac{\hbar}{i}\nabla' = i\hbar\beta\frac{\partial}{\partial t} - \beta c\vec{\alpha} \cdot \frac{\hbar}{i}\nabla \qquad (15.245)$$

since the scalar product of two 4-vectors is an invariant. This implies that

$$\hat{\psi}(\vec{r}\,', t') = \psi(\vec{r}, t) = \text{ Lorentz scalar} \qquad (15.246)$$

i.e., they both satisfy the same equation when $\vec{r}\,', t'$ and $\vec{r}, t$ are the same space-time point.

It turns out, however, that a more convenient equation to use in the new frame is one that still involves the old β and $\vec{\alpha}$ matrices, i.e., β' and $\vec{\alpha}\,'$ are represented by the same matrices as β and $\vec{\alpha}$. We can find this other equation as follows. We have

$$i\hbar\beta'\frac{\partial\hat{\psi}(\vec{r}\,',t')}{\partial t'} = \beta' c\vec{\alpha}\,'\cdot\frac{\hbar}{i}\nabla'\hat{\psi}(\vec{r}\,',t') + mc^2\hat{\psi}(\vec{r}\,',t')$$

$$i\hbar L_v\beta L_v^{-1}\frac{\partial\hat{\psi}(\vec{r}\,',t')}{\partial t'} = L_v\beta c\vec{\alpha}L_v^{-1}\cdot\frac{\hbar}{i}\nabla\,'\hat{\psi}(\vec{r}\,',t') + mc^2\hat{\psi}(\vec{r}\,',t')$$

$$i\hbar\beta L_v^{-1}\frac{\partial\hat{\psi}(\vec{r}\,',t')}{\partial t'} = \beta c\vec{\alpha}L_v^{-1}\cdot\frac{\hbar}{i}\nabla'\hat{\psi}(\vec{r}\,',t') + mc^2 L_v^{-1}\hat{\psi}(\vec{r}\,',t')$$

If we define

$$\psi'(\vec{r}\,',t') = L_v^{-1}\hat{\psi}(\vec{r}\,',t') = L_v^{-1}\psi(\vec{r},t) \tag{15.247}$$

we have the equation

$$i\hbar\beta\frac{\partial\psi'(\vec{r}\,',t')}{\partial t'} = \beta c\vec{\alpha}\cdot\frac{\hbar}{i}\nabla'\psi'(\vec{r}\,',t') + mc^2\psi'(\vec{r}\,',t') \tag{15.248}$$

This form of the equation has the same matrices β and $\vec{\alpha}$ in all frames with the wave function in the new frame related to the wave function in the old frame by the Lorentz transformation.

Alternatively, we can write the Dirac equation in covariant form. The Dirac equation is

$$i\hbar\frac{\partial\psi}{\partial t} = \left[c\vec{\alpha}\cdot\frac{\hbar}{i}\nabla + \beta mc^2\right]\psi \tag{15.249}$$

which we can rewrite as

$$-i\hbar\beta\partial_0\psi - i\hbar\beta\alpha^i\partial_i\psi + mc\psi = 0 \tag{15.250}$$

using the definition of the Dirac gamma matrices we have

$$\left(-i\gamma^\mu\partial_\mu + \frac{mc}{\hbar}\right)\psi = 0 \tag{15.251}$$

which is clearly covariant.

15.6.3 **Free Particle Solutions**

We start off by constructing solutions for a particle at rest. In this case, we have

$$\psi(\vec{r}, t) = e^{-iEt/\hbar} u \tag{15.252}$$

where u is a spinor independent of space and time. Substituting into the Dirac equation we have

$$Eu = \beta mc^2 u \tag{15.253}$$

The eigenvalues of β are ± 1. If u is an eigenstate of β with eigenvalue $+1$, then $E = +mc^2$ and if u is an eigenstate of β with eigenvalue -1, then $E = -mc^2$. So we find negative energy solutions again and we will associate them with particles and antiparticles as before. Their properties in the spin 1/2 case will be different, however.

We choose to write four linearly independent solutions to the free particle Dirac equation as:

$$u_{0\uparrow}^{(+)} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} , \; u_{0\downarrow}^{(+)} = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} , \; u_{0\downarrow}^{(-)} = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} , \; u_{0\uparrow}^{(-)} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$$

where the upper index $(\pm)$ denotes the eigenvalue of β, the 0 denotes that the particle is at rest $\vec{p} = 0$, and the arrow denotes the value of the spin associated physically with these states.

The spinors $u_{0\uparrow}^{(+)}$ and $u_{0\downarrow}^{(-)}$ are eigenstates of σ_z with eigenvalue $+1$ and $u_{0\downarrow}^{(+)}$ and $u_{0\uparrow}^{(-)}$ are eigenstates of σ_z with eigenvalue -1.

We are saying here that while $u_{0\uparrow}^{(-)}$ is the spinor of a negative energy particle with spin up, we will associate it with a positive energy antiparticle with spin down.

The states with $\beta = +1$ vary in time as $e^{-imc^2t/\hbar}$ and those with $\beta = -1$ vary in time as $e^{+imc^2t/\hbar}$. The positive and negative states have opposite parity(intrinsic).

We can now construct states for a particle with momentum $\vec{p}$ by starting with the particle at rest and applying a Lorentz transformation to take us to a frame moving with velocity

$$\vec{v} = -\frac{\vec{p}c^2}{E_p} \text{ where } E_p = +\sqrt{p^2c^2 + m^2c^4} \tag{15.254}$$

We showed earlier that

$$\psi'(\vec{r}', t') = L_v^{-1}\psi(\vec{r}, t) = e^{-\vec{\alpha}\cdot\vec{\omega}/2}\psi(\vec{r}, t) = e^{-\vec{\alpha}\cdot\vec{\omega}/2}e^{\mp imc^2t/\hbar}u_{0,\sigma}^{(\pm)} \tag{15.255}$$

Now $E'_pt' - \vec{p}' \cdot \vec{r}'$ is a Lorentz scalar (scalar product of two 4-vectors). In the rest frame it is equal to mc^2t. Therefore we can write

$$e^{\mp imc^2t/\hbar} = e^{\pm i(\vec{p}'\cdot\vec{r}' - E'_pt')/\hbar} \tag{15.256}$$

Dropping the superfluous primes we then have

$$\psi(\vec{r}, t) = e^{\pm i(\vec{p}\cdot\vec{r} - E_pt)/\hbar}e^{-\vec{\alpha}\cdot\vec{\omega}/2}u_{0,\sigma}^{(\pm)} \tag{15.257}$$

as the wave function for nonzero momentum. The new spinors are given by

$$u_{\vec{p},\sigma}^{(\pm)} = e^{-\vec{\alpha}\cdot\vec{\omega}/2} u_{0,\sigma}^{(\pm)} = \left[\cosh\frac{\omega}{2} - \vec{\alpha}\cdot\hat{v}\sinh\frac{\omega}{2}\right] u_{0,\sigma}^{(\pm)} \tag{15.258}$$

Using

$$\vec{v} = -\frac{\vec{p}c^2}{E_p} \tag{15.259}$$

we get

$$\cosh\frac{\omega}{2} = \sqrt{\frac{E_p + mc^2}{2mc^2}} \quad , \quad \hat{v}\tanh\frac{\omega}{2} = -\frac{\vec{p}c}{E_p + mc^2} \tag{15.260}$$

so that

$$u_{\vec{p},\sigma}^{(\pm)} = \sqrt{\frac{E_p + mc^2}{2mc^2}} \left[1 + \frac{c\vec{p}\cdot\vec{\alpha}}{E_p + mc^2}\right] u_{0,\sigma}^{(\pm)} \tag{15.261}$$

We then have (in the standard representation)

$$u^{(+)}_{\vec{p},\uparrow} = \sqrt{\frac{E_p + mc^2}{2mc^2}} \left[1 + \frac{c}{E_p + mc^2} \vec{p} \cdot \vec{\alpha}\right] u^{(+)}_{0,\uparrow} \qquad (15.262)$$

Now

$$\vec{p} \cdot \vec{\alpha} = p_x \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix} + p_y \begin{pmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \\ 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \end{pmatrix}$$
$$+ p_z \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix} \quad , \quad u^{(+)}_{0,\uparrow} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

and we get

$$u^{(+)}_{\vec{p},\uparrow} = \sqrt{\frac{E_p + mc^2}{2mc^2}} \left[\begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} + \frac{c}{E_p+mc^2} \left(p_x \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} + p_y \begin{pmatrix} 0 \\ 0 \\ 0 \\ i \end{pmatrix} + p_z \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} \right) \right]$$

$$= \sqrt{\frac{E_p + mc^2}{2mc^2}} \begin{pmatrix} 1 \\ 0 \\ \frac{cp_z}{E_p+mc^2} \\ \frac{c(p_x+ip_y)}{E_p+mc^2} \end{pmatrix} \tag{15.263}$$

and similarly

$$u^{(+)}_{\vec{p},\downarrow} = \sqrt{\frac{E_p + mc^2}{2mc^2}} \begin{pmatrix} 0 \\ 1 \\ \frac{c(p_x-ip_y)}{E_p+mc^2} \\ -\frac{cp_z}{E_p+mc^2} \end{pmatrix} \tag{15.264}$$

$$u_{\vec{p},\downarrow}^{(-)} = \sqrt{\frac{E_p + mc^2}{2mc^2}} \begin{pmatrix} \frac{cp_z}{E_p+mc^2} \\ \frac{c(p_x+ip_y)}{E_p+mc^2} \\ 1 \\ 0 \end{pmatrix} \tag{15.265}$$

$$u_{\vec{p},\uparrow}^{(-)} = \sqrt{\frac{E_p + mc^2}{2mc^2}} \begin{pmatrix} \frac{c(p_x-ip_y)}{E_p+mc^2} \\ -\frac{cp_z}{E_p+mc^2} \\ 0 \\ 1 \end{pmatrix} \tag{15.266}$$

Remember that the arrow refers to the spin associated with the state in the rest frame, which is minus the σ_z eigenvalue for the $(-)$ spinors. We see that a particle in a σ_z eigenstate in its rest frame appears to be in a σ_z eigenstate to an observer moving with respect to the particle only if the observer is moving along the $z-$direction, i.e., if $p_x = p_y = 0$ we have

$$
\begin{aligned}
u^{(+)}_{\vec{p},\uparrow} &= \sqrt{\frac{E_p + mc^2}{2mc^2}} \begin{pmatrix} 1 \\ 0 \\ \frac{cp_z}{E_p+mc^2} \\ 0 \end{pmatrix} \\
&= \sqrt{\frac{E_p + mc^2}{2mc^2}} \left[u^{(+)}_{0,\uparrow} + \frac{cp_z}{E_p + mc^2} u^{(-)}_{0,\downarrow} \right] \qquad (15.267)
\end{aligned}
$$

which is a sum of a particle and an antiparticle where both have spin up!

The positive energy solutions $u^{(+)}_{\vec{p}\sigma} e^{i(\vec{p}\cdot\vec{r} - E_p t)/\hbar}$ correspond to particles with momentum $\vec{p}$, energy E_p and spin orientation σ. The negative energy solutions $u^{(-)}_{\vec{p}\sigma} e^{-i(\vec{p}\cdot\vec{r} - E_p t)/\hbar}$ correspond to particles with momentum $-\vec{p}$, energy $-E_p$ and spin orientation $-\sigma$ which we will soon associate with antiparticles with momentum $\vec{p}$, energy E_p and spin orientation σ.

The nonzero momentum spinors are orthogonal but not normalized to one (as is the case with the zero momentum spinors). Since $L^+ \neq L^{-1}$, in general, the Lorentz transformations are not represented by a unitary operator and hence the lengths of vectors or normalizations change. In particular. The normalization is given by

$$u^{(\pm)+}_{\vec{p}\sigma} u^{(\pm)}_{\vec{p}\sigma} = \frac{E_p}{mc^2} \tag{15.268}$$

Since $\vec{\alpha}$ is Hermitian, we have $L^+ = L$.

Thus, if $u_{\vec{p}} = L^{-1} u_0$, then $(u_{\vec{p}})^+ = (u_0)^+ (L^{-1})^+ = (u_0)^+ L^{-1}$ and $u^+_{\vec{p}} u_{\vec{p}} = u^+_0 (L^{-1})^2 u_0$.

It is possible to define a normalization that is invariant under a Lorentz transformation. Since β anticommutes with $\vec{\alpha}$, we can write

$$(L^{-1})^+ \beta = L^{-1} \beta = e^{\vec{\alpha}\cdot\vec{\omega}/2} \beta = \beta e^{-\vec{\alpha}\cdot\vec{\omega}/2} = \beta L \tag{15.269}$$

Now, if the spinor u transforms as $u' = L^{-1}u$, then the spinor $\bar{u} = u^{+}\beta$ is given in the new frame by

$$\bar{u}' = u'^{+}\beta' = u'^{+}\beta = u^{+}(L^{-1})^{+}\beta = u^{+}L^{-1}\beta = u^{+}\beta L = \bar{u}L \tag{15.270}$$

This means that the product $\bar{u}_1 u_2$ of any two spinors is a Lorentz invariant, i.e.,

$$\bar{u}_1' u_2' = (\bar{u}_1 L)(L^{-1}u_2) = \bar{u}_1 u_2 \tag{15.271}$$

In the rest frame

$$u_{0\sigma}^{(b)+} u_{0\sigma'}^{(b')} = b\delta_{bb'}\delta_{\sigma\sigma'} \quad , \quad b = \pm \tag{15.272}$$

which says that the same relation is true for all momentum $\vec{p}$

$$u_{\vec{p}\sigma}^{(b)+} u_{\vec{p}\sigma'}^{(b')} = b\delta_{bb'}\delta_{\sigma\sigma'} \quad , \quad b = \pm \tag{15.273}$$

The spinors $u_{\vec{p}\sigma}^{(\pm)}$ obey the completeness relation that says that the 4×4 identity matrix can be written as the sum of the outer products of the four spinors, i.e.,

$$\sum_{b,\sigma} b u_{\vec{p}\sigma}^{(b)} \bar{u}_{\vec{p}\sigma}^{(b)} = 1 \tag{15.274}$$

The spinors $u_{\vec{p}\sigma}^{(\pm)}$ obey

$$(\beta E_p - c\beta\vec{\alpha}\cdot\vec{p})u_{\vec{p}\sigma}^{(\pm)} = \pm mc^2 u_{\vec{p}\sigma}^{(\pm)} \tag{15.275}$$

and

$$u_{\vec{p}\sigma}^{(\pm)+}(\beta E_p - c\vec{\alpha}\cdot\vec{p}\beta) = \pm mc^2 u_{\vec{p}\sigma}^{(\pm)+} \tag{15.276}$$

Multiplying the last equation on the right by β we have the equation satisfied by $\bar{u}_{\vec{p}\sigma}^{(\pm)}$

$$\bar{u}_{\vec{p}\sigma}^{(\pm)}(\beta E_p - c\beta\vec{\alpha}\cdot\vec{p}) = \pm mc^2 \bar{u}_{\vec{p}\sigma}^{(\pm)} \tag{15.277}$$

15.6.4 **More About Currents**

As we have seen, the solution of the Dirac equation $\psi(\vec{r}, t)$ has the following behavior under a Lorentz transformation

$$\psi(\vec{r}, t) \rightarrow \psi'(\vec{r}', t') = L^{-1}\psi(\vec{r}, t) \tag{15.278}$$

The spinor $\bar{\psi}(\vec{r}, t) = \psi^{+}(\vec{r}, t)\beta$ transforms like

$$\bar{\psi}(\vec{r}, t) \rightarrow \bar{\psi}'(\vec{r}', t') = [L^{-1}\psi(\vec{r}, t)]^{+}\beta = \bar{\psi}(\vec{r}, t)L \tag{15.279}$$

This says that the product $\bar{\psi}(\vec{r}, t)\psi(\vec{r}, t)$ transforms like a Lorentz scalar.

Now the γ^{μ} transform as the components of a 4-vector, i.e., $\gamma^{\mu} \rightarrow L\gamma^{\mu}L^{-1}$. Therefore, the product

$$\bar{\psi}(\vec{r}, t)\gamma^{\mu}\psi(\vec{r}, t) = \left(\rho(\vec{r}, t), \frac{1}{c}\vec{j}(\vec{r}, t)\right) \tag{15.280}$$

transforms like a 4-vector under a Lorentz transformation. It is the particle 4-current multiplied by $1/c$. In the same manner,

$$\bar{\psi}\sigma^{\mu\nu}\psi \rightarrow \text{ second -rank tensor}$$
$$\bar{\psi}\gamma_5\gamma^{\mu}\psi \rightarrow \text{ axial vector}$$
$$\bar{\psi}\gamma_5\psi \rightarrow \text{ pseudo - scalar}$$

The positive density $\rho(\vec{r},t) = \psi^{+}(\vec{r},t)\psi(\vec{r},t)$ and the current $\vec{j}(\vec{r},t) = c\psi^{+}(\vec{r},t)\vec{\alpha}\psi(\vec{r},t)$ satisfy the continuity equation

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \vec{j} = 0 \tag{15.281}$$

which implies that the quantity

$$\int \rho(\vec{r},t)d^3r \tag{15.282}$$

is a constant of the motion.

In this case, we can interpret $\rho(\vec{r},t)$ as a probability density (same as in nonrelativistic case). Remember in the spin zero case this was not so since the corresponding conserved density needed to be interpreted as a charge density which could be positive and negative.

One important consequence in the spin zero case was that it is impossible for a particle to make a transition from a state normalized to $+1$ to a state normalized to -1 since the normalization remains constant in time. We associated the negative energy states with particles and the negatively normalized states with antiparticles. We then see that the impossibility of a transition between positive and negative energy states just corresponds to charge conservation.

In the spin$-1/2$ case, however, both positive and negative energy states have positive normalization so that there is nothing in the theory (so far) that prevents a particle in a positive energy state from making a transition to a negative energy state radiating away several high energy photons in the process. A difficulty in the theory that we must return to later!

Let us say some more about the position and velocity operators in the Dirac theory.

The position operator has strange features similar to those of the Klein-Gordon theory. If we apply the position operator to a wave packet made up of positive energy free particle states we get

$$\begin{aligned}
\vec{r}\psi^{(+)}(\vec{r}) &= \vec{r}\left(\sum_\sigma \int \frac{d^3p}{(2\pi\hbar)^3} a_{\vec{p}\sigma} u^{(+)}_{\vec{p}\sigma} e^{i\vec{p}\cdot\vec{r}/\hbar}\right) \\
&= \sum_\sigma \int \frac{d^3p}{(2\pi\hbar)^3} a_{\vec{p}\sigma} u^{(+)}_{\vec{p}\sigma} \frac{\hbar}{i} \nabla_{\vec{p}} e^{i\vec{p}\cdot\vec{r}/\hbar} \\
&= \sum_\sigma \int \frac{d^3p}{(2\pi\hbar)^3} (i\hbar\nabla_{\vec{p}} a_{\vec{p}\sigma}) u^{(+)}_{\vec{p}\sigma} e^{i\vec{p}\cdot\vec{r}/\hbar} \\
&\quad + \sum_\sigma \int \frac{d^3p}{(2\pi\hbar)^3} a_{\vec{p}\sigma} (i\hbar\nabla_{\vec{p}} u^{(+)}_{\vec{p}\sigma}) e^{i\vec{p}\cdot\vec{r}/\hbar}
\end{aligned}$$

where we have integrated by parts to get the last two terms.

The first term contains only positive energy components. The second term, however, contains the factor $i\hbar\nabla_{\vec{p}}u^{(+)}_{\vec{p}\sigma}$, which generates both positive and negative components (explicitly do the derivatives on the column vectors we derived earlier). If we define, as before

$$\vec{r} = \vec{r}_{(+)} + \vec{r}_{(-)} \tag{15.283}$$

then, as before, the even part $\vec{r}_{(+)}$ acting on the wave packet of positive energy free particle states produces only positive energy free particle states and acting on the wave packet of negative energy free particle states produces only negative energy free particle states, while the odd part $\vec{r}_{(-)}$ turns positive positive energy states to negative energy states and vice versa.

As in the Klein-Gordon case, both positive and negative energy free particle solutions are needed to produce a localized wave packet.

Looking at the current expression $\vec{j}(\vec{r},t) = c\psi^{+}(\vec{r},t)\vec{\alpha}\psi(\vec{r},t)$ we see that the operator $c\vec{\alpha}$ acts as a velocity operator.

This interpretation also agrees with the commutator relation

$$-i\hbar\left[\vec{r},\hat{H}\right] = c\vec{\alpha} \tag{15.284}$$

which leads to the Heisenberg representation operator equation

$$\frac{d\vec{r}}{dt} = c\vec{\alpha} \tag{15.285}$$

If, however, we consider the $z-$component of this velocity operator we get $(c\alpha_z)^2 = c^2\alpha_z^2 = c^2$. Thus the eigenvalues of each component of the velocity operator are $\pm c$, which says that a particle in an eigenstate of the velocity operator travels at the speed of light!

This means that the velocity operator is not simply related to the momentum operator relativistically. The eigenstates of any component of $\vec{\alpha}$ are linear combinations of positive and negative energy free particle states and thus cannot be realized in any physical situation! For any arbitrary state the expectation value of $c\vec{\alpha}$ has a magnitude between 0 and c.

15.6.5 Non-relativistic Limit

We now derive corrections to the Pauli equation. Earlier we had

$$\vec{\tau} \cdot \left(c\vec{p} - e\vec{A} \right) \psi_B + mc^2 \psi_A = (E - e\Phi)\, \psi_A \tag{15.286}$$

$$\vec{\tau} \cdot \left(c\vec{p} - e\vec{A} \right) \psi_A - mc^2 \psi_B = (E - e\Phi)\, \psi_B \tag{15.287}$$

or

$$\vec{\tau} \cdot \left(\frac{\hbar}{i}\nabla - \frac{e}{c}\vec{A} \right) \psi_B + mc\psi_A = \frac{1}{c}\left(i\hbar\frac{\partial}{\partial t} - e\Phi \right) \psi_A \tag{15.288}$$

$$\vec{\tau} \cdot \left(\frac{\hbar}{i}\nabla - \frac{e}{c}\vec{A} \right) \psi_A - mc\psi_B = \frac{1}{c}\left(i\hbar\frac{\partial}{\partial t} - e\Phi \right) \psi_B \tag{15.289}$$

The second equation of the above pair gives (an exact equation)

$$\psi_B = \frac{1}{2mc}\left(\frac{\hbar}{i}\nabla - \frac{e}{c}\vec{A} \right) \cdot \vec{\tau}\psi_A - \frac{1}{2mc^2}\left(i\hbar\frac{\partial}{\partial t} - mc^2 - e\Phi \right) \psi_B \tag{15.290}$$

Now the ψ_A term is much larger than the ψ_B term on the right. Thus, we get the first correction by iterating once, i.e.

$$\psi_B = \frac{1}{2mc}\left(\frac{\hbar}{i}\nabla - \frac{e}{c}\vec{A}\right)\cdot\vec{\tau}\psi_A \\ - \frac{1}{4m^2c^3}\left(i\hbar\frac{\partial}{\partial t} - mc^2 - e\Phi\right)\left(\frac{\hbar}{i}\nabla - \frac{e}{c}\vec{A}\right)\cdot\vec{\tau}\psi_A \tag{15.291}$$

Substituting this expression into the first equation of the pair we get the first relativistic correction term to the Pauli equation

$$-\frac{1}{4m^2c^3}\left(\frac{\hbar}{i}\nabla - \frac{e}{c}\vec{A}\right)\cdot\vec{\tau}\left(i\hbar\frac{\partial}{\partial t} - mc^2 - e\Phi\right)\left(\frac{\hbar}{i}\nabla - \frac{e}{c}\vec{A}\right)\cdot\vec{\tau}\psi_A \tag{15.292}$$

which is $\approx (v/c)^2$ smaller than the kinetic energy term $p^2/2m$.

The correction term can be rewritten as

$$
- \frac{1}{4m^2c^3} \left(\left(\frac{\hbar}{i} \nabla - \frac{e}{c} \vec{A} \right) \cdot \vec{\tau} \right)^2 \left(i\hbar \frac{\partial}{\partial t} - mc^2 - e\Phi \right) \psi_A
$$

$$
- \frac{ie\hbar}{4m^2c^3} \left(\left(\frac{\hbar}{i} \nabla - \frac{e}{c} \vec{A} \right) \cdot \vec{\tau} \right) (\vec{\varepsilon} \cdot \vec{\tau}) \, \psi_A
$$

where

$$
\vec{\varepsilon} = -\nabla\Phi - \frac{1}{c} \frac{\partial \vec{A}}{\partial t} = \text{ electric field} \tag{15.293}
$$

To lowest order in (v/c) we have

$$
\left(i\hbar \frac{\partial}{\partial t} - mc^2 - e\Phi \right) \psi_A = \frac{p^2}{2m} \psi_A \tag{15.294}
$$

Using this relation with the identity

$$
(\vec{\tau} \cdot \vec{a})(\vec{\tau} \cdot \vec{b}) = \vec{a} \cdot \vec{b} + i\vec{\tau} \cdot \left(\vec{a} \times \vec{b} \right) \tag{15.295}
$$

the correction becomes

$$-\left[\frac{p^4}{8m^3c^2} + \frac{e\hbar}{4m^2c^2}\vec{\tau}\cdot(\vec{\varepsilon}\times\vec{p}) + \frac{ie\hbar}{4m^2c^2}\vec{p}\cdot\vec{\varepsilon}\right] \tag{15.296}$$

The first term is the relativistic correction to the kinetic energy. The second term is the spin-orbit coupling. The third term is new and is not even Hermitian!

The reason for this non-Hermitian term is that we are only working to order $(v/c)^2$. Such a non-Hermitian term in the wave equation means that the normalization integral

$$\int \psi_A^+ \psi_A d^3r$$

can change in time. Now the full Dirac equation obeys the normalization condition

$$\int \psi^+\psi d^3r = \int [\psi_A^+\psi_A + \psi_B^+\psi_B] d^3r = 1 \tag{15.297}$$

To lowest order, however,

$$\psi_B = \frac{\hbar}{2imc}\nabla \cdot \vec{\tau}\psi_A \to \psi_B^+\psi_B = \psi_A^+\frac{p^2}{4m^2c^2}\psi_A \qquad (15.298)$$

Thus, the integral stays constant to order $(v/c)^2$. It is the integral

$$\int \psi_A^+\left[1+\frac{p^2}{4m^2c^2}\right]\psi_A d^3r = \int \left[\left[1+\frac{p^2}{8m^2c^2}\right]\psi_A\right]^+\left[\left[1+\frac{p^2}{8m^2c^2}\right]\psi_A\right]$$

to order $(v/c)^2$, that remains constant and equal to 1. This implies that the correct nonrelativistic limit of the Dirac wave function (the limit whose normalization remains constant in time) is

$$\psi(\vec{r},t) = \left[1+\frac{p^2}{8m^2c^2}\right]\psi_A(\vec{r},t) \to \int \psi^+\psi d^3r = 1 \qquad (15.299)$$

The equation for this form of the wave function will not have any non-Hermitian terms. A large amount of algebra gives the equation for $\psi(\vec{r}, t)$ as

$$i\hbar\frac{\partial\psi}{\partial t} = \left[mc^2 + \frac{1}{2m}\left(\vec{p} - \frac{e}{c}\vec{A}\right)^2 - \frac{p^4}{8m^3c^2}\right]\psi \qquad (15.300)$$
$$- \left[\frac{e\hbar}{2mc}\vec{\tau}\cdot\vec{B} + \frac{e\hbar}{4m^2c^2}\vec{\tau}\cdot(\vec{\varepsilon}\times\vec{p})\right]\psi + \left[e\Phi + \frac{\hbar^2}{8m^2c^2}(\nabla^2 e\Phi)\right]$$

This is the correct nonrelativistic limit of the Dirac equation. All terms are Hermitian.

The terms on the right-hand side are

[rest energy + kinetic energy(to order $(v/c)^2$)]
− [Pauli magnetic moment energy + spin-orbit energy]
+ [correction to the potential energy term]

Spin-Orbit Term - Letting $\vec{A} = 0$ for simplicity we have

$$\frac{e\hbar}{4m^2c^2}\vec{\tau}\cdot(\vec{\varepsilon}\times\vec{p}) = -\frac{e\hbar}{4m^2c^2}\vec{\tau}\cdot(\nabla\Phi\times\vec{p}) \tag{15.301}$$

If we assume the potential is spherically symmetric, then

$$\nabla\Phi = \frac{1}{r}\frac{d\Phi}{dr}\vec{r} \tag{15.302}$$

and we get

$$\frac{e\hbar}{4m^2c^2}\vec{\tau}\cdot(\vec{\varepsilon}\times\vec{p}) = -\frac{e\hbar}{4m^2c^2r}\frac{d\Phi}{dr}\vec{\tau}\cdot(\vec{r}\times\vec{p}) = -\frac{e}{2m^2c^2r}\frac{d\Phi}{dr}\vec{S}\cdot\vec{L} \tag{15.303}$$

which is the spin-orbit energy. It correctly contains the Thomas precession correction! We do not have to add any terms in an ad hoc manner!

Correction to the Potential - This is called the *Darwin term*. Now, from Poisson's equation we have

$$\nabla^2 e\Phi(\vec{r}) = -4\pi e Q(\vec{r}) \quad , \quad Q(\vec{r}) = \text{ charge density producing } \Phi(\vec{r})$$

For a Coulomb potential we get

$$\frac{\hbar^2}{8m^2c^2}(\nabla^2 e\Phi) = \frac{\pi\hbar^2}{2m^2c^2} Z e^2 \delta(\vec{r}) \tag{15.304}$$

This term tends to raise the energy of s-states since they do not vanish at the origin.

15.6.6 **The Dirac Hydrogen Atom**

We start with the equations

$$\vec{\sigma} \cdot \left(c\vec{p} - e\vec{A} \right) \psi_B + mc^2 \psi_A = (E - e\Phi)\, \psi_A \tag{15.305}$$

$$\vec{\sigma} \cdot \left(c\vec{p} - e\vec{A} \right) \psi_A - mc^2 \psi_B = (E - e\Phi)\, \psi_B \tag{15.306}$$

where we have substituted $\vec{\sigma}$ for $\vec{\tau}$. The potential function is $e\Phi = -Ze^2/r$ and we let $\vec{A} = 0$. Writing

$$\psi_A = \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} \quad , \quad \psi_B = \begin{pmatrix} u_3 \\ u_4 \end{pmatrix} \tag{15.307}$$

we get

$$-\frac{i}{\hbar c} \left[E + \frac{Ze^2}{r} - mc^2 \right] u_1 + \frac{\partial u_4}{\partial x} - i \frac{\partial u_4}{\partial y} + \frac{\partial u_3}{\partial z} = 0 \tag{15.308}$$

$$-\frac{i}{\hbar c} \left[E + \frac{Ze^2}{r} - mc^2 \right] u_2 + \frac{\partial u_3}{\partial x} + i \frac{\partial u_3}{\partial y} - \frac{\partial u_4}{\partial z} = 0 \tag{15.309}$$

$$-\frac{i}{\hbar c} \left[E + \frac{Ze^2}{r} + mc^2 \right] u_3 + \frac{\partial u_2}{\partial x} - i \frac{\partial u_2}{\partial y} + \frac{\partial u_2}{\partial z} = 0 \tag{15.310}$$

$$-\frac{i}{\hbar c} \left[E + \frac{Ze^2}{r} + mc^2 \right] u_4 + \frac{\partial u_1}{\partial x} + i \frac{\partial u_1}{\partial y} - \frac{\partial u_2}{\partial z} = 0 \tag{15.311}$$

We now use another clever trick I learned from Professor Hans Bethe at Cornell University to find a solution.

If we consider only large components, i.e., set the small components to zero, then $\left[\vec{L}, \hat{H}\right]$, which is proportional to $\vec{\alpha} \times \vec{p}$, will be zero, since $\vec{\alpha}$ connects the small and large components. This means that ψ_A will be an eigenfunction of $\vec{L}$. In addition, it must contain one spin component with spin up and another with spin down.

Of course, $\vec{j}$ and j_z are constants of the motion. Hence, for $j = \ell + 1/2$ we can set

$$u_1 = g(r)\sqrt{\frac{\ell + m + \frac{1}{2}}{2\ell + 1}} Y_\ell^{m-\frac{1}{2}}(\Omega) \tag{15.312}$$

$$u_2 = -g(r)\sqrt{\frac{\ell - m + \frac{1}{2}}{2\ell + 1}} Y_\ell^{m+\frac{1}{2}}(\Omega) \tag{15.313}$$

where the unknown function $g(r)$ will be the solution of some relativistic radial equation.

To get the small components we recall the equation

$$\psi_B = \frac{1}{E' - e\Phi + 2mc^2}\vec{\tau}\cdot\left(c\vec{p} - e\vec{A}\right)\psi_A \qquad (15.314)$$

and note that the operator which gives the small component from the large component has odd parity ($\vec{p}$ is odd, $\vec{A} = 0$ and everything else is even) and commutes with $\vec{j}$. Hence, ψ_B must belong to the same j value as ψ_A but must have a different ℓ.

Corresponding to $j = \ell + 1/2$ the only other possible value of the orbital angular momentum is $\ell' = \ell + 1$. Therefore, we set (remembering the appropriate Clebsch-Gordon coefficients)

$$u_3 = if(r)\sqrt{\frac{\ell - m + \frac{3}{2}}{2\ell + 3}}Y_{\ell+1}^{m-\frac{1}{2}}(\Omega) \tag{15.315}$$

$$u_4 = -if(r)\sqrt{\frac{\ell + m + \frac{3}{2}}{2\ell + 3}}Y_{\ell+1}^{m+\frac{1}{2}}(\Omega) \tag{15.316}$$

where the unknown function $f(r)$ will be the solution of some relativistic radial equation. Inserting these solution guesses into the 4 coupled equations we find that for $j = \ell + 1/2$ the connection between f and g is given by

$$\frac{1}{\hbar c}\left[E + \frac{Ze^2}{r} + mc^2\right] f = \frac{dg}{dr} - \ell\frac{g}{r} \tag{15.317}$$

$$\frac{1}{\hbar c}\left[E + \frac{Ze^2}{r} - mc^2\right] g = -\frac{df}{dr} - (\ell + 2)\frac{f}{r} \tag{15.318}$$

In an analogous way for $j = \ell - 1/2$ we have

$$u_1 = g(r)\sqrt{\frac{\ell - m + \frac{1}{2}}{2\ell + 1}}Y_\ell^{m-\frac{1}{2}}(\Omega) \tag{15.319}$$

$$u_2 = g(r)\sqrt{\frac{\ell + m + \frac{1}{2}}{2\ell + 1}}Y_\ell^{m+\frac{1}{2}}(\Omega) \tag{15.320}$$

$$u_3 = -if(r)\sqrt{\frac{\ell + m - \frac{1}{2}}{2\ell - 1}}Y_{\ell-1}^{m-\frac{1}{2}}(\Omega) \tag{15.321}$$

$$u_4 = if(r)\sqrt{\frac{\ell - m - \frac{1}{2}}{2\ell - 1}}Y_{\ell-1}^{m+\frac{1}{2}}(\Omega) \tag{15.322}$$

and

$$\frac{1}{\hbar c}\left[E + \frac{Ze^2}{r} + mc^2\right]f = \frac{dg}{dr} + (\ell + 1)\frac{g}{r} \tag{15.323}$$

$$\frac{1}{\hbar c}\left[E + \frac{Ze^2}{r} - mc^2\right]g = -\frac{df}{dr} + (\ell - 1)\frac{f}{r} \tag{15.324}$$

We now define

$$k = \begin{cases} -(\ell+1) & \text{if} \quad j = \ell + 1/2 \\ \ell & \text{if} \quad j = \ell + 1/2 \end{cases} \tag{15.325}$$

i.e.,

$$k = \begin{cases} -1, -2, ... & \text{if} \quad j = \ell + 1/2 \\ 1, 2, ... & \text{if} \quad j = \ell + 1/2 \end{cases} \tag{15.326}$$

We can then combine the 4 equations for f and g into 2 equations as

$$\frac{1}{\hbar c}\left[E + \frac{Ze^2}{r} + mc^2\right] f - \left(\frac{dg}{dr} + (1+k)\frac{g}{r}\right) = 0 \tag{15.327}$$

$$\frac{1}{\hbar c}\left[E + \frac{Ze^2}{r} - mc^2\right] g + \left(\frac{df}{dr} + (1-k)\frac{f}{r}\right) = 0 \tag{15.328}$$

Setting

$$F = rf \quad , \quad G = rg$$

$$\alpha_1 = \frac{mc^2 + E}{\hbar c} \quad , \quad \alpha_2 = \frac{mc^2 - E}{\hbar c}$$

$$\alpha = (\alpha_1 \alpha_2)^{1/2} \quad , \quad \gamma = \frac{Ze^2}{\hbar c} \quad , \quad \rho = \alpha r$$

we get

$$\left(\frac{d}{d\rho} + \frac{k}{\rho}\right) G - \left(\frac{\alpha_1}{\alpha} + \frac{\gamma}{\rho}\right) F = 0 \tag{15.329}$$

$$\left(\frac{d}{d\rho} - \frac{k}{\rho}\right) F - \left(\frac{\alpha_2}{\alpha} - \frac{\gamma}{\rho}\right) G = 0 \tag{15.330}$$

We now solve these coupled equations using the standard series method to obtain the positive energy bound state solutions.

We substitute

$$F = \phi(\rho) e^{-\rho} \quad , \quad F = \chi(\rho) e^{-\rho} \tag{15.331}$$

and obtain

$$\chi' - \chi + \frac{k}{\rho}\chi - \left(\frac{\alpha_1}{\alpha} + \frac{\gamma}{\rho}\right)\phi = 0 \tag{15.332}$$

$$\phi' - \phi - \frac{k}{\rho}\phi - \left(\frac{\alpha_2}{\alpha} - \frac{\gamma}{\rho}\right)\chi = 0 \tag{15.333}$$

We now substitute the series

$$\phi = \rho^s \sum_{m=0}^{\infty} a_m \rho^m \quad , \; a_0 \neq 0 \quad , \quad \chi = \rho^s \sum_{m=0}^{\infty} b_m \rho^m \quad , \; b_0 \neq 0 \tag{15.334}$$

the requirement that f and g be finite everywhere turns out to be impossible to satisfy. Instead, we require that the integrated probability density be finite, i.e.,

$$\int_0^{\infty} \left[|F(\rho)|^2 + |G(\rho)|^2\right] d\rho < \infty \tag{15.335}$$

This makes sure that $s \neq -\infty$. Substituting the series and equating coefficients of the same power of ρ we get the recursion relations

$$(s+\nu+k)b_\nu - b_{\nu-1} - \gamma a_\nu - \frac{\alpha_1}{\alpha} a_{\nu-1} = 0 \tag{15.336}$$

$$(s+\nu-k)a_\nu - a_{\nu-1} + \gamma b_\nu - \frac{\alpha_2}{\alpha} b_{\nu-1} = 0 \tag{15.337}$$

For $\nu = 0$ we get

$$(s+k)b_0 - \gamma a_0 = 0 = (s-k)a_0 + \gamma b_0 \tag{15.338}$$

These equations have a nontrivial solution if and only if

$$s = \pm(k^2 - \gamma^2)^{1/2} \tag{15.339}$$

First we look at the negative root. For small ρ the integrand for the integrated probability density is $\sim \rho^{2s}$ and we must have $2s > -1$ or $(k^2 - \gamma^2)^{1/2} > 1/2$. The minimum s occurs when $k^2 = 1$. This corresponds to $Z \geq 109$. For $k^2 > 1$, no value of Z will permit the negative root.

Restricting ourselves to $Z < 109$, we choose the positive root $s = (k^2 - \gamma^2)^{1/2}$. For $k = 1$, $s < 1$, f and g diverge at the origin. The probability density integral converges, however.

The recursion relations lead to function of the order $e^{2\rho}$ (the probability density integral would diverge) unless the series terminate. Suppose the series terminate for $\nu = n'$, i.e., $a_{n'+1} = b_{n'+1} = 0$. We then have from the recursion relations that

$$\alpha_1 a_{n'} = -\alpha b_{n'} \quad , \quad n' = 0, 1, 2, ... \tag{15.340}$$

We now multiply the first recursion relation by α and the second by α_1 and subtract them to get

$$b_\nu[\alpha(s + \nu + k) - \alpha_1\gamma] = a_\nu[\alpha_1(s + \nu - k) + \alpha\gamma] \tag{15.341}$$

Inserting $\nu = n'$ and using $\alpha_1 a_{n'} = -\alpha b_{n'}$ we get

$$2\alpha(s + n') = \gamma(\alpha_1 - \alpha_2) = \frac{2E\gamma}{\hbar c} \tag{15.342}$$

Putting everything together we get

$$E = mc^2 \left[1 + \frac{\gamma^2}{(s+n')^2}\right]^{-1/2} = mc^2 \left[1 + \frac{\gamma^2}{\left(n' + \sqrt{k^2 - \gamma^2}\right)^2}\right]^{-1/2} \tag{15.343}$$

Since $|k| = j + \frac{1}{2}$ we get

$$E = mc^2 \left[1 + \frac{\gamma^2}{\left(n' + \sqrt{(j+\frac{1}{2})^2 - \gamma^2}\right)^2}\right]^{-1/2}$$

$$n' = 0, 1, 2... \; j + \tfrac{1}{2} = 1, 2, 3, ... \tag{15.344}$$

where $\gamma = Ze^2/\hbar c$.

Before looking at the physics in this result let us investigate an alternative approach involving a second-order Dirac Equation. The first-order Dirac equation is

$$\beta\left(i\hbar\frac{\partial}{\partial t}-\hat{H}\right)\psi(\vec{r},t)=0 \quad , \quad \hat{H}=c\vec{\alpha}\cdot\left(\frac{\hbar}{i}\nabla-\frac{e}{c}\vec{A}\right)+\beta mc^2+e\Phi \tag{15.345}$$

We now define the projection operator $\hat{P}$ as

$$\hat{P}=\frac{\beta\left(i\hbar\frac{\partial}{\partial t}-\hat{H}\right)+2mc^2}{2mc^2} \tag{15.346}$$

and operate on the Dirac equation from the left. After some algebra we get

$$\left[\frac{1}{c^2}\left(i\hbar\frac{\partial}{\partial t}-e\Phi\right)^2-\left(\frac{\hbar}{i}\nabla-\frac{e}{c}\vec{A}\right)^2 -m^2c^2+\frac{e\hbar}{c}\left(\vec{\sigma}\cdot\vec{B}-i\vec{\alpha}\cdot\vec{\varepsilon}\right)\right]\psi=0 \tag{15.347}$$

where we have used the relations

$$\left[\vec{\alpha}\cdot\left(\frac{\hbar}{i}\nabla - \frac{e}{c}\vec{A}\right)\right]^2 = \left(\frac{\hbar}{i}\nabla - \frac{e}{c}\vec{A}\right)^2 - \frac{e\hbar}{c}\vec{\sigma}\cdot\vec{B} \qquad (15.348)$$

and

$$\left[\frac{\hbar}{i}\nabla - \frac{e}{c}\vec{A}, i\hbar\frac{\partial}{\partial t} - e\Phi\right] = -i\hbar e\vec{\varepsilon} \qquad (15.349)$$

The new second-order equation is just the Klein-Gordon equation with an additional term $\left(\vec{\sigma}\cdot\vec{B} - i\vec{\alpha}\cdot\vec{\varepsilon}\right)$, which represents the direct coupling of the electromagnetic fields to the magnetic(and electric) moments of the particle.

Every solution of the Dirac equation is a solution of this new second-order equation, but every solution of the second-order equation in not necessarily a solution of the Dirac equation.

If, however, ψ is a solution of the second-order equation, then $\phi = \hat{P}\psi$ is a solution of the Dirac equation. We can see this as follows. The second-order equation can be written as

$$\hat{P}\beta\left(i\hbar\frac{\partial}{\partial t}-\hat{H}\right)\psi(\vec{r},t)=\beta\left(i\hbar\frac{\partial}{\partial t}-\hat{H}\right)\hat{P}\psi(\vec{r},t)=0 \quad (15.350)$$

or the second order equation is equivalent to

$$\left(i\hbar\frac{\partial}{\partial t}-\hat{H}\right)\psi(\vec{r},t)=\left(i\hbar\frac{\partial}{\partial t}-\hat{H}\right)\phi(\vec{r},t)=0 \qquad (15.351)$$

This says that $\hat{P}$ acts as a projection operator, which reduces solutions of the second-order equation to solutions of the first-order Dirac equation.

Let us now use the second-order equation to find the energy levels of the Dirac hydrogen atom (Glauber, et al PR **109**,1307(1958)). For a stationary state of energy E in the Coulomb potential the second-order equation becomes

$$\left[\frac{1}{c^2}\left(E+\frac{Ze^2}{r}\right)^2-\left(\frac{\hbar}{i}\nabla\right)^2-m^2c^2+\frac{i\hbar Ze^2}{r^2c}\alpha_r\right]\psi=0 \qquad (15.352)$$

where $\alpha_r = \vec{\alpha} \cdot \hat{r}$. We now write

$$\left(\frac{\hbar}{i}\nabla\right)^2 = -\frac{\hbar^2}{r^2}\frac{\partial^2}{\partial r^2}r^2 + \frac{\hat{L}^2}{r^2} \tag{15.353}$$

and get the equation

$$\left[\frac{E^2 - m^2c^4}{c^2} + \frac{2EZe^2}{rc^2} + \frac{\hbar^2}{r^2}\frac{\partial^2}{\partial r^2}r^2 \right.$$
$$\left. - \frac{\hat{L}^2 - \left(\frac{Ze^2}{c}\right)^2 - i\hbar\left(\frac{Ze^2}{c}\right)\alpha_r}{r^2}\right]\psi = 0 \tag{15.354}$$

We now use a few tricks to change this equation, which is almost in the same form as the Klein-Gordon equation for the Coulomb potential, into exactly the same form.

We first define the operator

$$\hat{K} = \beta\left(1 + \vec{\sigma}\cdot\frac{\vec{L}}{\hbar}\right) \tag{15.355}$$

with these properties

$$\left[\hat{K}, \vec{\alpha}\cdot\vec{p}\right] = 0 \quad , \quad \left[\hat{K}, \vec{\alpha}\cdot\vec{r}\right] = 0 \quad , \quad \left[\hat{K}, r^2\right] = 0 \tag{15.356}$$

$$\left[\hat{K}, \vec{J}\right] = 0 \quad , \quad \vec{J} = \vec{L} + \frac{\hbar}{2}\vec{\sigma} \tag{15.357}$$

These imply that $\hat{K}$ commutes with the Hamiltonian

$$\hat{H} = c\vec{\alpha}\cdot\vec{p} + \beta mc^2 - \frac{Ze^2}{r} \tag{15.358}$$

for the relativistic hydrogen atom.

This says that $\hat{K}$ is a constant of the motion and since it also commutes with the total angular momentum we can label the common eigenstates or energy levels of the hydrogen atom by the eigenvalues of $\hat{K}$, $\hat{J}^2$ and $\hat{J}_z$.

$\hat{K}$ is a constant of the motion for any spherically symmetric, spin-independent potential and physically it measures the degree to which the spin and the orbital angular momentum of the particle are aligned.

Let us find the eigenvalues k of $\hat{K}$. We note that

$$\begin{aligned}
\hat{K}^2 &= \left(1 + \vec{\sigma} \cdot \frac{\vec{L}}{\hbar}\right)^2 = 1 + \left(\vec{\sigma} \cdot \frac{\vec{L}}{\hbar}\right)^2 + 2\vec{\sigma} \cdot \frac{\vec{L}}{\hbar} \\
&= 1 + \left(\frac{\vec{L} \cdot \vec{L}}{\hbar^2} + \frac{i}{\hbar^2}\vec{\sigma} \cdot (\vec{L} \times \vec{L})\right) + 2\vec{\sigma} \cdot \frac{\vec{L}}{\hbar} \\
&= 1 + \left(\frac{\vec{L} \cdot \vec{L}}{\hbar^2} + \frac{i}{\hbar^2}\vec{\sigma} \cdot (i\hbar\vec{L})\right) + 2\vec{\sigma} \cdot \frac{\vec{L}}{\hbar} \\
&= 1 + \frac{L^2}{\hbar^2} + \vec{\sigma} \cdot \frac{\vec{L}}{\hbar} = \frac{1}{\hbar^2}\left(\vec{L} + \frac{\hbar}{2}\vec{\sigma}\right)^2 + \frac{1}{4} \\
&= \frac{\hat{J}^2}{\hbar^2} + \frac{1}{4}
\end{aligned} \tag{15.359}$$

where we have used

$$(\vec{\sigma} \cdot \vec{A})(\vec{\sigma} \cdot \vec{B}) = \vec{A} \cdot \vec{B} + i\vec{\sigma} \cdot (\vec{A} \times \vec{B})$$

$$\vec{L} \times \vec{L} = i\hbar\vec{L} \quad , \quad \vec{J} = \vec{L} + \vec{S} \quad , \quad \vec{S} = \frac{\hbar}{2}\vec{\sigma}$$

Therefore, we have

$$k^2 = j(j+1) + \frac{1}{4} = (j + \tfrac{1}{2})^2 \tag{15.360}$$

Now, since $\left\{\hat{K}, \gamma_5\right\} = 0$ we find that, if k is an eigenvalue of $\hat{K}$, i.e.,

$$\hat{K} |k\rangle = k |k\rangle \tag{15.361}$$

then

$$\hat{K}\gamma_5 |k\rangle = -\gamma_5\hat{K} |k\rangle = -k\gamma_5 |k\rangle \tag{15.362}$$

which says that $-k$ is also an eigenvalue of $\hat{K}$. The eigenvalues are then

$$k = \pm 1 \ , \ \pm 2 \ , \ \pm 3 \ , ... \tag{15.363}$$

since $j = 1/2, 3/2, 5/2, \ldots\ldots..$ Note that zero is not an eigenvalue of $\hat{K}$. In addition, an eigenstate of $\hat{K}$ with eigenvalue k is an eigenstate of $\hat{J}^2$ with eigenvalue $j = |k| - 1/2$.

We now find the energy eigenvalues. Define the operator

$$\hat{\Lambda} = -\beta\hat{K} - i\frac{Ze^2}{\hbar c}\alpha_r \tag{15.364}$$

with the properties

$$\left[\hat{\Lambda}, \hat{K}\right] = 0 \quad , \quad \left[\hat{\Lambda}, \vec{J}\right] = 0 \quad , \quad \Lambda^2 = K^2 - \left(\frac{Ze^2}{\hbar c}\right)^2 \tag{15.365}$$

A little algebra then shows that

$$\hbar^2\hat{\Lambda}(\hat{\Lambda} + 1) = \hat{L}^2 - \left(\frac{Ze^2}{c}\right)^2 - i\hbar\left(\frac{Ze^2}{c}\right)\alpha_r \tag{15.366}$$

which is the operator in the last term of the second-order equation. We can then write

$$\left[\frac{E^2 - m^2c^4}{c^2} + \frac{2EZe^2}{rc^2} + \frac{\hbar^2}{r^2}\frac{\partial^2}{\partial r^2}r^2 - \frac{\hbar^2\hat{\Lambda}(\hat{\Lambda}+1)}{r^2}\right]\psi = 0 \tag{15.367}$$

This is exactly the same form as the Klein-Gordon equation except that

$$\ell'(\ell'+1) \to \hat{\Lambda}(\hat{\Lambda}+1) \tag{15.368}$$

or a number has been replaced by an operator. Now if $\psi(\vec{r})$ is an eigenstate of $\hat{\Lambda}(\hat{\Lambda}+1)$ then the operator $\hat{\Lambda}(\hat{\Lambda}+1)$ in the equation is replaced by its eigenvalue which we can write as $\ell'(\ell'+1)$. This says that the energy eigenvalues are given by the same formula as in the spin zero case, i.e.,

$$E = \frac{mc^2}{\left[1 + \left(\frac{Ze^2}{\hbar cn'}\right)^2\right]^{1/2}} \quad , \quad n' = \ell' + 1 + \nu \quad , \quad \nu = 0, 1, 2, ... \tag{15.369}$$

Since $\hat{\Lambda}$, $\hat{K}$, $\hat{J}^2$ and $\hat{J}_z$ all commute, we can construct solutions which are eigenstates of $\hat{K}$, $\hat{J}^2$ and $\hat{J}_z$ as well as $\hat{\Lambda}$.

$\hat{\Lambda}$ does not commute with $\hat{H}$ however. This means that the solutions we have found for the second order equation cannot directly be eigenfunctions of $\hat{H}$. Instead, since

$$\hat{H}(\hat{P}\psi) = E(\hat{P}\psi) \tag{15.370}$$

i.e., the energy eigenvalues from the second-order equation are also the eigenvalues of $\hat{H}$, we can find eigenfunctions of $\hat{H}$ by using the projection operator $\hat{P}$. Since $\hat{P}$ and $\hat{\Lambda}$ do not commute, the eigenfunction of $\hat{H}$, namely $\hat{P}\psi$, will generally be a linear combination of different $\hat{\Lambda}$ eigenfunctions.

To find the energy eigenvalues we need to know the eigenvalues of $\hat{\Lambda}$. Consider an eigenstate of $\hat{\Lambda}$ and $\hat{K}$ with eigenvalues k. We then have

$$\hat{\Lambda}^2 |k\rangle = \lambda^2 |k\rangle = \left(\hat{K}^2 - \left(\frac{Ze^2}{\hbar c}\right)^2\right) |k\rangle = \left(k^2 - \left(\frac{Ze^2}{\hbar c}\right)^2\right) |k\rangle \tag{15.371}$$

or

$$\lambda = \left(k^2 - \left(\frac{Ze^2}{\hbar c}\right)^2\right)^{1/2} \tag{15.372}$$

and the possible eigenvalues of $\hat{\Lambda}$ are $\pm\lambda$. When $\hat{\Lambda}(\hat{\Lambda}+1)$ acts on a $(\hat{\Lambda}\ , \hat{K})$ eigenstate it has the eigenvalue $\pm\lambda(\pm\lambda+1) = \ell'(\ell'+1)$. This leads to two possible ℓ' values for each eigenvalue of $\hat{\Lambda}$:

$$\ell' = \begin{cases} \lambda,\ -\lambda-1 & \text{for } \Lambda = \lambda \\ -\lambda,\ \lambda-1 & \text{for } \Lambda = -\lambda \end{cases} \tag{15.373}$$

For each eigenvalue of $\hat{\Lambda}$, the two ℓ' solutions add up to -1. The smaller of the two solutions $-lambda$ and $-\lambda-1$ are eliminated because they are not normalizable (behavior near the origin). This leave two cases to consider:

$$\begin{aligned} &(1) \quad \Lambda = \lambda \quad , \quad \ell' = \lambda \\ &(2) \quad \Lambda = -\lambda \quad , \quad \ell' = \lambda - 1 \end{aligned}$$

The possible energy eigenvalues are given by

$$E = \frac{mc^2}{\left[1 + \left(\frac{Ze^2}{\hbar c n'}\right)^2\right]^{1/2}} \quad , \quad n' = \ell' + 1 + \nu \quad , \quad \nu = 0, 1, 2, ... \tag{15.374}$$

or redefining some quantities

$$n' = n - |k| + \lambda = n - j - \tfrac{1}{2} + \sqrt{\left(j + \tfrac{1}{2}\right)^2 - \left(\frac{Ze^2}{\hbar c}\right)^2} \tag{15.375}$$

so that n takes on the values

$$n = |k| \;,\; |k| + 1 \;,\; |k| + 2 \;,\; ....\text{for}\Lambda = -\lambda$$
$$n = |k| + 1 \;,\; |k| + 2 \;,\; |k| + 3 \;,\; ....\text{for}\Lambda = \lambda$$

the energy levels are then given by

$$E = mc^2 \left[1 + \frac{\left(\frac{Ze^2}{\hbar c}\right)^2}{\left[n - j - \frac{1}{2} - \sqrt{\left(j+\frac{1}{2}\right)^2 - \left(\frac{Ze^2}{\hbar c}\right)^2} \right]^2} \right]^{-1/2} \tag{15.376}$$

The quantum number n is just the principal quantum number of the hydrogen atom.

The energy level structure looks like the figure below.

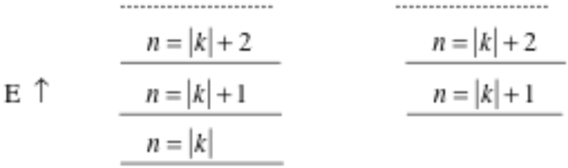

Figure: Dirac hydrogen energy level structure where the left sequence corresponds to $\Lambda = -\lambda$ and the right sequence to $\Lambda = \lambda$.

Some Features

The energy levels for the spin 1/2 particle are the same as those found for the spin 0 particle with $\ell \to j$. The energy is real only if

$$j + \tfrac{1}{2} < \frac{Ze^2}{\hbar c} \tag{15.377}$$

which corresponds to $Z < 137$ for $j = 1/2$.

The Dirac theory leads to an accidental degeneracy in ℓ, i.e., states with the same j but different ℓ have the same energy. This degeneracy is removed by the Lamb shift, which is due to the interaction of the electron with its own field. As we shall see later, for $j = 1/2$, the effect is one order of magnitude smaller then the fine structure splitting. For $j \geq 3/2$, it is two orders of magnitude smaller.

An expansion in powers of $Z\alpha$, where

$$\alpha = \frac{e^2}{\hbar c} = \text{ fine structure constant} \tag{15.378}$$

looks like

$$E_{n,j} = mc^2 \left[1 - \frac{Z^2\alpha^2}{2n^2} - \frac{(Z\alpha)^4}{2n^3}\left(\frac{1}{j+\frac{1}{2}} - \frac{3}{4n}\right) + O((Z\alpha)^6)\right] \tag{15.379}$$

which agrees with the perturbation calculations we carried out earlier.

Some Details about the Energy Levels

The solutions of the Dirac equation are not $\hat{\Lambda}$ eigenstates but they are $\hat{K}$ eigenstates and $\hat{K}$ is a constant of the motion (it commutes with the Hamiltonian). The total orbital angular momentum $\vec{L}$ is not a constant of the motion and neither is $\hat{L}^2$. We need to come up with some way to classify the energy levels in the relativistic hydrogen atom using the eigenvalues k.

To get a handle on how to proceed we look at the nonrelativistic limit where

$$\hat{\Lambda} \to -\beta\hat{K} \to -\hat{K} \text{ for positive energy states} \tag{15.380}$$

We expect the solutions of the second order equation with one sign of $\hat{\Lambda}$ to correspond to solutions of the first-order equation with the opposite sign of $\hat{K}$. This means that

$$\begin{aligned}
n &= |k| \ , \ |k|+1 \ , \ |k|+2 \ , \ .... \text{ for } \Lambda = -\lambda \to k > 0 \\
n &= |k|+1 \ , \ |k|+2 \ , \ |k|+3 \ , \ .... \text{ for } \Lambda = \lambda \to k < 0
\end{aligned}$$

It turns out to be convenient to still label the solutions by the ℓ value that they would have in the nonrelativistic limit. To find this ℓ value we use

$$\begin{aligned}
\hat{K}^2 &= 1 + \frac{\hat{L}^2}{\hbar^2} + \vec{\sigma}\cdot\frac{\vec{L}}{\hbar} = \beta\hat{K} + \frac{\hat{L}^2}{\hbar^2} \\
\hat{K}(\hat{K}-\beta) &= \frac{\hat{L}^2}{\hbar^2}
\end{aligned}$$

In the nonrelativistic limit, $\beta \to 1$ and we have

$$\hat{K}(\hat{K}-1) = \frac{\hat{L}^2}{\hbar^2} \to k(k-1) = \ell(\ell+1) \tag{15.381}$$

so that ℓ becomes the total orbital angular momentum quantum number in the nonrelativistic limit. Solving for ℓ in terms of k we get

$$\ell = \begin{cases} k-1 = j-1/2 & \text{for } k > 0 \\ |k| = j+1/2 & \text{for } k < 0 \end{cases} \tag{15.382}$$

Now K measures the alignment of the spin and the orbital angular momentum. The above results say that for $k > 0$, they are essentially parallel and so $j = \ell + 1/2$ and for $k < 0$ they are essentially antiparallel so $j = \ell - 1/2$.

A detailed calculation of the wave functions shows that the upper two components of the wave function (the large components) are eigenstates of total orbital angular momentum with eigenvalue ℓ, while the lower two components (the small components) are eigenstates of total orbital angular momentum with eigenvalue $\ell + 1$ for $k > 0$ and with $\ell - 1$ for $k < 0$.

The complete energy level scheme for the relativistic hydrogen atom for $n = 1$, 2, and 3 looks like Figure 14.3 below.

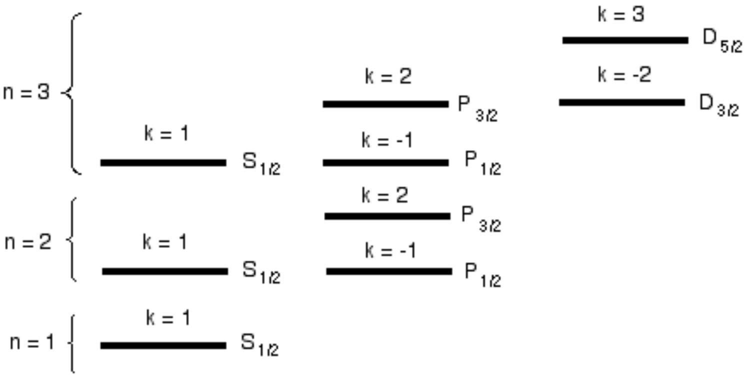

Figure: Energy level structure for relativistic hydrogen

The complete degeneracy of a given n in the nonrelativistic case is lifted by relativistic effects.

The degeneracy between states like $1S_{1/2}$, $2P_{3/2}$, $3D_{5/2}$, $4F_{7/2}$, etc is now broken. The degeneracy still remains between states like $2S_{1/2}$ and $2P_{1/2}$, $3S_{1/2}$ and $3P_{1/2}$, $3P_{3/2}$ and $3D_{3/2}$, etc., levels.

All levels except $1S_{1/2}$, $2P_{3/2}$, $3D_{5/2}$, etc., are 2-fold degenerate because they are the eigenstates of of K with opposite eigenvalues, i.e., $2P_{3/2} \rightarrow k = 2$, $2D_{3/2} \rightarrow k = -2$.

Hyperfine Structure

The are two corrections that modify the energy level results from the Dirac equation. The two-fold degeneracy is removed by the interaction of the electron with vacuum fluctuations of the electromagnetic radiation field. This effect is called the Lamb shift. In addition, there is also a hyperfine interaction which splits every level into two, It is due to the interaction of the electron with the magnetic moment of the proton. We consider hyperfine splitting first.

As an example we derive the hyperfine splitting of an $s-$state using nonrelativistic first-order perturbation theory. The interaction of the electron spin with the magnetic moment of the proton is given by

$$\hat{H}' = \frac{|e|\,\hbar}{2mc}\vec{\sigma}\cdot\vec{B}(\vec{r}) = \mu_B\vec{\sigma}\cdot\vec{B}(\vec{r}) \tag{15.383}$$

where $\vec{B}(\vec{r})$ is the magnetic field due to the magnetic moment of the proton. This magnetic moment is given by

$$\vec{M}_p = \frac{|e|\,\hbar g_p}{4m_p c}\vec{\sigma}_p = \frac{1}{2}g_p\mu_p\vec{\sigma}_p \tag{15.384}$$

where g_p is the gyromagnetic ratio of the proton, m_p is the proton mass and $\hbar\vec{\sigma}_p/2$ is the spin of the proton. The magnetic field from this magnetic moment (assuming the proton is fixed at the origin) is given by the relations

$$\vec{A}(\vec{r}) = -\vec{M}_p \times \nabla \left(\frac{1}{r}\right) = \text{ vector potential} \tag{15.385}$$

$$\vec{B}(\vec{r}) = \nabla \times \vec{A}(\vec{r}) \tag{15.386}$$

$$\vec{B}(\vec{r}) = -\nabla \times (\vec{\sigma}_p \times \nabla)\frac{g_p \mu_p}{2r} \tag{15.387}$$

This gives

$$\begin{aligned}
\hat{H}' &= -g_p \mu_B \mu_p \vec{\sigma} \cdot \left(\nabla \times (\vec{\sigma}_p \times \nabla)\frac{1}{2r}\right) \\
&= -g_p \mu_B \mu_p \vec{\sigma} \cdot (\vec{\sigma}_p (\nabla \cdot \nabla) - \nabla(\vec{\sigma}_p \cdot \nabla))\,\frac{1}{2r} \\
&= -g_p \mu_B \mu_p \left((\vec{\sigma} \cdot \vec{\sigma}_p)(\nabla \cdot \nabla) - (\vec{\sigma} \cdot \nabla)(\vec{\sigma}_p \cdot \nabla)\right)\frac{1}{2r}
\end{aligned} \tag{15.388}$$

The first-order shift of the level is

$$\left\langle \hat{H}' \right\rangle = -g_p \mu_B \mu_p \int d^3r \times$$

$$|\psi(\vec{r})|^2 \left[\left(\langle \vec{\sigma} \cdot \vec{\sigma}_p \rangle (\nabla \cdot \nabla) - \langle (\vec{\sigma} \cdot \nabla)(\vec{\sigma}_p \cdot \nabla) \rangle \right) \frac{1}{2r} \right] \tag{15.389}$$

where the brackets $\langle .....\rangle$ denote the expectation value in the relative spin state of the electron and proton and $\psi(\vec{r})$ is the nonrelativistic wave function of the level. If we only consider $s-$states, which are spherically symmetric, then

$$\langle (\vec{\sigma} \cdot \nabla)(\vec{\sigma}_p \cdot \nabla) \rangle = \frac{1}{3} \langle (\vec{\sigma} \cdot \vec{\sigma}_p) \rangle \nabla^2 \tag{15.390}$$

and we get

$$\begin{aligned}\left\langle \hat{H}' \right\rangle &= -\frac{1}{3} g_p \mu_B \mu_p \int d^3r \, |\psi(\vec{r})|^2 \left\langle (\vec{\sigma} \cdot \vec{\sigma}_p) \right\rangle \left(\nabla^2 \frac{1}{2r} \right) \\ &= \frac{4\pi}{3} g_p \mu_B \mu_p \left\langle (\vec{\sigma} \cdot \vec{\sigma}_p) \right\rangle \int d^3r \, |\psi(\vec{r})|^2 \delta(\vec{r}) \\ &= \frac{4\pi}{3} g_p \mu_B \mu_p \left\langle (\vec{\sigma} \cdot \vec{\sigma}_p) \right\rangle |\psi(0)|^2 \end{aligned} \tag{15.391}$$

where we have used

$$\nabla^2 \frac{1}{r} = -4\pi\delta(\vec{r}) \tag{15.392}$$

For the hydrogen atom $s-$state

$$|\psi(0)|^2 = \frac{1}{\pi(na_0)^3} \tag{15.393}$$

and we get

$$\left\langle \hat{H}' \right\rangle = \frac{2}{3} \left(\frac{e^2}{2a_0} \right) g_p \frac{m}{m_p} \frac{\alpha^2}{n^3} \left\langle (\vec{\sigma} \cdot \vec{\sigma}_p) \right\rangle \tag{15.394}$$

We then have

$$\vec{F} = \vec{S} + \vec{I} = \text{ total spin} \tag{15.395}$$

For $S = \frac{1}{2}$, $I = \frac{1}{2}$, we have $F = 0$(singlet) , 1(triplet). But

$$\vec{F} = \vec{S} + \vec{I} \rightarrow \vec{F}^2 = \vec{S}^2 + \vec{I}^2 + 2\vec{S} \cdot \vec{I} \tag{15.396}$$

$$\vec{S} \cdot \vec{I} = \frac{\hbar^2}{4} \vec{\sigma} \cdot \vec{\sigma}_p = \frac{\hbar^2}{2} (F(F+1) - 3/2) \tag{15.397}$$

We then have for a relative triplet state $\langle (\vec{\sigma} \cdot \vec{\sigma}_p) \rangle = 1$ and for a relative singlet state $\langle (\vec{\sigma} \cdot \vec{\sigma}_p) \rangle = -3$. This says that the singlet state lies lower than the triplet.

The total splitting of the *ground state* is

$$\Delta E = \frac{8}{3} \left(\frac{e^2}{2a_0} \right) g_p \frac{m}{m_p} \alpha^2 \tag{15.398}$$

between the triplet and singlet.

The transition between these two levels generates radiation with a frequency of $1420\,MHz$ and a wavelength of $21.4\,cm$. This radiation is very important in astronomy. From its intensity, Doppler broadening, and Doppler shift, one obtains information concerning the density, temperature, and motion of interstellar and intergalactic hydrogen clouds.

The Lamb Shift

The coupling

$$\hat{H}_{\text{int}} = -\frac{e}{c}\int d^3r\,\vec{j}(\vec{r})\cdot\vec{A}(\vec{r}) \tag{15.399}$$

of the electron to the quantum mechanical radiation field causes a shift in the energy levels of the hydrogen atom. Although not an exact calculation, we can get some idea of the fundamental difficulties in quantum electrodynamics by doing a nonrelativistic second-order perturbation calculation.

We consider an electron in the state $|n\rangle$ with energy ε_n. Because of the above interaction (see last part of this chapter) the electron is able to spontaneously emit a photon thereby going to some state $|n'\rangle$. This produces a second-order shift in the energy given by

$$\Delta E_n = \sum_{n'} \sum_{\vec{k}\vec{\lambda}} \frac{\left| \left\langle n', \vec{k}\vec{\lambda} \right| \hat{H}_{\rm int} \left| n, 0 \right\rangle \right|^2}{\varepsilon_n - \varepsilon_{n'} - ck} \tag{15.400}$$

where $|n, 0\rangle$ is the initial state with the electron in $|n\rangle$ with no photons present, and $\left| n', \vec{k}\vec{\lambda} \right\rangle$ is the intermediate state with an electron in $|n'\rangle$ and on photon of momentum $\vec{k}$ and polarization $\vec{\lambda}$ present. The energy of this intermediate state is $\varepsilon_{n'} + ck$.

From the quantum theory of electromagnetic radiation (see end of this chapter) we have that

$$\left\langle n', \vec{k}\vec{\lambda} \right| \hat{H}_{\rm int} \left| n, 0 \right\rangle = -\frac{e}{c}\sqrt{\frac{2\pi\hbar^2 c^2}{\omega_k V}} \left\langle n' \right| \vec{j}_{\vec{k}} \cdot \vec{\lambda}^* \left| n \right\rangle \tag{15.401}$$

where $\vec{j}_{\vec{k}}$ is the k^{th} Fourier component of the current $\vec{j}(\vec{r})$. Therefore,

$$\Delta E_n = \int \frac{d^3k}{(2\pi\hbar)^3} \frac{2\pi\hbar^2 e^2}{ck} \sum_{n'} \frac{\sum_{\vec{\lambda}} \left| \langle n' | \, \vec{j}_{\vec{k}} \cdot \vec{\lambda}^* \, | n \rangle \right|^2}{\varepsilon_n - \varepsilon_{n'} - ck}$$

$$= \int \frac{k^2 dk}{4\pi^2\hbar} \frac{e^2}{ck} \sum_{n'} \frac{\int d\Omega \sum_{\vec{\lambda}} \left| \langle n' | \, \vec{j}_{\vec{k}} \cdot \vec{\lambda}^* \, | n \rangle \right|^2}{\varepsilon_n - \varepsilon_{n'} - ck} \qquad (15.402)$$

In the dipole approximation, we can use

$$\vec{j}_{\vec{k}} \to \vec{j}_0 = \frac{\vec{p}}{m} \quad , \quad \vec{p} = \text{ electron momentum operator} \qquad (15.403)$$

The angular integration over the polarizations is given by

$$\int d\Omega \sum_{\vec{\lambda}} \left| \langle n' | \, \vec{j}_{\vec{k}} \cdot \vec{\lambda}^* \, | n \rangle \right|^2 = \frac{1}{m} \int d\Omega \sum_{\vec{\lambda}} \left| \langle n' | \, \vec{p} \cdot \vec{\lambda}^* \, | n \rangle \right|^2$$

$$= \frac{4\pi}{m} \frac{2}{3} \left| \langle n' | \, \vec{p} \, | n \rangle \right|^2$$

where the factor 2/3 comes from the fact that there are only 2 independent polarizations for each $\vec{k}$ value. This gives

$$\Delta E_n = \frac{2e^2}{3\pi\hbar c^3 m^2} \int_0^\infty \omega d\omega \sum_{n'} \frac{\left| \langle n' | \, \vec{p} \, | n \rangle \right|^2}{\varepsilon_n - \varepsilon_{n'} - \omega} \quad , \quad \omega = ck \quad (15.404)$$

The first problem we encounter is that the ω integral diverges!! This means that the interaction with the radiation field produces an *infinite shift downward* in the energy of the electron.

This result presented theoretical physics with a great difficulty for many years. In the late 1940's it was resolved due to the work of Feynman, Schwinger and Tomonaga in producing new calculation rules within the context of quantum electrodynamics and by Bethe and Weisskopf who actually carried out the calculation using the new rules and got a finite number agreeing with experiment.

Let us try to understand some aspects of what happened.

If we do a similar calculation for a free electron, then one gets an infinite result again. In the dipole approximation, we can evaluate the energy shift for a free electron in a momentum state $|\vec{p}\rangle$. We get

$$\Delta E_{\vec{p}} = \frac{2e^2}{3\pi\hbar c^3 m^2} \int\limits_0^\infty \omega d\omega \sum_{\vec{q}} \frac{|\langle\vec{q}|\,\vec{p}\,|\vec{p}\rangle|^2}{\varepsilon_q - \varepsilon_p - \omega} \tag{15.405}$$

Since this is a free particle $\varepsilon_q - \varepsilon_p = 0$ and we have

$$\Delta E_{\vec{p}} = -\frac{2e^2}{3\pi\hbar c^3 m^2}\int\limits_0^\infty \omega d\omega \frac{\left|\langle\vec{p}|\,\vec{p}\,|\vec{p}\rangle\right|^2}{\omega} = -\frac{2e^2}{3\pi\hbar c^3 m^2} p^2 \int\limits_0^\infty d\omega \tag{15.406}$$

which is infinite. What Bethe and Weisskopf noticed was that this expression is proportional to p^2. In their development of quantum electrodynamics, Feynman, Schwinger and Tomonaga had similar problems which they were able to deal with be redefining the electron parameters that appeared in the theory (like mass and charge). The process is called *renormalization*. In this process all infinite expression are consistently incorporated into the mass or charge parameters and then these are defined to have the known experimental values.

In our case, we can interpret the infinite result as redefining the mass, i.e., as representing a shift of the mass of the electron. In terms of the mathematics, this means the following.

If we say that m_0 is the mass and $p^2/2m_0$ is the kinetic energy of a free electron of momentum $\vec{p}$ neglecting the electromagnetic interactions, then the energy including the effects of the electromagnetic interactions is given by

$$\frac{p^2}{2m_0} + \Delta E_{\vec{p}} = \left(\frac{1}{m_0} - \frac{2e^2}{3\pi\hbar c^3 m^2} \int_0^{\infty} d\omega \right) \frac{p^2}{2} = \frac{1}{m} \frac{p^2}{2} \quad (15.407)$$

i.e., we have *renormalized* the electron mass. The so-called electromagnetic self-energy of the electron can thus be interpreted as giving a shift of the mass of the electron from its *bare* (no electromagnetic interactions) value m_0 to its *observed* (measured in the laboratory where all interactions are present) value m.

We then argue that the reason the interacting electron has an infinite energy shift is that it includes the infinite energy change that we already have counted once when we use the observed mass m rather than the bare mass in the calculation and, thus, we are double counting.

In other words, we should really start out with the Hamiltonian for the hydrogen atom in the presence of the radiation field given by

$$\hat{H} = \frac{p^2}{2m_0} - \frac{e^2}{r} + \hat{H}_{\text{int}} \tag{15.408}$$

Then using the corrected expression for m we get

$$\hat{H} = \frac{p^2}{2m} - \frac{e^2}{r} + \left(\hat{H}_{\text{int}} + \frac{2e^2}{3\pi\hbar c^3 m^2} \int_0^\infty d\omega \right) \tag{15.409}$$

This means that if we write the observed free particle mass in the kinetic energy (which we always do) we should not count that part of $\hat{H}_{\text{int}}$ that produces the infinite mass shift, i.e., we should regard

$$\hat{H}_{\text{int}} + \frac{2e^2}{3\pi\hbar c^3 m^2} \int_0^\infty d\omega \tag{15.410}$$

as the effective interaction of an electron of renormalized mass m with the radiation field.

It is now finite to second-order of our calculation. Feynman, et al, showed that this could be done to all orders of perturbation theory!!

We therefore modify our calculation by adding in the required term. We get

$$\Delta E_n' = \frac{2e^2}{3\pi\hbar c^3 m^2} \int_0^\infty \omega d\omega \left(\sum_{n'} \frac{\left|\langle n'|\, \vec{p}\,|n\rangle\right|^2}{\varepsilon_n - \varepsilon_{n'} - \omega} + \frac{\left|\langle n|\, \vec{p}\,|n\rangle\right|^2}{\omega} \right) \tag{15.411}$$

Using completeness, we have

$$\langle n|\, p^2\,|n\rangle = \sum_{n'} \langle n|\, p\,|n'\rangle \langle n'|\, p\,|n\rangle = \sum_{n'} \left|\langle n'|\, p\,|n\rangle\right|^2 \tag{15.412}$$

so that

$$\Delta E_n' = \frac{2e^2}{3\pi\hbar c^3 m^2} \sum_{n'} \left|\langle n'|\, p\,|n\rangle\right|^2 \int_0^\infty d\omega \frac{\varepsilon_{n'} - \varepsilon_n}{\varepsilon_n - \varepsilon_{n'} - \omega} \tag{15.413}$$

The integral is still divergent but only logarithmically and, in fact, not at all in more sophisticated relativistic calculations. We can imagine that the correct calculation would yield a similar result but with a convergent integral. We can simulate this result by integrating to some cutoff value (and not to infinity) say at $\hbar\omega = mc^2$. We then get

$$\Delta E_n' = \frac{2e^2}{3\pi\hbar c^3 m^2} \sum_{n'} \left| \langle n' | \, p \, | n \rangle \right|^2 (\varepsilon_{n'} - \varepsilon_n) \ell n \left| \frac{mc^2}{\varepsilon_{n'} - \varepsilon_n} \right| \quad (15.414)$$

where we have neglected quantities the size of $\varepsilon_{n'} - \varepsilon_n$ in comparison to mc^2.

Bethe evaluated this result numerically and obtained $\Delta E_n' = +1040$ megacycles (the $2P_{1/2}$ level turns out to be shifted downward) and the observed value equals $+1057$ megacycles, which is remarkable agreement!

Taking into account both the Lamb shift and the hyperfine splitting we have the level scheme shown in the figure below for $n = 2$:

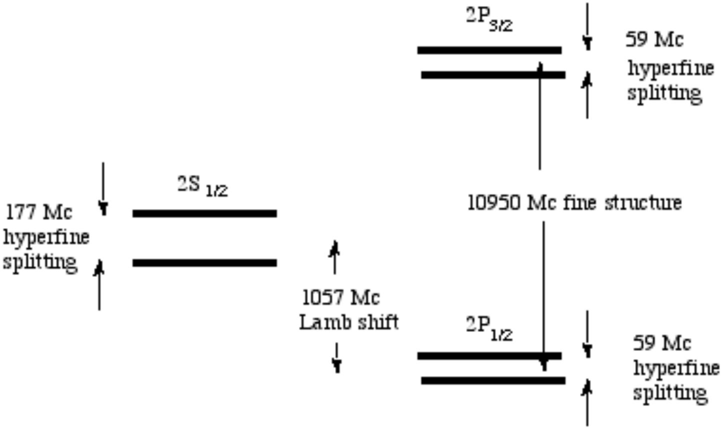

Figure: $n = 2$ Energy level structure for relativistic hydrogen

Dirac Hole Theory

Finally, we tackle the problem of the negative energy states in the Dirac theory.

As we said earlier, there is no simple conservation law that prevents an electron or any other spin 1/2 particle in a positive energy state from making a radiative transition to a negative energy state. This means all atoms must be unstable! An energy diagram is shown in the figure below.

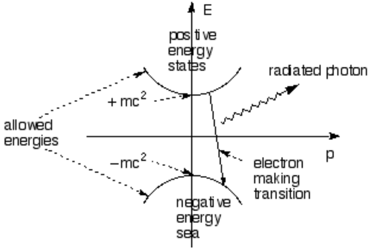

Figure: $n = 2$ Energy level structure for relativistic hydrogen

The properties of the positive energy states show remarkable agreement with experiment. Can we simply ignore the negative energy states? The answer is no because an arbitrary wave packet, as we saw earlier will always contain negative energy components via interactions even if we start off only with positive energy components.

Dirac proposed a clever way out of this dilemma : since spin $1/2$ particles obey the exclusion principle, all one needs to do to insure stability is to say that the negative energy states are completely filled. Then a particle cannot make a transition from a positive to a negative energy state for this would put two particles into the same (negative energy) state. The vacuum state in this picture consists of an *infinite sea* of particles in negative energy states.

The particle and charge density at every point is infinite. This is not a problem for the physical theory since Dirac contended that we only measure deviations from the vacuum. In the absence of any potential, the charge density of the negative sea is uniform and Dirac argued that this charge density can produce no forces, since by isotropy, the forces have no special direction to point!

Now this theory has some very useful special property. Suppose that we remove a negative energy electron from the vacuum. What is left behind is a *hole* in the negative energy sea. Measured with respect to the vacuum, the hole would appear to have positive charge and positive energy,i.e., since it is the absence of negative charge and negative energy. Dirac interpreted it as a positron, which is the electron antiparticle.

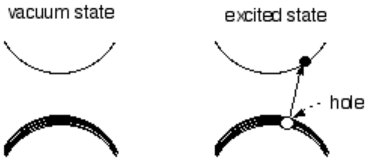

Figure: A hole appears

Let me say that again..... an excited state of the vacuum arises as shown in the figure. A negative energy electron is excited into a positive energy state, leaving behind a hole with charge $-(-e) = +e$ and the same mass as the electron, which is the antiparticle. It looks like a positive charge since if we apply an electric field the infinite sea of electron translates opposite to the field direction, which is unobservable since the sea is infinite. However, the hole seems to be traveling in the direction of the field like a positive charge! In this way, antiparticles appear in the Dirac theory as unoccupied negative energy states, which is very different from the way they appear in the spin zero theory.

This Dirac hole theory gives a simple description for pair production. Suppose that a photon of energy $> 2mc^2$ traveling through the vacuum is absorbed by a negative energy electron and the negative energy electron gets excited to a positive energy state. What remains, as we have said, is a hole in the negative energy sea, i.e., a positive energy positron and a positive energy electron. This says that pair production is simply the excitation of a particle from a negative to a positive energy state.

Since we could exchange the roles of positrons and electrons in the entire Dirac theory, electrons would appear as holes in a positron sea. This forces us to conclude that negative energy seas cannot have any physical reality. The *hole theory* is simply a mathematical model that allows us to do the correct *bookkeeping* within the framework of a single-particle Dirac theory.

With a filled negative energy sea, the Dirac theory would become a many-particle theory in which we are unable to take into account the interactions between these particles. The Dirac theory gives valid results only when these interactions can be neglected. For example, in the hydrogen atom, the modification of the Coulomb potential by vacuum polarization accounts for about 2.5% of the Lamb shift.

If we second-quantized the Dirac theory, we can treat both particles and antiparticles on the same basis.

The full relativistic quantum field theory of the electrons and positrons and their interactions with photons was carried out by Feynman, et al in a theory which is beyond the scope of these volumes.

15.7 **Electromagnetic Radiation and Matter**

15.7.1 Interacting with the Classical Radiation Field

We assume *classical* EM radiation in the *transverse gauge*, where

$$\phi(\vec{r},t) = 0 \quad , \quad \nabla \cdot \vec{A}(\vec{r},t) = 0 \tag{15.415}$$

The electric and magnetic fields are given in terms of the vector potential (in this gauge) by

$$\vec{\varepsilon}(\vec{r},t) = -\frac{1}{c}\frac{\partial \vec{A}(\vec{r},t)}{\partial t} \quad , \quad \vec{B}(\vec{r},t) = \nabla \times \vec{A}(\vec{r},t) \tag{15.416}$$

The electromagnetic energy is given by

$$E = \int d^3\vec{r}\,\frac{\varepsilon^2(\vec{r},t) + B^2(\vec{r},t)}{8\pi} \tag{15.417}$$

and the rate and direction of energy transport is given by the Poynting vector

$$\vec{\wp}(\vec{r},t) = \frac{c}{4\pi}\vec{\varepsilon}(\vec{r},t) \times \vec{B}(\vec{r},t) \tag{15.418}$$

The radiation field generated by a classical current $\vec{j}(\vec{r},t)$ is given by

$$\left(\nabla^2 - \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\right)\vec{A}(\vec{r},t) = -\frac{4\pi}{c}j_\perp(\vec{r},t) \tag{15.419}$$

where $\perp$ means the transverse/divergence-free part.

We first consider the *monochromatic plane wave* solution of this equation. It takes the form

$$\vec{A}(\vec{r},t) = \alpha\vec{\lambda}e^{i\vec{k}\cdot\vec{r}-i\omega t} + \alpha^*\vec{\lambda}^*e^{-i\vec{k}\cdot\vec{r}+i\omega t} \tag{15.420}$$

where

$$\omega = ck$$

$$\vec{\lambda} = \text{ polarization vector with } \left|\vec{\lambda}\right|^2 = 1$$

$$\alpha = \text{ amplitude} = \text{constant}$$

To insure that $\nabla \cdot \vec{A}(\vec{r},t) = 0$ we require $\vec{\lambda} \cdot \vec{k} = 0$ which corresponds to transverse polarizations only.

The energy per unit volume in the electromagnetic wave is

$$\frac{\varepsilon^2 + B^2}{8\pi} = \frac{\omega^2}{2\pi c^2}\left[|\alpha|^2 - \mathrm{Re}\left(\alpha^2\lambda^2 e^{2i\vec{k}\cdot\vec{r} - 2i\omega t}\right)\right] \tag{15.421}$$

The quantity Re(..) oscillates in time and averages to zero so that the average energy density is

$$\frac{E}{volume} = \frac{\omega^2}{2\pi c^2}\,|\alpha|^2 \tag{15.422}$$

In a similar way the time average of the Poynting vector is

$$\frac{\omega^2}{2\pi c}\,|\alpha|^2\,\hat{k} \tag{15.423}$$

Any general wave solution is a *linear superposition* of these monochromatic wave solutions.

$$\vec{A}(\vec{r},t) = \sum_{\vec{k}\vec{\lambda}} \left[A_{\vec{k}\vec{\lambda}} \vec{\lambda} \frac{e^{i\vec{k}\cdot\vec{r}-i\omega t}}{\sqrt{V}} + A^*_{\vec{k}\vec{\lambda}} \vec{\lambda}^* \frac{e^{-i\vec{k}\cdot\vec{r}+i\omega t}}{\sqrt{V}} \right] \tag{15.424}$$

where the sum is over all allowed $\vec{k}$ values and over the two orthogonal $\vec{\lambda}$ polarizations for each $\vec{k}$ such that $\vec{\lambda}\cdot\vec{k} = 0$ and we have assumed that the universe is a very large box of volume V. The total energy in this wave solution is

$$E = \sum_{\vec{k}\vec{\lambda}} \frac{\omega^2}{2\pi c^2} \left| A_{\vec{k}\vec{\lambda}} \right|^2 \tag{15.425}$$

How does this classical electromagnetic field interact with a quantum mechanical particle?

In general (no transverse gauge at this point), the classical Hamiltonian is

$$\hat{H} = \frac{\left(\vec{p} - \frac{e}{c}\vec{A}(\vec{r},t)\right)^2}{2m} + e\phi(\vec{r},t) + V(\vec{r},t) \tag{15.426}$$

where $V(\vec{r},t)$ represents all the other potentials seen by the particle.

We get to quantum mechanics via the standard substitutions

$$\vec{r} \rightarrow \vec{r}_{op} \quad , \quad \vec{p} \rightarrow \vec{p}_{op} = \frac{\hbar}{i}\nabla \tag{15.427}$$

Substituting, we get the Schrodinger equation for an electron in an electromagnetic field

$$i\hbar\frac{\partial\psi(\vec{r},t)}{\partial t} = \left[\frac{1}{2m}\left(\frac{\hbar}{i}\nabla - \frac{e}{c}\vec{A}(\vec{r},t)\right)^2 + e\phi(\vec{r},t) + V(\vec{r},t)\right]\psi(\vec{r},t) \tag{15.428}$$

15.7.2 **Relation to Gauge Invariance**

In order to have the Schrodinger equation invariant under a gauge transformation, the wave function has to change by a phase factor,i.e.,

$$\psi'(\vec{r},t) = e^{i\frac{e}{\hbar c}\chi(\vec{r},t)}\psi(\vec{r},t) \tag{15.429}$$

where $\chi(\vec{r},t)$ is the some scalar function.

This means that the solutions of the gauge-transformed Schrodinger equation will still describe the same physical states.

The wave functions or state vectors differ by a phase factor that depends on space and time and thus, the invariance is $LOCAL$ rather than $GLOBAL$ (a phase factor independent of space and time).

It is then clear that it is NOT the canonical momentum $\hat{p} \to -i\hbar\nabla$ (whose expectation value is NOT gauge invariant), but the genuine kinetic momentum

$$\hat{p} - \frac{q}{c}\vec{A}(\hat{r},t) \tag{15.430}$$

(whose expectation value *IS* gauge invariant), that represents a *measurable* quantity.

In any physical system, if the momentum operator $\hat{p}$ appears, then it must always be replaced by

$$\psi'(\vec{r},t) = e^{i\frac{e}{\hbar c}\chi(\vec{r},t)}\psi(\vec{r},t) \tag{15.431}$$

if we turn on an electromagnetic fields. This is the only way to guarantee gauge invariance in quantum mechanics.

Quantum mechanics + electromagnetism requires *minimal coupling* for gauge invariance to be valid.

15.7.3 **Interactions**

We now write

$$\hat{H} = \hat{H}_0 + \hat{H}_{int} \tag{15.432}$$

where

$$\hat{H}_0 = \frac{\vec{p}^2}{2m} + V(\vec{r},t) \tag{15.433}$$

is the Hamiltonian in the absence of electromagnetic fields and

$$\hat{H}_{\text{int}} = -\frac{e}{2mc}\left(\vec{p}\cdot\vec{A}(\vec{r},t) + \vec{A}(\vec{r},t)\cdot\vec{p}\right) + \frac{e^2}{2mc^2}\vec{A}^2(\vec{r},t) + e\phi(\vec{r},t) \tag{15.434}$$

is the operator giving the *interaction between matter and radiation.*

One must treat the term $\vec{p}\cdot\vec{A}(\vec{r},t) + \vec{A}(\vec{r},t)\cdot\vec{p}$ with care since $[x_i, p_j] = i\hbar\delta_{ij}$. In general, we can show that

$$\vec{p}\cdot\vec{A}(\vec{r},t) - \vec{A}(\vec{r},t)\cdot\vec{p} = -i\hbar\left(\nabla\cdot\vec{A}(\vec{r},t)\right) \tag{15.435}$$

which says that

$$\vec{p}\cdot\vec{A}(\vec{r},t) = \vec{A}(\vec{r},t)\cdot\vec{p} \text{ only when } \nabla\cdot\vec{A} = 0 \tag{15.436}$$

or when we are operating in the transverse gauge.

For multi-electron atoms we have

$$\hat{H} = \sum_{i=1}^{N} \frac{\left(\vec{p}_i - \frac{e}{c}\vec{A}(\vec{r}_i,t)\right)^2}{2m} + e\sum_{i=1}^{N}\phi(\vec{r}_i,t) + V \tag{15.437}$$

and

$$\hat{H}_{int} = \sum_{i=1}^{N}\left\{-\frac{e}{2mc}\left(\vec{p}_i\cdot\vec{A}(\vec{r}_i,t) + \vec{A}(\vec{r}_i,t)\cdot\vec{p}_i\right) + \frac{e^2}{2mc^2}\vec{A}^2(\vec{r}_i,t) + e\phi(\vec{r}_i,t)\right\} \tag{15.438}$$

We now define a particle number density

$$\rho(\vec{r}) = \sum_i \delta(\vec{r}-\vec{r}_i) \tag{15.439}$$

and a current density

$$\vec{j}(\vec{r}) = \frac{1}{2}\sum_i\left(\frac{\vec{p}_i}{m}\delta(\vec{r}-\vec{r}_i) + \delta(\vec{r}-\vec{r}_i)\frac{\vec{p}_i}{m}\right) \tag{15.440}$$

where we constructed a symmetric combination of the terms so that the operator would be Hermitian.

These quantities imply that

$$\sum_i e\phi(\vec{r}_i,t) = \sum_i \int d^3\vec{r}\, e\delta(\vec{r}-\vec{r}_i)\phi(\vec{r},t) = \int d^3\vec{r}\, e\rho(\vec{r})\phi(\vec{r},t) \tag{15.441}$$

where $\phi(\vec{r},t) \neq$ operator (all operators are in $\rho(\vec{r})$) and

$$\int d^3\vec{r}\rho(\vec{r}) = N = \text{ total number of particles} \tag{15.442}$$

Finally, we have

$$\sum_{i=1}^{N}\left\{-\frac{e}{2mc}\left(\vec{p}_i\cdot\vec{A}(\vec{r}_i,t)+\vec{A}(\vec{r}_i,t)\cdot\vec{p}_i\right)\right\} = -\frac{e}{c}\int d^3\vec{r}\vec{j}(\vec{r})\cdot\vec{A}(\vec{r},t) \tag{15.443}$$

Since

$$\vec{v}_i = \frac{\vec{p}_i}{m} - \frac{e}{mc}\vec{A} \tag{15.444}$$

when an electromagnetic field is present, the true current operator is

$$\vec{J}(\vec{r}) = \vec{j}(\vec{r}) - \frac{e}{mc}\vec{A}(\vec{r},t)\rho(\vec{r}) = \text{(paramagnetic + diamagnetic) currents} \tag{15.445}$$

and therefore,

$$\hat{H}_{\text{int}} = \int d^3\vec{r}\left[-\frac{e}{c}\vec{j}(\vec{r})\cdot\vec{A}(\vec{r},t) + \frac{e^2}{2mc^2}\rho(\vec{r})\vec{A}^2(\vec{r},t) + e\phi(\vec{r},t)\rho(\vec{r})\right] \tag{15.446}$$

15.7.4 **Induced Absorption and Emission**

We will now use the transverse gauge, which says that the $\phi(\vec{r},t)$ term is zero. We also assume that the radiation fields are small compared to the fields inside the atom, i.e., $\left|\vec{A}\right| << e^2/a_0$, which implies that we can neglect the $\vec{A}^2$ term compared to the $\vec{j}\cdot\vec{A}$ term. Therefore, we have

$$\hat{H}_{int} = -\frac{e}{c}\int d^3\vec{r}\,\vec{j}(\vec{r})\cdot\vec{A}(\vec{r},t) \tag{15.447}$$

For $\vec{A}$ as a linear superposition of monochromatic plane waves we then have

$$\begin{aligned}
\hat{H}_{int} &= -\frac{e}{c}\int d^3\vec{r}\left(\frac{1}{2}\sum_i\left(\frac{\vec{p}_i}{m}\delta(\vec{r}-\vec{r}_i)+\delta(\vec{r}-\vec{r}_i)\frac{\vec{p}_i}{m}\right)\right) \\
&\qquad\times\left(\sum_{\vec{k}\vec{\lambda}}\left[A_{\vec{k}\vec{\lambda}}\vec{\lambda}\frac{e^{i\vec{k}\cdot\vec{r}-i\omega t}}{\sqrt{V}}+A^*_{\vec{k}\vec{\lambda}}\vec{\lambda}^*\frac{e^{-i\vec{k}\cdot\vec{r}+i\omega t}}{\sqrt{V}}\right]\right) \\
&= -\frac{e}{2c\sqrt{V}}\sum_{\vec{k}\vec{\lambda}}\sum_i\left(\begin{array}{c} A_{\vec{k}\vec{\lambda}}\vec{\lambda}\frac{\vec{p}_i}{m}e^{i\vec{k}\cdot\vec{r}_i-i\omega t}+A^*_{\vec{k}\vec{\lambda}}\vec{\lambda}^*\frac{\vec{p}_i}{m}e^{-i\vec{k}\cdot\vec{r}_i+i\omega t} \\ +A_{\vec{k}\vec{\lambda}}\vec{\lambda}e^{i\vec{k}\cdot\vec{r}_i-i\omega t}\frac{\vec{p}_i}{m}+A^*_{\vec{k}\vec{\lambda}}\vec{\lambda}^*e^{-i\vec{k}\cdot\vec{r}_i+i\omega t}\frac{\vec{p}_i}{m}\end{array}\right) \\
&= -\frac{e}{c\sqrt{V}}\sum_{\vec{k}\vec{\lambda}}\left[A_{\vec{k}\vec{\lambda}}\vec{j}_{-\vec{k}}\cdot\vec{\lambda}e^{-i\omega t}+A^*_{\vec{k}\vec{\lambda}}\vec{j}_{\vec{k}}\cdot\vec{\lambda}^*e^{i\omega t}\right] \qquad (15.448)
\end{aligned}$$

where

$$\vec{j}_{\vec{k}} = \frac{1}{2}\sum_i\left(\frac{\vec{p}_i}{m}e^{-i\vec{k}\cdot\vec{r}_i}+e^{-i\vec{k}\cdot\vec{r}_i}\frac{\vec{p}_i}{m}\right) = \int d^3\vec{r}e^{-i\vec{k}\cdot\vec{r}}\vec{j}(\vec{r}) \qquad (15.449)$$

As we saw in the discussion of time-dependent perturbation theory for a harmonic perturbation, the $e^{-i\omega t}$ term implies an absorption of radiation process and the $e^{i\omega t}$ term implies and emission of radiation process. Following the same steps as that case, we have for the absorption transition rate

$$\Gamma^{abs}_{0\rightarrow n;\vec{k}\vec{\lambda}} = \frac{2\pi}{\hbar}\delta(\varepsilon_n - \varepsilon_0 - \hbar\omega)\frac{e^2}{Vc^2}\left|A_{\vec{k}\vec{\lambda}}\right|^2\left|\langle n|\,\vec{j}_{\vec{k}}\cdot\vec{\lambda}\,|0\rangle\right|^2 \quad (15.450)$$

To find the total rate of transition we must sum over $\vec{k}$ and $\vec{\lambda}$ (2 polarizations for each $\vec{k}$) to get

$$\Gamma^{abs}_{0\rightarrow n} = \frac{2\pi}{\hbar V}\sum_{\vec{k}\vec{\lambda}}\delta(\varepsilon_n - \varepsilon_0 - \hbar\omega)\frac{e^2}{c^2}\left|A_{\vec{k}\vec{\lambda}}\right|^2\left|\langle n|\,\vec{j}_{-\vec{k}}\cdot\vec{\lambda}\,|0\rangle\right|^2 \quad (15.451)$$

Now we can write

$$\frac{1}{V}\sum_{\vec{k}} \rightarrow \int\frac{k^2dkd\Omega}{(2\pi)^3} = \int\frac{\omega^2d\omega d\Omega}{(2\pi c)^3} \quad (15.452)$$

so that

$$\Gamma_{0\to n}^{abs} = \frac{2\pi e^2}{\hbar^2 c^2}\frac{\omega^2}{2\pi c^3}\int d\Omega \sum_{\vec{\lambda}} \left|A_{\vec{k}\vec{\lambda}}\right|^2 \left|\langle n|\,\vec{j}_{\vec{k}}\cdot\vec{\lambda}\,|0\rangle\right|^2 \qquad (15.453)$$

where

$$\omega = \frac{\varepsilon_n - \varepsilon_0}{\hbar} \text{ (from the } \delta - \text{ function)} \qquad (15.454)$$

If the incident light beam subtends a solid angle $d\Omega$ and it is polarized with polarization vector $\vec{\lambda}$, then the total rate of energy transport in the beam is the time average of the Poynting vector which is given by

$$\frac{1}{V}\sum_{\vec{k}} \frac{\omega^2}{2\pi c}\left|A_{\vec{k}\vec{\lambda}}\right|^2 = d\Omega \int d\omega \frac{\omega^4}{(2\pi c)^4}\left|A_{\vec{k}\vec{\lambda}}\right|^2 \qquad (15.455)$$

Now

$$\begin{aligned} I(\omega) &= d\Omega \frac{\omega^4}{(2\pi c)^4} \left| A_{\vec{k}\vec{\lambda}} \right|^2 \\ &= \text{ intensity of the incident beam per unit frequency} \end{aligned} \tag{15.456}$$

In a similar way

$$\Gamma^{ind\ emis}_{n \to 0} = \frac{4\pi^2 e^2}{\hbar^2 c \omega^2} I(\omega) \left| \langle n | \, \vec{j}_{\vec{k}} \cdot \vec{\lambda}^* \, |0\rangle \right|^2 \tag{15.457}$$

Since

$$\langle n | \, \vec{j}_{\vec{k}} \cdot \vec{\lambda}^* \, |0\rangle = \langle n | \, \vec{j}_{-\vec{k}} \cdot \vec{\lambda} \, |0\rangle^* \tag{15.458}$$

we have

$$\Gamma^{abs}_{0 \to n} = \Gamma^{ind\ emis}_{n \to 0} \tag{15.459}$$

(this is the origin of the Einstein A and B coefficients).

In the absorption process, the absorption of one photon of energy $\hbar\omega = \varepsilon_n - \varepsilon_0$ causes an upward transition. The electron gains energy and the electromagnetic field loses energy. Induced emission is just the opposite.

Now a photon of frequency ω and energy $\hbar\omega$ and therefore, the total energy in the incident beam is

$$E = \sum_{\vec{k}\vec{\lambda}} \hbar\omega N_{\vec{k}\vec{\lambda}} \tag{15.460}$$

where $N_{\vec{k}\vec{\lambda}}$ = the number of photons in the $(\vec{k}, \vec{\lambda})$ mode in the beam. But we already have

$$E = \sum_{\vec{k}\vec{\lambda}} \frac{\omega^2}{2\pi c^2} \left|A_{\vec{k}\vec{\lambda}}\right|^2 \tag{15.461}$$

which says that

$$\left|A_{\vec{k}\vec{\lambda}}\right|^2 = \frac{2\pi\hbar c^2}{\omega} N_{\vec{k}\vec{\lambda}} \tag{15.462}$$

and thus

$$\Gamma^{abs}_{0\to n} = \Gamma^{ind\ emis}_{n\to 0} = \sum_{\vec{k}\vec{\lambda}} \frac{4\pi^2 e^2}{\omega V} \delta(\varepsilon_n - \varepsilon_0 - \hbar\omega) \left| \langle n| \vec{j}_{-\vec{k}} \cdot \vec{\lambda} \,|0\rangle \right|^2 N_{\vec{k}\vec{\lambda}} \tag{15.463}$$

15.7.5 Quantized Radiation Field and Spontaneous Emission

Up to this point we have been treating the electromagnetic field classically as a wave. We have mentioned the idea of photons, but have not created any formal quantum mechanical structure to describe them, i.e., we have been considering what happens to the atom and ignoring what is happening to the EM field during these processes.

To bring out the structure of the theory in terms of photons, we must now describe these processes in terms of state vectors, such that, in the absorption process the atom makes a transition from $|0\rangle \to |n\rangle$ while the electromagnetic field makes a transition from an initial state to a state with *one less photon* (it has been absorbed).

All of our development so far has involved what is physically called an incoherent beam of light.

We related $\left|A_{\vec{k}\vec{\lambda}}\right|$ and $N_{\vec{k}\vec{\lambda}}$ so that knowledge of the $N_{\vec{k}\vec{\lambda}}$ clearly does not imply any information about the relative phases of the $A_{\vec{k}\vec{\lambda}}$ which is the meaning of the term incoherent.

An incoherent beam, therefore, is completely specified by the photon numbers, i.e., the $N_{\vec{k}\vec{\lambda}}$. It is in this sense that we can write the initial state(normalized) of the electromagnetic field as

$$\left|N_{\vec{k}_1\vec{\lambda}_1}, N_{\vec{k}_2\vec{\lambda}_2}, ..., N_{\vec{k}\vec{\lambda}}, ...\right\rangle \tag{15.464}$$

where, as before, the $N_{\vec{k}\vec{\lambda}}$ = the number of photons in the mode $(\vec{k}, \vec{\lambda})$.

Any two of these states are orthogonal if they differ in the number of photons in any mode.

The final state of the electromagnetic field after photon absorption of a photon in the mode $(\vec{k}, \vec{\lambda})$ is

$$\left|N_{\vec{k}_1\vec{\lambda}_1}, N_{\vec{k}_2\vec{\lambda}_2}, ..., N_{\vec{k}\vec{\lambda}} - 1, ...\right\rangle \tag{15.465}$$

We assume that there exists some $\hat{H}_{int}$ that causes both transitions (atom and electromagnetic field) as it couples the electromagnetic field to matter. We define

$$\text{initial state } = |0\rangle \left|N_{\vec{k}_1\vec{\lambda}_1}, N_{\vec{k}_2\vec{\lambda}_2}, ..., N_{\vec{k}\vec{\lambda}}, ...\right\rangle \tag{15.466}$$

$$\text{final state } = |n\rangle \left|N_{\vec{k}_1\vec{\lambda}_1}, N_{\vec{k}_2\vec{\lambda}_2}, ..., N_{\vec{k}\vec{\lambda}} - 1, ...\right\rangle \tag{15.467}$$

so that

$$E_{initial} = \varepsilon_0 + \sum_{\vec{k}'\vec{\lambda}'} \hbar c k' N_{\vec{k}'\vec{\lambda}'} \tag{15.468}$$

$$E_{final} = \varepsilon_n + \sum_{\vec{k}'\vec{\lambda}'} \hbar c k' N_{\vec{k}'\vec{\lambda}'} - \hbar c k \tag{15.469}$$

The transition rate between the two states is given by Fermi's golden rule as

$$\frac{2\pi}{\hbar}\delta(\varepsilon_n - \varepsilon_0 - \hbar\omega)\left|\langle final|\,\hat{H}_{\rm int}\,|initial\rangle\right|^2 \tag{15.470}$$

This must be the same as our earlier result (20.463) which implies that we must have

$$\begin{aligned}\left|\langle final|\,\hat{H}_{int}\,|initial\rangle\right|^2 &= \frac{e^2}{Vc^2}\left|A_{\vec{k}\vec{\lambda}}\right|^2\left|\langle n|\,\vec{j}_{-\vec{k}}\cdot\vec{\lambda}\,|0\rangle\right|^2 \\ &= \frac{e^2}{Vc^2}\frac{2\pi\hbar c^2}{\omega}N_{\vec{k}\vec{\lambda}}\left|\langle n|\,\vec{j}_{-\vec{k}}\cdot\vec{\lambda}\,|0\rangle\right|^2\end{aligned} \tag{15.471}$$

This implies that as yet undetermined operator $\hat{H}_{int}$ must have the following properties:

1. it must include a part $\vec{j}_{-\vec{k}} \cdot \vec{\lambda}$ that acts on the atom
2. it must have a part that decreases the number of photons in the $(\vec{k}, \vec{\lambda})$ mode by 1
3. it must be Hermitian

One way of doing this is to write

$$\hat{H}_{int} = \frac{e}{c\sqrt{V}} \sum_{\vec{k}'\vec{\lambda}'} \left(\vec{j}_{-\vec{k}'} \cdot \vec{\lambda}' A^{(op)}_{\vec{k}'\vec{\lambda}'} + \vec{j}_{\vec{k}'} \cdot \vec{\lambda}'^{*} A^{(op)+}_{\vec{k}'\vec{\lambda}'} \right) \tag{15.472}$$

where $A^{(op)}_{\vec{k}\vec{\lambda}}$ *reduces the number of photons* in the $(\vec{k}, \vec{\lambda})$ mode by 1. It is a photon in mode $(\vec{k}, \vec{\lambda})$ *annihilation operator*.

The second term is required to make $\hat{H}_{int}$ Hermitian. Using this model we then have

$$
\begin{aligned}
&\langle final|\, \hat{H}_{int}\, |initial\rangle \\
&\quad = \left\langle n; N_{\vec{k}_1\vec{\lambda}_1}, N_{\vec{k}_2\vec{\lambda}_2}, ..., N_{\vec{k}\vec{\lambda}} - 1, ...\right| \hat{H}_{\rm int} \left| 0; N_{\vec{k}_1\vec{\lambda}_1}, N_{\vec{k}_2\vec{\lambda}_2}, ..., N_{\vec{k}\vec{\lambda}}, ...\right\rangle \\
&\quad = -\frac{e}{c}\, \langle n|\, \vec{j}_{-\vec{k}} \cdot \vec{\lambda}\, |0\rangle \\
&\qquad \times \left\langle N_{\vec{k}_1\vec{\lambda}_1}, N_{\vec{k}_2\vec{\lambda}_2}, ..., N_{\vec{k}\vec{\lambda}} - 1, ...\right| A^{(op)}_{\vec{k}\vec{\lambda}} \left| N_{\vec{k}_1\vec{\lambda}_1}, N_{\vec{k}_2\vec{\lambda}_2}, ..., N_{\vec{k}\vec{\lambda}}, ...\right\rangle
\end{aligned}
\tag{15.473}
$$

For agreement with the earlier result we must have

$$
\begin{aligned}
&\left\langle N_{\vec{k}_1\vec{\lambda}_1}, N_{\vec{k}_2\vec{\lambda}_2}, ..., N_{\vec{k}\vec{\lambda}} - 1, ...\right| A^{(op)}_{\vec{k}\vec{\lambda}} \left| N_{\vec{k}_1\vec{\lambda}_1}, N_{\vec{k}_2\vec{\lambda}_2}, ..., N_{\vec{k}\vec{\lambda}}, ...\right\rangle \\
&\qquad = \sqrt{\frac{2\pi\hbar c^2}{\omega}} \sqrt{N_{\vec{k}\vec{\lambda}}}
\end{aligned}
\tag{15.474}
$$

This matrix element of $A^{(op)}_{\vec{k}\vec{\lambda}}$ corresponds to the $A_{\vec{k}\vec{\lambda}}$ term in the classical field picture.

The matrix element implies that

$$\left\langle N_{\vec{k}_1\vec{\lambda}_1}, N_{\vec{k}_2\vec{\lambda}_2}, ..., N_{\vec{k}\vec{\lambda}} - 1, ... \right| A^{(op)}_{\vec{k}\vec{\lambda}} \left| N_{\vec{k}_1\vec{\lambda}_1}, N_{\vec{k}_2\vec{\lambda}_2}, ..., N_{\vec{k}\vec{\lambda}}, ... \right\rangle^*$$
$$= \left\langle N_{\vec{k}_1\vec{\lambda}_1}, N_{\vec{k}_2\vec{\lambda}_2}, ..., N_{\vec{k}\vec{\lambda}}, ... \right| A^{(op)+}_{\vec{k}\vec{\lambda}} \left| N_{\vec{k}_1\vec{\lambda}_1}, N_{\vec{k}_2\vec{\lambda}_2}, ..., N_{\vec{k}\vec{\lambda}} - 1, ... \right\rangle$$
$$= \sqrt{\frac{2\pi\hbar c^2}{\omega}} \sqrt{N_{\vec{k}\vec{\lambda}}} \tag{15.475}$$

which says that $A^{(op)+}_{\vec{k}\vec{\lambda}}$ is an operator that increases the number of photons in the $(\vec{k}, \vec{\lambda})$ mode by 1. It is a photon in mode $(\vec{k}, \vec{\lambda})$ *creation operator*. We thus have

$$A^{(op)}_{\vec{k}\vec{\lambda}} \left| N_{\vec{k}_1\vec{\lambda}_1}, N_{\vec{k}_2\vec{\lambda}_2}, ..., N_{\vec{k}\vec{\lambda}}, ... \right\rangle$$
$$= \sqrt{\frac{2\pi\hbar c^2}{\omega}} \sqrt{N_{\vec{k}\vec{\lambda}}} \left| N_{\vec{k}_1\vec{\lambda}_1}, N_{\vec{k}_2\vec{\lambda}_2}, ..., N_{\vec{k}\vec{\lambda}} - 1, ... \right\rangle \tag{15.476}$$

$$A^{(op)+}_{\vec{k}\vec{\lambda}} \left| N_{\vec{k}_1\vec{\lambda}_1}, N_{\vec{k}_2\vec{\lambda}_2}, ..., N_{\vec{k}\vec{\lambda}}, ... \right\rangle$$
$$= \sqrt{\frac{2\pi\hbar c^2}{\omega}} \sqrt{N_{\vec{k}\vec{\lambda}} + 1} \left| N_{\vec{k}_1\vec{\lambda}_1}, N_{\vec{k}_2\vec{\lambda}_2}, ..., N_{\vec{k}\vec{\lambda}} + 1, ... \right\rangle \tag{15.477}$$

This behavior is identical (aside from the $\sqrt{2\pi\hbar c^2/\omega}$ factor) to that of the $\hat{a}$ and $\hat{a}^+$ operators in the harmonic oscillator problem.

This model gives a quantum mechanical picture of the electromagnetic radiation field as an infinite number of *harmonic oscillators* - one per mode and the quanta associated with these oscillators are photons.

If we define a Hermitian electromagnetic field operator as

$$\vec{A}^{(op)}(\vec{r}) = \sum_{\vec{k}\vec{\lambda}} \left[A^{(op)}_{\vec{k}\vec{\lambda}} \vec{\lambda} \frac{e^{i\vec{k}\bullet\vec{r}}}{\sqrt{V}} + A^{(op)+}_{\vec{k}\vec{\lambda}} \vec{\lambda}^* \frac{e^{-i\vec{k}\bullet\vec{r}}}{\sqrt{V}} \right] \tag{15.478}$$

we have

$$\hat{H}_{int} = \int d^3\vec{r} \left[-\frac{e}{c}\vec{j}(\vec{r}) \cdot \vec{A}^{(op)}(\vec{r}) + \frac{e^2}{2mc^2}\rho(\vec{r}) \left(\vec{A}^{(op)}(\vec{r}) \right)^2 \right] \tag{15.479}$$

In the interaction representation $\vec{A}^{(op)}(\vec{r},t)$ has the time dependence

$$\vec{A}^{(op)}(\vec{r},t) = e^{\frac{i}{\hbar}\hat{H}_{em}t}\vec{A}^{(op)}(\vec{r})e^{-\frac{i}{\hbar}\hat{H}_{em}t} \tag{15.480}$$

where $\hat{H}_{em}$ = Hamiltonian for free radiation. We then have

$$\hat{H}_{em} = \frac{1}{8\pi}\int d^3\vec{r}\left(\vec{\varepsilon}^2 + \vec{B}^2\right) = \sum_{\vec{k}\vec{\lambda}}\hbar ck\left(A^{(op)+}_{\vec{k}\vec{\lambda}}A^{(op)}_{\vec{k}\vec{\lambda}} + \frac{1}{2}\right) \tag{15.481}$$

The operator algebra similarity to the $\hat{a}$ and $\hat{a}^+$ problem then allows us to write

$$\left[A^{(op)}_{\vec{k}\vec{\lambda}}, A^{(op)+}_{\vec{k}'\vec{\lambda}'}\right] = \frac{2\pi\hbar c^2}{\omega}\delta_{\vec{k}\vec{k}'}\delta_{\vec{\lambda}\vec{\lambda}'} \quad , \quad \left[A^{(op)}_{\vec{k}\vec{\lambda}}, A^{(op)}_{\vec{k}'\vec{\lambda}'}\right] = 0 \tag{15.482}$$

and

$$\left|N_{\vec{k}_1\vec{\lambda}_1}, N_{\vec{k}_2\vec{\lambda}_2}, ..., N_{\vec{k}\vec{\lambda}}, ...\right\rangle = \frac{1}{\sqrt{N_{\vec{k}\vec{\lambda}}!}}\left(A^{(op)+}_{\vec{k}\vec{\lambda}}\right)^{N_{\vec{k}\vec{\lambda}}}\left|N_{\vec{k}_1\vec{\lambda}_1}, N_{\vec{k}_2\vec{\lambda}_2}, ..., 0, ...\right\rangle \quad (15.483)$$

and $\hat{H} = \hat{H}_0 + \hat{H}_{em} + \hat{H}_{int}$ where $\hat{H}_0$ = Hamiltonian for the electrons.

We then have

$$\begin{aligned}
& e^{\frac{i}{\hbar}\hat{H}_{em}t} A^{(op)}_{\vec{k}\vec{\lambda}} e^{-\frac{i}{\hbar}\hat{H}_{em}t}\left|....., N_{\vec{k}\vec{\lambda}}, ...\right\rangle \\
&\qquad = e^{\frac{i}{\hbar}\hat{H}_{em}t} A^{(op)}_{\vec{k}\vec{\lambda}} e^{-i(N_{\vec{k}\vec{\lambda}}+\frac{1}{2})t}\left|....., N_{\vec{k}\vec{\lambda}}, ...\right\rangle \\
&\qquad = e^{\frac{i}{\hbar}\hat{H}_{em}t} e^{-i(N_{\vec{k}\vec{\lambda}}+\frac{1}{2})t}\sqrt{N_{\vec{k}\vec{\lambda}}}\left|....., N_{\vec{k}\vec{\lambda}}-1, ...\right\rangle \\
&\qquad = e^{i(N_{\vec{k}\vec{\lambda}}-1+\frac{1}{2})t} e^{-i(N_{\vec{k}\vec{\lambda}}+\frac{1}{2})t}\sqrt{N_{\vec{k}\vec{\lambda}}}\left|....., N_{\vec{k}\vec{\lambda}}-1, ...\right\rangle \\
&\qquad = e^{-ickt} A^{(op)}_{\vec{k}\vec{\lambda}}\left|....., N_{\vec{k}\vec{\lambda}}, ...\right\rangle \qquad (15.484)
\end{aligned}$$

or

$$e^{\frac{i}{\hbar}\hat{H}_{em}t}A^{(op)}_{\vec{k}\vec{\lambda}}e^{-\frac{i}{\hbar}\hat{H}_{em}t} = e^{-ickt}A^{(op)}_{\vec{k}\vec{\lambda}} \tag{15.485}$$

and similarly

$$e^{\frac{i}{\hbar}\hat{H}_{em}t}A^{(op)+}_{\vec{k}\vec{\lambda}}e^{-\frac{i}{\hbar}\hat{H}_{em}t} = e^{ickt}A^{(op)+}_{\vec{k}\vec{\lambda}} \tag{15.486}$$

Putting this all together we have

$$\vec{A}^{(op)}(\vec{r},t) = \sum_{\vec{k}\vec{\lambda}}\left[A^{(op)}_{\vec{k}\vec{\lambda}}\vec{\lambda}\frac{e^{i\vec{k}\cdot\vec{r}-i\omega t}}{\sqrt{V}} + A^{(op)+}_{\vec{k}\vec{\lambda}}\vec{\lambda}^*\frac{e^{-i\vec{k}\cdot\vec{r}+i\omega t}}{\sqrt{V}}\right] \tag{15.487}$$

By construction, we have forced the quantum mechanical description of absorption of the electromagnetic field in terms of the photon to be identical to the description in terms of the classical electromagnetic field for the induced absorption process.

We now apply the formalism to the emission process. This corresponds to the transition between the states

$$\text{initial state } = |0\rangle \left| N_{\vec{k}_1\vec{\lambda}_1}, N_{\vec{k}_2\vec{\lambda}_2}, ..., N_{\vec{k}\vec{\lambda}}, ... \right\rangle \tag{15.488}$$

$$\text{final state } = |n\rangle \left| N_{\vec{k}_1\vec{\lambda}_1}, N_{\vec{k}_2\vec{\lambda}_2}, ..., N_{\vec{k}\vec{\lambda}} + 1, ... \right\rangle \tag{15.489}$$

so that

$$E_{initial} = \varepsilon_0 + \sum_{\vec{k}\,'\vec{\lambda}\,'} \hbar c k' N_{\vec{k}\,'\vec{\lambda}\,'} \tag{15.490}$$

$$E_{final} = \varepsilon_n + \sum_{\vec{k}\,'\vec{\lambda}\,'} \hbar c k' N_{\vec{k}\,'\vec{\lambda}\,'} + \hbar c k \tag{15.491}$$

The transition rate is

$$\frac{2\pi}{\hbar}\delta(\varepsilon_n - \varepsilon_0 - \hbar c k) \left| \left\langle 0; ....N_{\vec{k}\vec{\lambda}} + 1, ...\right| \hat{H}_{\text{int}} \left| n; ....N_{\vec{k}\vec{\lambda}}, ...\right\rangle \right|^2 \tag{15.492}$$

where

$$\left\langle 0; ....N_{\vec{k}\vec{\lambda}}+1, ...\right| \hat{H}_{int} \left| n; ....N_{\vec{k}\vec{\lambda}}, ...\right\rangle$$
$$= -\frac{e}{c\sqrt{V}} \left\langle 0 \right| \vec{j}_{\vec{k}} \cdot \vec{\lambda}^* \left| n \right\rangle \left\langle ....N_{\vec{k}\vec{\lambda}}+1, ...\right| A^{(op)+}_{\vec{k}\vec{\lambda}} \left| ....N_{\vec{k}\vec{\lambda}}, ...\right\rangle$$
$$= -\frac{e}{c}\sqrt{\frac{2\pi\hbar c}{\omega V}} \left\langle 0 \right| \vec{j}_{\vec{k}} \cdot \vec{\lambda}^* \left| n \right\rangle \sqrt{N_{\vec{k}\vec{\lambda}}+1} \qquad (15.493)$$

We no longer have any features that are unknown and hence adjustable. Forcing agreement with induced absorption makes the results for the emission process a prediction!

We get

$$\Gamma^{emis}_{n\to 0;\vec{k}\vec{\lambda}} = \frac{4\pi^2 e^2}{\omega V}\delta(\varepsilon_n - \varepsilon_0 - \hbar ck) \left| \left\langle 0 \right| \vec{j}_{\vec{k}} \cdot \vec{\lambda}^* \left| n \right\rangle \right|^2 \left(N_{\vec{k}\vec{\lambda}}+1 \right) \neq \Gamma^{abs}_{0\to n;\vec{k}\vec{\lambda}} \qquad (15.494)$$

which disagrees with the classical field result but agrees with experiment.

The $N_{\vec{k}\vec{\lambda}}$ part corresponds to the classical result.

The $+1$ part is a purely quantum mechanical effect.

This term implies that there is an emission process that can take place even if there is *no external field* present.

This process is called *spontaneous emission.* A clear victory for the quantum approach.