Quantum Theory 2015/16

4. Relativistic Quantum Theory

4.1 Quick Review of Special Relativity

Four-Vector Notation: The coordinates of an object or ‘event’ in four-dimensional space-time, Minkowski space, form a *contravariant* four-vector whose components have ‘upper’ indices:

$$x^\mu \equiv (x^0,\, x^1,\, x^2,\, x^3) \equiv (ct,\, \underline{x})$$

Similarly, we define a *covariant* four-vector whose components have ‘lower’ indices:

$$x_\mu \equiv (x_0,\, x_1,\, x_2,\, x_3) \equiv (ct,\, -\underline{x})$$

A general four-vector a^μ is defined in the same way:

$$\begin{aligned} a^\mu &\equiv (a^0,\, a^1,\, a^2,\, a^3) \equiv (a^0,\, \underline{a}) \\ a_\mu &\equiv (a_0,\, a_1,\, a_2,\, a_3) \equiv (a^0,\, -\underline{a}) \end{aligned}$$

so that $a^0 = a_0$ and $a^i = -a_i,\ i = 1, 2, 3$. Upper and lower indices are related by the *metric tensor* $g^{\mu\nu}$:

$$a^\mu = g^{\mu\nu}\, a_\nu \qquad\qquad a_\mu = g_{\mu\nu}\, a^\nu$$

where

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

and we use the Einstein summation convention where there is an implicit sum over the *repeated index*: $\nu = 0, 1, 2, 3$.

The *scalar product* in Minkowski space is defined, for general 4-vectors a^μ and b^μ by

$$\begin{aligned} a \cdot b &\equiv a^\mu b_\mu = a_\mu b^\mu = a_\mu b_\nu g^{\mu\nu} = a^\mu b^\nu g_{\mu\nu} \\ &= a^0 b^0 - \underline{a} \cdot \underline{b} \end{aligned}$$

where $\underline{a}$ and $\underline{b}$ are ordinary 3-vectors.

NB we **do *not* underline** 4-vectors; every pair of repeated indices is implicitly summed over and each pair consists of one upper & one lower index. An expression with two identical upper (or lower) indices (eg $a^\mu b^\mu$) is simply **wrong**!

Lorentz transformations: Lorentz transformations are linear transformations on the components of 4-vectors which leave invariant this scalar product:

$$a'^{\,\mu} = \Lambda^\mu{}_\nu\, a^\nu \quad \text{eg} \quad x'^{\,\mu} = \Lambda^\mu{}_\nu\, x^\nu$$

Strictly, these are *homogeneous* Lorentz transformations – translations are not included.

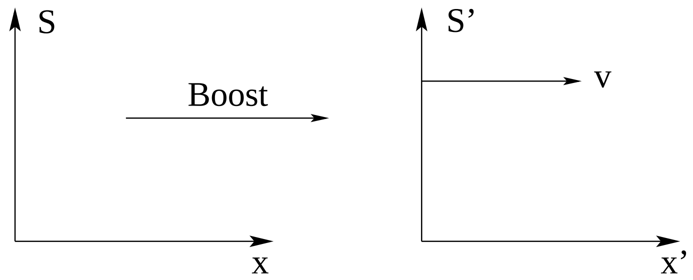
The 'standard' Lorentz transformation is a 'boost' along the x direction

$$\Lambda^{\mu}{}_{\nu} \;=\; \begin{pmatrix} \cosh\omega & -\sinh\omega & 0 & 0 \\ -\sinh\omega & \cosh\omega & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

where the 'rapidity' ω satisfies

$$\begin{aligned} \tanh\omega &\equiv \beta \equiv v/c \\ \cosh\omega &\equiv \gamma = (1-\beta^2)^{-1/2} \;=\; (1-(v/c)^2)^{-1/2} \\ \sinh\omega &= \gamma\,\beta \end{aligned}$$

Hence $ct' = \gamma\,(ct - (v/c)x)$ and $x' = \gamma\,(x - vt)$ as usual, relating the time and space co-ordinates of a given event in two inertial frames in relative motion:



Differential operators

$$\begin{aligned} \partial_\mu &\equiv \frac{\partial}{\partial x^\mu} = \left(\frac{1}{c}\frac{\partial}{\partial t},\, \underline{\nabla}\right) \\ \partial^\mu &\equiv \frac{\partial}{\partial x_\mu} \;=\; \left(\frac{1}{c}\frac{\partial}{\partial t},\, -\underline{\nabla}\right) \end{aligned}$$

$$\text{d'Alembertian:} \qquad \partial_\mu\,\partial^\mu \;=\; \partial^\mu\,\partial_\mu \;=\; \partial^2 \;=\; \frac{1}{c^2}\frac{\partial^2}{\partial t^2} \;-\; \nabla^2 \qquad (\;=\;\Box)$$

(NB sometimes $\Box$ is called $\Box^2$, so we will almost always use ∂^2.)

Momentum and energy: The conserved 4-momentum is denoted by:

$$p^\mu \;\equiv\; \left(\frac{E}{c},\, \underline{p}\right)$$

$$\begin{aligned} p^2 &= \frac{E^2}{c^2} \;-\; \underline{p}\cdot\underline{p} \;=\; m^2c^2 \quad \text{for a free particle} \\ \text{or} \quad E^2 &= |\underline{p}|^2c^2 \;+\; m^2c^4 \end{aligned}$$

where m is the mass of the particle.

We shall follow the historical development of relativistic quantum mechanics, beginning with the standard simple-minded approach to making the Schrödinger equation consistent with special relativity.

4.2 The Klein-Gordon equation

Recall that the Schrödinger equation for a free particle

$$i\hbar\frac{\partial}{\partial t}\psi(\underline{r},t) \;=\; \left\{-\frac{\hbar^2}{2m}\nabla^2\right\}\psi(\underline{r},t)$$

can be obtained from the (non-relativistic) classical total energy

$$E \;=\; H \;=\; \frac{|\underline{p}|^2}{2m}$$

by means of the operator substitution prescriptions

$$E \to i\hbar\frac{\partial}{\partial t} \qquad \text{and} \qquad \underline{p} \to -i\hbar\underline{\nabla}$$

The relativistic expression for the total energy of a free particle is

$$E^2 \;=\; |\underline{p}|^2c^2 \;+\; m^2c^4$$

Schrödinger (& Klein, Gordon, & Fock) suggested this as a starting point, thus obtaining

$$-\hbar^2\frac{\partial^2}{\partial t^2}\phi(\underline{r},t) \;=\; -\,\hbar^2\,c^2\nabla^2\phi(\underline{r},t) \;+\; m^2c^4\phi(\underline{r},t) \qquad (1)$$

which is the Klein Gordon (KG) equation for the wavefunction $\phi(\underline{r},t)$ of a free relativistic particle.[1] We can write this in a manifestly covariant form as

$$\left(\partial^2 \;+\; \frac{m^2c^2}{\hbar^2}\right)\phi(x) \;=\; 0$$

where x is the four-vector $(ct,\, x^1,\, x^2,\, x^3)$, so the operator prescription in covariant form is

$$p^\mu \;\;\to\;\; \hat{p}^\mu \;=\; i\hbar\left\{\frac{1}{c}\frac{\partial}{\partial t},\; -\underline{\nabla}\right\} \;=\; i\hbar\frac{\partial}{\partial x_\mu} \;=\; i\hbar\partial^\mu$$

For a *massless* particle, $m = 0$, the KG equation reduces to the classical wave equation $\partial^2\phi = 0$.

Free particle solutions: By substitution into the KG equation (1) we see it has plane-wave solutions

$$\phi(\underline{r},t) \;=\; \exp\{i\underline{k}\cdot\underline{r} \;-\; i\omega\, t\}$$

provided that ω, $\underline{k}$ & m are related by

$$\hbar^2\omega^2 \;=\; \hbar^2c^2|\underline{k}|^2 \;+\; m^2c^4$$

Taking the square-root, we get: $\hbar\omega \;=\; \pm\left\{\hbar^2c^2|\underline{k}|^2 \;+\; m^2c^4\right\}^{1/2}$.

Such solutions are readily seen to be eigenfunctions of the momentum and energy operators, with eigenvalues $\underline{p} \equiv \hbar\underline{k}$ and $E \equiv \hbar\omega$, respectively.

[1] The KG equation was first written down by Schrödinger but, due to the problems we will discover below, he discarded it in favour of the non-relativistic equation that bears his name.

Thus, if we interpret $\hbar\omega$ as an allowed total energy of the free particle solution, there is an ambiguity in the *sign* of the total energy: there are both +ve and −ve energy solutions, and these have energy

$$E \;=\; \pm\sqrt{|\underline{p}|^2c^2 + m^2c^4}$$

The positive-energy eigenvalues are in agreement with the classical relativistic relation between energy, mass, and momentum, but what should we make of particles with negative total energy?

If we define the four-vector $k^\mu \equiv (\frac{\omega}{c}, \underline{k})$ we can write the solution in covariant form

$$\phi(x) \;\equiv\; \exp(-ik\cdot x) \;\equiv\; \exp(-ik^\mu x_\mu) \;\equiv \exp(-ip^\mu x_\mu/\hbar)$$

and thus interpret the four-momentum as $p^\mu = \hbar k^\mu$.

Continuity equation and probability interpretation

Denote the Schrödinger equation by (SE) and its complex-conjugate by (SE)*. Considering

$$\psi^*\,(\mathrm{SE}) \;-\; \psi\,(\mathrm{SE})^*\,,$$

gives a continuity equation $\quad \dfrac{\partial}{\partial t}\rho \;+\; \underline{\nabla}\cdot\underline{j} \;=\; 0$

where $\quad \rho \;=\; \psi^*\,\psi \quad$ and $\quad \underline{j} \;=\; -\dfrac{i\hbar}{2m}\,(\psi^*\underline{\nabla}\psi \;-\; \psi\underline{\nabla}\psi^*)$

are the probability density and probability current density, respectively. (Integrate over any volume, and use the divergence theorem to see why – tutorial.) If we repeat this for the Klein Gordon equation, we obtain the quantities

$$\rho \;=\; \frac{i\hbar}{2mc^2}\left(\phi^*\frac{\partial\phi}{\partial t} \;-\; \phi\frac{\partial\phi^*}{\partial t}\right) \qquad \text{and} \qquad \underline{j} \;=\; -\,\frac{i\hbar}{2m}\,(\phi^*\underline{\nabla}\phi \;-\; \phi\underline{\nabla}\phi^*)$$

Note:

1. $\underline{j}$ is *identical* in form to the non-relativistic Schrödinger current density (we have *chosen* to normalise $\underline{j}$ so that this is the case.).
2. ρ can be shown to reduce to $\phi^*\phi$ in the non-relativistic limit.
3. The candidate for the probability density, $\rho(x)$, is no longer positive definite – negative energy solutions have $\rho < 0$ (exercise). Therefore there is no obvious probability-density interpretation.

Summary: The Klein Gordon (KG) equation is the simplest relativistically-covariant generalisation of the Schrödinger equation. Its solutions have the usual desirable properties for the description of a relativistic quantum particle, but they also describe particles of negative total energy, together with negative probabilities for finding them!

Considering the positive energy solutions only, the KG equation with a Coulomb potential can be solved exactly for the energy levels of the hydrogen atom. The non-relativistic expansion reproduces exactly the relativistic kinetic energy correction ΔE_{KE} obtained in time-independent perturbation theory, but it doesn't account for the spin-orbit correction or the Darwin term, so something else is required. . .

4.3 The Dirac Equation

Dirac tried to avoid the twin difficulties of negative energy and negative probability by proposing a relativistic wave equation which, like the Schrödinger equation, is *linear* in $\frac{\partial}{\partial t}$, hoping to avoid the sign ambiguity in the square-root of E^2, and also the presence of time derivatives in the 'probability density'. Relativity then dictates that the equation should also be linear in the spatial derivatives in order to treat space and time on an equal footing.

Following Dirac, we start with a Hamiltonian equation of the form

$$i\hbar \frac{\partial}{\partial t} \psi(\underline{r}, t) \;=\; \hat{H}\, \psi(\underline{r}, t)$$

and write

$$i\hbar \frac{\partial}{\partial t} \psi(\underline{r}, t) \;=\; -i\hbar c \left\{ \alpha^1 \frac{\partial}{\partial x^1} \;+\; \alpha^2 \frac{\partial}{\partial x^2} \;+\; \alpha^3 \frac{\partial}{\partial x^3} \right\} \psi(\underline{r},\, t) \;+\; \beta\, mc^2\, \psi(\underline{r},\, t) \quad (2)$$

$$= \left\{ c\, \underline{\alpha} \cdot \underline{\hat{p}} \;+\; \beta\, mc^2 \right\} \psi(\underline{r},\, t) \;=\; \hat{H} \psi(\underline{r},\, t) \quad (3)$$

$$\text{where} \quad \underline{\alpha} \cdot \underline{\hat{p}} \;\equiv\; \alpha^i\, \hat{p}^i \;=\; -\, i\hbar \alpha^i \frac{\partial}{\partial x^i} \qquad \left(\text{with} \quad \alpha^i\, \hat{p}^i \;\equiv\; \sum_{i=1}^{3} \alpha^i\, \hat{p}^i \text{ etc.} \right)$$

Initially, we attempt to construct an equation for a *free particle*, so no terms in the Hamiltonian $\hat{H}$ should depend on $\underline{r}$ or t as these would describe forces. By assumption, the quantities α^i and β are independent of derivatives, therefore α^i and β commute with $\underline{r}$, t, $\underline{\hat{p}}$ and E but not necessarily with each other.

Since relativistic invariance must be maintained, *ie* $E^2 \;=\; |\underline{p}|^2 c^2 \;+\; m^2 c^4$, Dirac demanded that

$$\hat{H}^2\, \psi(\underline{r}, t) \;=\; \left(c^2\, |\underline{\hat{p}}|^2 \;+\; m^2 c^4 \right)\, \psi(\underline{r}, t) \quad (4)$$

From equation (3) we have

$$\hat{H}^2\, \psi(\underline{r},\, t) \;=\; \left\{ c\, \underline{\alpha} \cdot \underline{\hat{p}} \;+\; \beta\, mc^2 \right\} \left\{ c\, \underline{\alpha} \cdot \underline{\hat{p}} \;+\; \beta\, mc^2 \right\}\, \psi(\underline{r},\, t)$$

Expand the RHS of this equation, being careful about the ordering of the, as yet undetermined, quantities α^i and β

$$\begin{aligned} &\hat{H}^2\, \psi(\underline{r},\, t) \\ &\quad = \left\{ c^2 \left[(\alpha^1)^2\, (\hat{p}^1)^2 \;+\; (\alpha^2)^2\, (\hat{p}^2)^2 \;+\; (\alpha^3)^2\, (\hat{p}^3)^2 \right] \;+\; m^2 c^4\, \beta^2 \right\} \psi(\underline{r}, t) \\ &\qquad + \; c^2 \left\{ \left(\alpha^1 \alpha^2 \;+\; \alpha^2 \alpha^1 \right) \hat{p}^1 \hat{p}^2 \;+\; \left(\alpha^2 \alpha^3 \;+\; \alpha^3 \alpha^2 \right) \hat{p}^2 \hat{p}^3 \;+\; \left(\alpha^3 \alpha^1 \;+\; \alpha^1 \alpha^3 \right) \hat{p}^1 \hat{p}^3 \right\} \psi(\underline{r}, t) \\ &\qquad + \; mc^3 \left\{ \left(\alpha^1 \beta \;+\; \beta \alpha^1 \right) \hat{p}^1 \;+\; \left(\alpha^2 \beta \;+\; \beta \alpha^2 \right) \hat{p}^2 \;+\; \left(\alpha^3 \beta \;+\; \beta \alpha^3 \right) \hat{p}^3 \right\} \psi(\underline{r}, t) \end{aligned}$$

Condition (4) is satisfied if

$$\begin{aligned} (\alpha^1)^2 \;=\; (\alpha^2)^2 \;=\; (\alpha^3)^2 \;=\; \beta^2 \;&=\; 1 \\ \alpha^i\, \alpha^j \;+\; \alpha^j\, \alpha^i \;&=\; 0 \qquad (i \neq j) \\ \alpha^i\, \beta \;+\; \beta\, \alpha^i \;&=\; 0 \end{aligned}$$

or, more compactly,

$$\begin{aligned} \left\{\alpha^i,\, \alpha^j\right\} &= 2\,\delta^{ij} \qquad \text{the } \textit{anticommutator} \text{ of } \alpha^i \text{ and } \alpha^j \\ \left\{\alpha^i,\, \beta\right\} &= 0 \quad , \qquad \beta^2 \;=\; 1 \end{aligned}$$

1. From these relations it's clear that the α^i and β cannot be ordinary numbers. If we assume they're *matrices*, then since $\hat{H}$ is hermitian, α^i and β must also be hermitian (and therefore *square*) $n \times n$ matrices.

2. The matrices α^i and β are hermitian so their eigenvalues are all real. Therefore, since $(\alpha^i)^2 = \beta^2 = I$ (the unit matrix), all the eigenvalues must be ± 1 (exercise).

3. $\mathrm{Tr}\ (\alpha^i) \;=\; \mathrm{Tr}\ (\beta) \;=\; 0$.

   Proof:
   $$\begin{aligned} \mathrm{Tr}\ (\alpha^i) &= \mathrm{Tr}\ (\beta^2\,\alpha^i) \;=\; \mathrm{Tr}\ (\beta\,\alpha^i\,\beta) \qquad (\text{using } \mathrm{Tr}\ (AB) \;=\; \mathrm{Tr}\ (BA)\ ) \\ &= -\mathrm{Tr}\ (\alpha^i\,\beta^2) \qquad (\text{using } \alpha^i\,\beta \;=\; -\,\beta\alpha^i) \\ &= -\mathrm{Tr}\ (\alpha^i) \;=\; 0 \end{aligned}$$

Since the eigenvalues are ± 1, and the trace is the sum of the eigenvalues, n must be *even.* It's not possible to find a set of 4 traceless hermitian 2×2 matrices which satisfy the anti-commutation relations; the 3 Pauli matrices σ^i satisfy $\{\sigma^i, \sigma^j\} \;=\; 2\delta^{ij}$, but there is no 4^{th} matrix.

The smallest representation of α^i and β is 4×4, and may be constructed using the Pauli matrices σ^i as sub-matrices. The *standard representation* has β diagonal:

$$\beta \;=\; \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \qquad \alpha^i \;=\; \begin{pmatrix} 0 & \sigma^i \\ \sigma^i & 0 \end{pmatrix} \qquad \text{or} \qquad \underline{\alpha} \;=\; \begin{pmatrix} 0 & \underline{\sigma} \\ \underline{\sigma} & 0 \end{pmatrix}$$

where each element is a 2×2 submatrix, and $\underline{\alpha}$ is shorthand for a 'three vector' of 4×4 matrices α^i.

Writing these out in full gives

$$\beta \;=\; \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$$

$$\alpha^1 \;=\; \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix} \qquad \alpha^2 \;=\; \begin{pmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \\ 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \end{pmatrix} \qquad \alpha^3 \;=\; \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix}$$

Exercise: Check that these matrices satisfy the correct anti-commutation relations.

Since the Hamiltonian is a 4×4 matrix, the wave-function $\psi(\underline{r}, t)$ it acts on is naturally a 4-*component column matrix*:

$$\psi(\underline{r}, t) \;=\; \begin{pmatrix} \psi_1(\underline{r}, t) \\ \psi_2(\underline{r}, t) \\ \psi_3(\underline{r}, t) \\ \psi_4(\underline{r}, t) \end{pmatrix}$$

Probability Density

The Dirac equation for a free particle is

$$i\hbar\frac{\partial}{\partial t}\,\psi(\underline{r},t) \;=\; \left(-i\hbar c\,\underline{\alpha}\cdot\underline{\nabla} \;+\; \beta\, mc^2\right)\psi(\underline{r},t) \tag{5}$$

Construction of the probability density is straightforward. Take the Hermitian conjugate of equation (5) (*ie* complex conjugate and transpose)

$$-i\hbar\frac{\partial}{\partial t}\,\psi^\dagger(\underline{r},t) \;=\; \psi^\dagger(\underline{r},t)\left(i\hbar c\,\underline{\alpha}\cdot\overleftarrow{\underline{\nabla}} \;+\; \beta\, mc^2\right) \tag{6}$$

Note that $\psi^\dagger$ is a row vector whose components are the complex conjugates of the components of ψ. Now multiply (5) by $\psi^\dagger$ from the left and (6) by ψ from the right and subtract:

$$\begin{aligned}
i\hbar\frac{\partial}{\partial t}\left(\psi^\dagger\,\psi\right) &= -i\hbar c\left(\psi^\dagger\underline{\alpha}\cdot\underline{\nabla}\psi \;+\; \psi^\dagger\underline{\alpha}\cdot\overleftarrow{\underline{\nabla}}\psi\right)\\
&= -i\hbar c\left(\psi^\dagger\underline{\alpha}\cdot\underline{\nabla}\psi \;+\; \left(\underline{\nabla}\psi^\dagger\right)\cdot\underline{\alpha}\,\psi\right)\\
&= -i\hbar c\,\underline{\nabla}\cdot\left(\psi^\dagger\,\underline{\alpha}\,\psi\right)
\end{aligned}$$

This can be written as a continuity equation

$$\frac{1}{c}\frac{\partial\rho}{\partial t} \;+\; \underline{\nabla}\cdot\underline{j} \;=\; 0$$

with

$$\rho \;=\; \psi^\dagger\psi \qquad\text{and}\qquad j^{\,i} \;=\; \psi^\dagger\,\alpha^i\,\psi \qquad \left(\text{or}\quad \underline{j} \;=\; \psi^\dagger\,\underline{\alpha}\,\psi\right)$$

where $\rho \;=\; \psi^\dagger\psi \;\equiv\; |\psi|^2$ is a positive definite quantity as required of a probability density.

We can write the continuity equation in covariant form as

$$\partial_\mu\, j^\mu \;=\; 0 \qquad\text{with}\qquad j^\mu \;=\; (\rho,\,\underline{j})$$

This is usually known as *probability-current density conservation* and it implies that $\psi^\dagger\psi$ transforms like the time-like component of a 4-vector, with $\psi^\dagger\,\underline{\alpha}\,\psi$ the corresponding space part, which we identify as the usual probability-current density.

Free Particle Solutions

Let's look for plane-wave solutions of the form

$$\begin{aligned}
\psi(\underline{r},t) &= \exp(-ik^\mu\,x_\mu)\,w(p)\\
&= \exp(-ik\cdot x)\,w(p) \;=\; \exp(-ip\cdot x/\hbar)\,w(p)\\
&= \exp\left\{-\frac{i}{\hbar}\left(cp^0t \;-\; \underline{p}\cdot\underline{r}\right)\right\}w(p)
\end{aligned}$$

where $w(p)$ is a 4-component column matrix.

Substituting into the Dirac equation (5) and dividing out by $c\exp(-ip\cdot x/\hbar)$, yields

$$p^0\,w(p) \;=\; \left(\underline{\alpha}\cdot\underline{p} \;+\; \beta mc\right)\,w(p) \tag{7}$$

which is sometimes called the momentum-space or 'p-space' Dirac equation. The trial solution presumably represents a particle of energy cp^0 and momentum $\underline{p}$.

Writing out equation (7) by substituting the matrices β and α^i gives a set of 4-simultaneous linear equations which we write in matrix form as:

$$\begin{pmatrix} (-p^0+mc) & 0 & p^3 & (p^1-ip^2) \\ 0 & (-p^0+mc) & (p^1+ip^2) & -p^3 \\ p^3 & (p^1-ip^2) & -(p^0+mc) & 0 \\ (p^1+ip^2) & -p^3 & 0 & -(p^0+mc) \end{pmatrix} \begin{pmatrix} w_1 \\ w_2 \\ w_3 \\ w_4 \end{pmatrix} = 0$$

The condition for non-trivial solutions for $w(p)$ is that the determinant of the matrix vanishes. On multiplying out the determinant, we find (slightly laborious exercise)

$$\left\{m^2c^2 \;+\; |\underline{p}|^2 \;-\; (p^0)^2\right\}^2 \;=\; 0 \tag{8}$$

which is the just the square of the required energy-momentum relation. Of course, this had to happen because we constructed the matrices α^i and β so that it would! Taking the square-root, we have

$$p^0 \;=\; \pm\left\{(m^2c^2 \;+\; |\underline{p}|^2\right\}^{1/2}$$

so the negative energy solutions are still with us.

Viewed more formally, equation (7) is an eigenvalue problem which we wish to solve for the *eigenvalues* p_0 and *eigenvectors* $w(p)$. The eigenvalue condition, equation (8), is a quartic equation whose four solutions are

$$p^0 \;=\; +\left\{(m^2c^2 \;+\; |\underline{p}|^2\right\}^{1/2} \quad \text{(twice)} \qquad \text{and} \qquad p^0 \;=\; -\left\{(m^2c^2 \;+\; |\underline{p}|^2\right\}^{1/2} \quad \text{(twice)}$$

The four eigenvalues p^0 come in two degenerate pairs of equal magnitude but opposite sign.

Two-by-two block form of the Dirac equation

The p-space Dirac equation

$$p^0\, w(p) \;=\; \left(\underline{\alpha}\cdot\underline{p} \;+\; \beta mc\right)\, w(p)$$

can be solved for $w(p)$ by brute force, but we shall introduce a more elegant formalism by writing the *four-component spinor* $w(p)$ in terms of two *two-component spinors* $\phi(p)$ and $\chi(p)$:

$$w(p) \;=\; \begin{pmatrix} \phi(p) \\ \chi(p) \end{pmatrix}$$

The p-space Dirac equation (7), becomes

$$p^0 \begin{pmatrix} \phi \\ \chi \end{pmatrix} \;=\; \begin{pmatrix} mc & \underline{\sigma}\cdot\underline{p} \\ \underline{\sigma}\cdot\underline{p} & -mc \end{pmatrix} \begin{pmatrix} \phi \\ \chi \end{pmatrix}$$

Note that the elements of the 2×2 *block matrix* are themselves 2×2 matrices: $\underline{\sigma}\cdot\underline{p}$ is the 2×2 matrix $\sum_{i=1}^{3}\sigma^i\, p^i$, mc is shorthand for $mc\, I$, where I is the 2×2 unit matrix, and hence

$$p^0\,\phi \;=\; mc\,\phi \;+\; \underline{\sigma}\cdot\underline{p}\,\chi \tag{9}$$

$$p^0\,\chi \;=\; \underline{\sigma}\cdot\underline{p}\,\phi \;-\; mc\,\chi \tag{10}$$

Positive energy solutions: Let us first choose $p^0 > 0$.

(From the previous section, we know this will give us

$$p^0 \;=\; +\,(m^2c^2 + |\underline{p}|^2)^{1/2} \equiv p^0_+ \;=\; \frac{E}{c} \quad (E > 0)$$

but we will re-derive this result here.)

Equation (10) can be used to solve for χ in terms of ϕ

$$\chi \;=\; \frac{\underline{\sigma} \cdot \underline{p}}{p^0 + mc}\,\phi \tag{11}$$

which we can substitute back into equation (9) to obtain

$$p^0\,\phi \;=\; \left\{ mc \;+\; \frac{(\underline{\sigma} \cdot \underline{p})^2}{p^0 + mc} \right\} \phi$$

but $(\underline{\sigma} \cdot \underline{p})^2 \;=\; |\underline{p}|^2 I$ (exercise), therefore $w(p)$ is a free particle solution of the Dirac equation for *all* two-component spinors ϕ if

$$(p^0)^2 \;+\; p^0 mc \;=\; p^0 mc \;+\; (mc)^2 \;+\; |\underline{p}|^2$$

which gives us the desired relation between energy & momentum.

The Dirac spinors $w^{(1),(2)}(p)$ corresponding to the two positive-energy plane-wave solutions can then be written as

$$w^{(1),(2)}(p) \;=\; \begin{pmatrix} \phi^{(1),(2)} \\ \left(\dfrac{c\,\underline{\sigma} \cdot \underline{p}}{E + mc^2} \right) \phi^{(1),(2)} \end{pmatrix}$$

It is conventional to *choose* the two linearly-independent two-spinors

$$\phi^{(1)} \;=\; \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad \text{and} \qquad \phi^{(2)} \;=\; \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

Negative energy solutions: Now choose $p^0 < 0$ [which will again give us

$$p^0 \;=\; -\,(m^2c^2 + |\underline{p}|^2)^{1/2} \equiv p^0_- \;=\; -\,\frac{E}{c} \quad (E > 0)\,]$$

It is conventional to write down the two negative energy solutions for negative spatial momenta $-\underline{p}$, *ie* for $p^\mu_- \;=\; (p^0_-, -\underline{p})$. By solving equation (9) for ϕ in terms of χ we obtain (exercise):

$$w^{(3),(4)}(-p) \;=\; \begin{pmatrix} \left(\dfrac{c\,\underline{\sigma} \cdot \underline{p}}{E + mc^2} \right) \chi^{(1),(2)} \\ \chi^{(1),(2)} \end{pmatrix}$$

For the negative energy solutions, it is conventional to choose the two linearly-independent two-spinors

$$\chi^{(1)} \;=\; \begin{pmatrix} 0 \\ 1 \end{pmatrix} \qquad \text{and} \qquad \chi^{(2)} \;=\; \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

The reason for the (apparently perverse) choice of negative momenta and two-spinors will become clearer when we try to interpret the negative energy states.

Summary: With the above conventions, the two positive energy solutions with four momenta $p_+^\mu = (E/c,\, \underline{p})$ have components

$$w^{(1)}(p) \;=\; \begin{pmatrix} 1 \\ 0 \\ \dfrac{cp^3}{E+mc^2} \\ \dfrac{c(p^1+ip^2)}{E+mc^2} \end{pmatrix} \qquad \text{and} \qquad w^{(2)}(p) \;=\; \begin{pmatrix} 0 \\ 1 \\ \dfrac{c(p^1-ip^2)}{E+mc^2} \\ \dfrac{-cp^3}{E+mc^2} \end{pmatrix}$$

and the two negative energy solutions with spatial momenta $-\underline{p}$, *ie* $p_-^\mu = (-E/c,\, -\underline{p}) = -p_+^\mu$, have components

$$w^{(3)}(-p) \;=\; \begin{pmatrix} \dfrac{c(p^1-ip^2)}{E+mc^2} \\ \dfrac{-cp^3}{E+mc^2} \\ 0 \\ 1 \end{pmatrix} \qquad \text{and} \qquad w^{(4)}(-p) \;=\; \begin{pmatrix} \dfrac{cp^3}{E+mc^2} \\ \dfrac{c(p^1+ip^2)}{E+mc^2} \\ 1 \\ 0 \end{pmatrix}$$

Note: Recall that we defined the quantity $E > 0$ in all equations above. Beware: conventions in labelling the spinors $w^{(i)}$ differ widely.

Rest-frame solutions, spin and angular momentum: When $\underline{p} = 0$ we have

$$w^{(1)} \;=\; \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} \qquad w^{(2)} \;=\; \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} \qquad w^{(3)} \;=\; \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} \qquad w^{(4)} \;=\; \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}$$

and the positive-energy solutions reduce to

$$\psi^{(1)} \;=\; \exp(-imc^2t/\hbar) \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} \qquad \text{and} \qquad \psi^{(2)} \;=\; \exp(-imc^2t/\hbar) \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}$$

which are degenerate in energy. Therefore, by the compatibility theorem, there must exist some other operator which commutes with the Hamiltonian (for $\underline{p} = 0$) and whose eigenvalues label (and distinguish) the two states. One such operator is

$$\Sigma^3 \;\equiv\; \begin{pmatrix} \sigma^3 & 0 \\ 0 & \sigma^3 \end{pmatrix} \;=\; \begin{pmatrix} 1 & & & \\ & -1 & & \\ & & 1 & \\ & & & -1 \end{pmatrix}$$

The rest-frame *four-component spinors* $w^{(i)}(0)$ are eigenvectors of Σ^3 with eigenvalues ± 1.

The appearance of the Pauli spin matrix σ^3 suggests that we interpret the Dirac equation as describing a spin 1/2 particle. If we introduce the three 4×4 matrices

$$\Sigma^i \;\equiv\; \begin{pmatrix} \sigma^i & 0 \\ 0 & \sigma^i \end{pmatrix} \qquad \text{or, in vector notation,} \qquad \underline{\Sigma} \;\equiv\; \begin{pmatrix} \underline{\sigma} & 0 \\ 0 & \underline{\sigma} \end{pmatrix}$$

$$\left.\begin{array}{llcl} \text{Then} & \left(\frac{1}{2}\hbar\,\underline{\Sigma}\right)\cdot\left(\frac{1}{2}\hbar\,\underline{\Sigma}\right) & = & \frac{3}{4}\hbar^2\,\hat{1} \;=\; s(s+1)\,\hbar^2\,\hat{1}\;\text{ with }\; s=\frac{1}{2} \\ \text{and} & \frac{1}{2}\hbar\,\Sigma^3 & & \text{has eigenvalues }\;\pm\,\tfrac{1}{2}\hbar \end{array}\right\}\;\Rightarrow\;\underline{\hat{s}}\;=\;\frac{1}{2}\hbar\,\underline{\Sigma}$$

We therefore interpret $\frac{1}{2}\hbar\underline{\Sigma}$ as the *spin operator* for the Dirac particle, which necessarily has an *intrinsic spin*, $s = 1/2$, that isn't related to ordinary orbital angular momentum.

However, $\underline{\Sigma}$ does *not* commute with the Hamiltonian $c\underline{\alpha}\cdot\underline{p}\,+\,\beta mc^2$ in any frame other than the rest frame, $\underline{p}=0$, so the expectation value of $\underline{\Sigma}$ is *not* a conserved quanity for $\underline{p}\neq 0$.

Similarly, the operator $\underline{\hat{L}}\,=\,\underline{\hat{r}}\times\underline{\hat{p}}$ does *not* commute with the Hamiltonian in any frame other than the rest frame, so orbital angular momentum isn't a conserved quantity either.

However, the operator

$$\underline{\hat{J}}\;=\;\underline{\hat{L}}\;+\;\frac{1}{2}\hbar\,\underline{\Sigma}$$

does commute with the Hamiltonian in all frames. This strongly suggests that $\underline{\hat{J}}$ should be interpreted as the operator for the *total* angular momentum, and this *is* conserved (tutorial).

Helicity: As we have seen, there are two degenerate linearly-independent states for any given four-momentum. A different (p-space) operator which commutes with $c\underline{\alpha}\cdot\underline{p}\,+\,\beta mc^2$, and which can be used to label, and therefore distinguish, the states is the *helicity operator*

$$\hat{h}(\underline{p})\;=\;\begin{pmatrix} \dfrac{\underline{\sigma}\cdot\underline{p}}{|\underline{p}|} & 0 \\ 0 & \dfrac{\underline{\sigma}\cdot\underline{p}}{|\underline{p}|} \end{pmatrix}$$

which has eigenvalues ± 1; these give the projection of the particle's spin along its direction of motion $\underline{p}/|\underline{p}|$. Plane wave states with $\underline{p}\neq 0$ can be chosen to be eigenstates of the helicity operator (see tutorial.)

Covariant form of the Dirac equation

In most applications of the Dirac equation, a covariant notation is used. Defining the 'natural' system of units, $\hbar = c = 1$, the Dirac equation for a free particle is

$$i\frac{\partial}{\partial t}\,\psi(\underline{r},t)\;=\;(\,-i\,\underline{\alpha}\cdot\underline{\nabla}\;+\;\beta\,m)\,\psi(\underline{r},t)$$

If we multiply by β

$$i\beta\frac{\partial}{\partial t}\,\psi(\underline{r},t)\;=\;(\,-i\,\beta\,\underline{\alpha}\cdot\underline{\nabla}\;+\;m)\,\psi(\underline{r},t) \qquad (12)$$

and introduce the matrices

$$\begin{aligned}\gamma^0 &\equiv \beta \\ \gamma^i &\equiv \beta\,\alpha^i\end{aligned}$$

we may rewrite equation (12) as

$$\left\{i\left(\gamma^0\,\frac{\partial}{\partial x^0}\;+\;\gamma^i\,\frac{\partial}{\partial x^i}\right)\;-\;m\right\}\,\psi(x)\;=\;0$$

where $x = x^\mu$ $(\mu = 0, \cdots, 3)$. More compactly,

$$\begin{aligned} (i\gamma^\mu \partial_\mu \; - \; m)\, \psi(x) &= 0 \\ \text{or} \qquad (i\partial\!\!\!/ \; - \; m)\, \psi(x) &= 0 \end{aligned}$$

where we have introduced the Feynman *slash* notation:

$$a\!\!\!/ \;\equiv\; \gamma^\mu\, a_\mu \;=\; \gamma_\mu\, a^\mu$$

is 'a-slash' (pronounced to rhyme with 'hay-slash'). Similarly, $\partial\!\!\!/$ is pronounced 'dee-slash'.

Positive energy plane-wave solutions of the type $\psi(x) = \exp(-ip \cdot x)\, u(p, s)$ satisfy

$$(\gamma^\mu p_\mu \;-\; m)\; u(p, s) \;=\; (p\!\!\!/ \;-\; m)\; u(p, s) \;=\; 0$$

where the positive energy spinors $u(p, s) \equiv w^{(s)}(p)$ for $s = 1, 2$. Similarly, negative energy (negative four-momentum) solutions $\psi(x) = \exp(+ip \cdot x)\, v(p, s)$ satisfy

$$(\gamma^\mu p_\mu \;+\; m)\; v(p, s) \;=\; (p\!\!\!/ \;+\; m)\; v(p, s) \;=\; 0$$

where $v(p, s) \equiv w^{(s+2)}(-p)$ for $s = 1, 2$.

It is easy to verify that the gamma matrices satisfy the anticommutation relations known as the *Clifford algebra*

$$\gamma^\mu\, \gamma^\nu \;+\; \gamma^\nu\, \gamma^\mu \;\equiv\; \{\gamma^\mu, \gamma^\nu\} \;=\; 2\, g^{\mu\nu}$$

In the standard representation of α^i and β

$$\gamma^i \;=\; \begin{pmatrix} 0 & \sigma^i \\ -\sigma^i & 0 \end{pmatrix} \qquad \text{and} \qquad \gamma^0 \;=\; \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

so that γ^0 is hermitian $\gamma^{0\dagger} = \gamma^0$, the γ^i are anti-hermitian $\gamma^{i\dagger} = -\gamma^i$, thus $(\gamma^0)^2 = 1$ and $(\gamma^i)^2 = -1$.

It is also convenient to work with

$$\begin{aligned} \overline{\psi} \;&\equiv\; \psi^\dagger\, \gamma^0 \\ \text{and similarly} \qquad \overline{u} \;&\equiv\; u^\dagger\, \gamma^0\,, \qquad \text{etc} \end{aligned}$$

where $\overline{\psi}$ is pronounced 'psi-bar'.

The new notation treats space and time on an (even more) equal basis, and is known as the *covariant formulation*. One can derive the properties of the Dirac wave-function $\psi(x)$ under Lorentz boosts and use them to verify explicitly that the conserved current

$$\begin{aligned} j^\mu \;&\equiv\; \left(\psi^\dagger \psi,\; \psi^\dagger\, \underline{\alpha}\, \psi\right) \\ &=\; \overline{\psi}\gamma^\mu\psi \end{aligned}$$

does indeed transform as a 4-vector under Lorentz transformations. Similarly, one can show that the quantity $\overline{\psi}\psi$ is invariant under Lorentz transformations, *ie* it's a Lorentz scalar.

Note: Since ∂_μ is a 4-vector operator, and $\partial_\mu\, j^\mu = 0$, then j^μ is a 4-vector by the quotient theorem. (See *Symmetries of Classical Mechanics*.)

General solutions for a free particle

The general solution of the Dirac equation for a free particle is a linear superposition of plane-wave solutions with both positive and negative energies

$$\psi(x) \;=\; \sum_{s=1,2} \int \frac{\mathrm{d}^3p}{(2\pi)^3}\,\frac{1}{2E_p}\left[a_s(\underline{p})\,u(p,s)\,\mathrm{e}^{-ip\cdot x/\hbar} + b_s^\dagger(\underline{p})\,v(p,s)\,\mathrm{e}^{ip\cdot x/\hbar}\right]$$

This is just a linear sum (integral) over solutions with momenta $\pm p^\mu$, and spin polarisations s. The normalisation factor $E_p \equiv +\sqrt{|\underline{p}|^2c^2 + m^2c^4}$ in the denominator is a convention, and the (arbitrary) coefficient functions $a_s(\underline{p})$ and $b_s^\dagger(\underline{p})$ will play a crucial role in quantum field theory – see RQFT.

The general solution of the Klein-Gordon equation may similarly be written as

$$\phi(x) \;=\; \int \frac{\mathrm{d}^3p}{(2\pi)^3}\,\frac{1}{2E_p}\left[a(\underline{p})\,e^{-ip\cdot x/\hbar} + b^\dagger(\underline{p})\,e^{ip\cdot x/\hbar}\right]$$

4.4 The Klein-Gordon and Dirac equations in an external electromagnetic field

The classical Hamiltonian for a free non-relativistic particle is

$$H = E = \frac{\left|\underline{p}\right|^2}{2m} \tag{13}$$

The Hamiltonian for a particle of charge q interacting with an electromagnetic field is

$$H_{\mathrm{em}} \;=\; \frac{\left|\underline{p} - q\underline{A}/c\right|^2}{2m} \;+\; q\,\Phi$$

in Heaviside-Lorentz units. (The Hamiltonian in SI units is the same, but without the factor of c.)

Clearly, the interacting Hamiltonian may be obtained from the free Hamiltonian by subtracting the term $q\Phi$ from the LHS of equation (13), and making the replacement

$$\underline{p} \to \underline{p} - q\underline{A}/c$$

on the RHS. In other words we let

$$E \to E \;-\; q\Phi \qquad \text{and} \qquad \underline{p} \to \underline{p} \;-\; q\underline{A}/c$$

This is known as the *minimal coupling prescription*.

The same prescription works in the relativistic case. In terms of four-vectors

$$p^\mu \to p^\mu \;-\; \frac{q}{c}A^\mu \qquad \text{where} \qquad A^\mu \;=\; (\Phi,\,\underline{A})$$

so the relativistic energy momentum relation becomes

$$(E \;-\; q\Phi)^2 \;=\; c^2\left(\underline{p} \;-\; \frac{q}{c}\underline{A}\right)^2 \;+\; m^2c^4\,.$$

If we perform operator substitution *á la* Klein-Gordon, we obtain

$$\left(i\hbar\frac{\partial}{\partial t} - q\Phi(x)\right)^2 \phi(x) \;=\; c^2\left(-i\hbar\underline{\nabla} \;-\; \frac{q}{c}\underline{A}(x)\right)^2 \phi(x) \;+\; m^2c^4\,\phi(x)$$

If the potentials are time-independent, then separable solutions of the form

$$\phi(\underline{r},t) \;=\; u(\underline{r})\,\exp(-iEt/\hbar)$$

are possible, giving

$$(E \;-\; q\Phi)^2\,u(\underline{r}) \;=\; \left\{-\hbar^2c^2\,\nabla^2 \;+\; 2iq\hbar c\,\underline{A}\cdot\underline{\nabla} \;+\; iq\hbar c\,\underline{\nabla}\cdot\underline{A} \;+\; q^2\,|\underline{A}|^2 \;+\; m^2c^4\right\} u(\underline{r})$$

Similarly, the Dirac equation for a particle of charge q interacting with an EM field A^μ may be obtained using the minimal coupling prescription:

$$\left\{i\hbar\frac{\partial}{\partial t} - q\Phi\right\}\psi(x) \;=\; \left\{c\,\underline{\alpha}\cdot\left(\hat{\underline{p}} \;-\; \frac{q}{c}\,\underline{A}\right) \;+\; \beta\,mc^2\right\}\psi(x) \tag{14}$$

$$\text{or}\quad i\hbar\frac{\partial}{\partial t}\,\psi(x) \;=\; \left\{c\,\underline{\alpha}\cdot\left(\hat{\underline{p}} \;-\; \frac{q}{c}\,\underline{A}\right) \;+\; \beta\,mc^2 \;+\; qA^0\right\}\psi(x) \tag{15}$$

where $A^0(x) \equiv \Phi(x)$. The covariant form is (exercise)

$$i\gamma^\mu\,(\partial_\mu \;+\; ieA_\mu)\,\psi(x) - m\psi(x) = 0\,. \tag{16}$$

The operator $D_\mu = \partial_\mu \;+\; ieA_\mu(x)$ is called the *covariant derivative*, whereupon the Dirac equation becomes simply

$$(i\not{D} \;-\; m)\;\psi(x) = 0 \tag{17}$$

4.5 Interpreting the negative energy solutions

As we saw, the plane wave solutions of the Dirac equation satisfy the energy-momentum relation

$$p^0c \;=\; \pm\sqrt{\left(|\underline{p}|^2c^2 \;+\; m^2c^4\right)}$$

therefore

$$\textbf{either}\quad p^0c \;\geq\; mc^2 \qquad \textbf{or}\quad p^0c \;\leq -mc^2$$

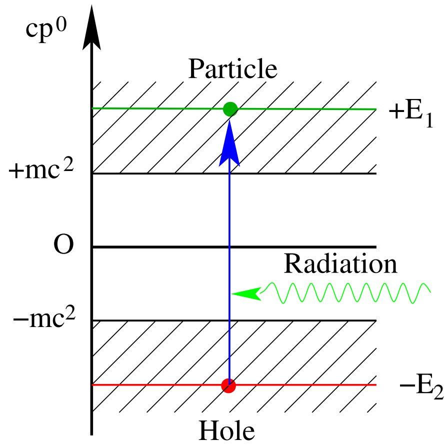
ie, there is a continuum of positive energy states starting at $p^0c = mc^2$, and a continuum of negative energy states going down from $p^0c = -mc^2$.

Since the Dirac equation appears to describe spin-half particles, let's assume these particles are electrons, and let's take the negative energy solutions seriously. The problem we must address is the following:

> What is to prevent a positive energy electron from making transitions under the influence of a perturbation to negative energy states?

A solution to this problem was suggested by Dirac in 1930.

The Dirac Sea: Dirac proposed that all negative energy states are filled, each energy level holding two electrons with opposite spins. Since electrons are fermions, he then evoked the Pauli exclusion principle to prevent any transition of a positive energy electron to a negative energy state. In this picture the ground state or 'vacuum' is an infinite sea of negative energy electrons – the Dirac sea. He then argued that the infinite negative energy and infinite negative charge of this 'vacuum', are unobservable – we can only measure finite changes of charge and energy *relative* to this vacuum.



Pair Production: An important consequence of this picture is that we can excite a negative energy particle from the 'sea' into a positive energy state.

Suppose an electron in the 'sea' absorbs photons[2] with sufficient energy ($> 2mc^2$) to make a transition to a state in the positive energy continuum. What we will observe is an electron of charge $-e$ and energy $+E_1$, say, together with a 'hole' in the sea. The 'hole' which is the *absence* of an electron with charge $-e$ and energy $-E_2$ would be interpreted by an observer as a *particle* of charge $+e$ and *energy* $+E_2$, in other words as a *positive* energy *anti-particle* or *positron*. Furthermore, the threshold for this process is just $2mc^2$, the size of the gap in the energy eigenvalue spectrum, and we have arrived at a model for electron-positron *pair production*. Thus Dirac predicted the existence of antiparticles.

Notes:

- Although we started with a single-particle wave equation, the Dirac theory forces us into a many-particle interpretation, for which quantum mechanics with a fixed number of particles is inadequate.
- The *absence* of a *negative energy* particle with spin *'up'* in its rest-frame is equivalent to the *presence* of a *positive-energy* particle with spin *'down'*. This is one reason for the 'apparently perverse' choice of negative-momentum solutions and two-component spinors we made on page 9.
- The Dirac-sea picture provides a *model* for how a many-particle relativistic quantum theory could work. The full multi-particle theory requires Relativistic Quantum Field Theory (RQFT).

[2]At least two photons must be absorbed to conserve 4-momentum.

- The Dirac sea picture doesn't work at all for bosons. There is no Pauli principle, therefore nothing can seemingly stop the positive energy particles decaying into oblivion. This is one of the reasons that lead Dirac to discard the Klein-Gordon equation for spinless particles. The problem is solved in RQFT, wherein there is no problem using the Klein-Gordon equation to describe bosons in RQFT. Indeed, if we multiply the troublesome putative probability density ρ by the particle charge, we can reinterpret it as the *electric charge density* which can of course be +ve or −ve.
- Dirac's ideas weren't universally popular at the time. Heisenberg once wrote:

  The saddest chapter of modern physics is and remains the Dirac theory. I regard the Dirac theory as learned trash which no one can take seriously.
- The positron was discovered four years later, thus confirming Dirac's prediction.

4.6 Quantum Field Theory (QFT) – non-examinable

Quantum Field Theory requires a lecture course of its own. It's surely impossible to give an idea of its flavour in a few minutes, but a fool can can try...

Motivation: The classical equation of motion for the electromagnetic field $A^\mu(x)$ (in the Lorenz gauge, $\partial_\mu A^\mu = 0$), is

$$\left(\frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \nabla^2\right) A^\mu(x) = \partial^2 A^\mu(x) = 0$$

Quantisation of the electromagnetic field using the operator formalism in the Heisenberg picture follows the standard route:

- Identify the fields $A^\mu(x)$ as the dynamical degrees of freedom, *i.e.* the equivalent of the generalised co-ordinates of particle mechanics.
- Identify the canonical momenta – these turn out to be simply the three components of the electric field $\underline{E}$.
- Impose equal-time commutation relations between the *operators* $\hat{A}^\mu$ and $\underline{\hat{E}}$. Choosing *axial gauge*, $\hat{A}^0 = 0$, we impose $[\hat{A}^i(\underline{r}, t),\, \hat{E}^j(\underline{r}', t)] \;=\; i\hbar\, \delta^{ij}\, \delta^{(3)}(\underline{r} - \underline{r}')$. These are the quantum field theory analogs of $[\hat{x}(t),\, \hat{p}(t)] = i\hbar$.
- Construct raising and lowering operators as in the harmonic oscillator, and use them to show that the physical states of the system are *photons* of energy $E = \hbar\omega$. One can then construct states of arbitrary many photons.

In order to treat radiation and matter on the same footing, we do the same with the Dirac and Klein-Gordon equations, which we now regard as classical field equations. In natural units $\hbar = c = 1$:

$$(i\gamma^\mu \partial_\mu \;-\; m)\, \psi(x) \;=\; 0\,, \qquad\qquad \left(\partial^2 + m^2\right) \phi(x) \;=\; 0$$

A *Lagrangian* approach is usually employed. We first define the action S and Lagrangian L of the free Dirac field in terms of the *Lagrangian density* $\mathcal{L}$:

$$S \;=\; \int dt L \;=\; \int dt \int d^3x\, \mathcal{L} \;=\; \int d^4x\, \overline{\psi}(x)\; (i\gamma^\mu \partial_\mu \;-\; m)\; \psi(x)$$

By applying Hamilton's principle $\delta S = 0$ to variations in $\overline{\psi}$, we get the equation of motion:

$$\frac{\partial \mathcal{L}}{\partial \overline{\psi}} = \partial_\mu \left(\frac{\partial \mathcal{L}}{\partial(\partial_\mu \overline{\psi})} \right) \quad \rightarrow \quad (i\gamma^\mu \, \partial_\mu \; - \; m) \, \psi(x) \; = \; 0$$

i.e. the Dirac equation is the *classical* equation of motion for the Dirac field $\psi(x)$. (The RHS is zero because $\mathcal{L}$ doesn't depend on $\partial_\mu \overline{\psi}$.) A similar equation holds for $\overline{\psi}$.

In canonical quantisation, the *fields* A^μ, ϕ, ψ and $\bar{\psi}$ *all* become quantum *operators.* We must identify the canonical momentum for each field, and impose the appropriate equal-time commutation relations – commutators for the electromagnetic and Klein-Gordon (bosonic) fields, and anticommutators for the Dirac (fermionic) field. When the dust settles, we find that the negative energy solutions of the Dirac and Klein-Gordon equations become negative 'frequency' solutions of the quantum field theory, whereas the eigenvalues of the field-theory Hamiltonian are all *positive*, and are identified as free particles and their anti-particles.

Finally, we may construct the Lagrangian density for Quantum Electrodynamics using minimal substitution $\partial_\mu \rightarrow \partial_\mu \; + \; ieA_\mu$:

$$\mathcal{L}_{\mathrm{QED}} \;=\; \overline{\psi}(x) \left(i\gamma^\mu \left(\partial_\mu \; + \; ieA_\mu \right) - m \right) \psi(x) \; - \; \frac{1}{4} \left(\partial_\mu \, A_\nu - \partial_\nu \, A_\mu \right)^2$$

where the last term is the Maxwell Lagrangian density $(E^2 - B^2)/2$, which gives a Hamiltonian density $(E^2 + B^2)/2$, *i.e.* the usual energy density for the electromagnetic field.

Canonical quantisation proceeds as sketched above.

Path-integral quantisation proceeds in much the same way as in ordinary quantum theory. The action is

$$S_{\mathrm{QED}} = \int d^4x \, \mathcal{L}_{\mathrm{QED}}$$

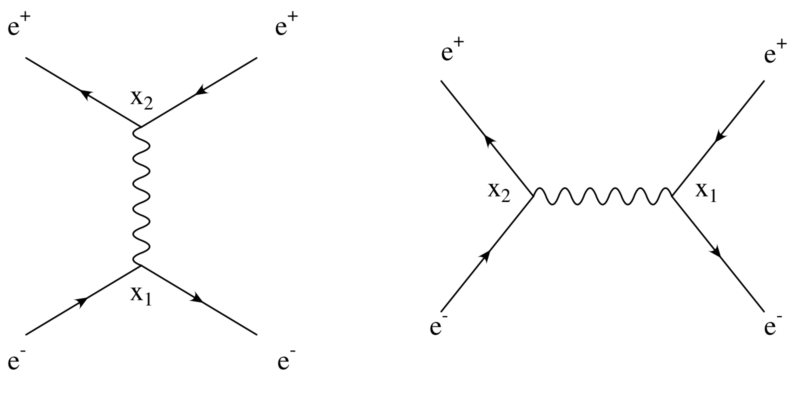
and we quantise by integrating over all field configurations in the path integral

$$Z = \int \mathcal{D}\psi \, \mathcal{D}\bar{\psi} \, \mathcal{D}A^\mu \, e^{iS_{\mathrm{QED}}/\hbar} \; .$$

Expanding this in powers of the electron-photon coupling, e, gives Feynman perturbation theory. The Feynman diagrams for electron-positron elastic scattering

$$e^+ + e^- \rightarrow e^+ + e^-$$

are



See RQFT for details.