Chapter 15

Relativistic Quantum Mechanics

The aim of this chapter is to introduce and explore some of the simplest aspects of relativistic quantum mechanics. Out of this analysis will emerge the Klein-Gordon and Dirac equations, and the concept of quantum mechanical spin. This introduction prepares the way for the construction of relativistic quantum field theories, aspects touched upon in our study of the quantum mechanics of the EM field. To prepare our discussion, we begin first with a survey of the motivations to seek a relativistic formulation of quantum mechanics, and some revision of the special theory of relativity.

Why study relativistic quantum mechanics? Firstly, there are many experimental phenomena which cannot be explained or understood within the purely non-relativistic domain. Secondly, aesthetically and intellectually it would be profoundly unsatisfactory if relativity and quantum mechanics could not be united. Finally there are theoretical reasons why one would expect new phenomena to appear at relativistic velocities.

When is a particle relativistic? Relativity impacts when the velocity approaches the speed of light, c or, more intrinsically, when its energy is large compared to its rest mass energy, mc^2. For instance, protons in the accelerator at CERN are accelerated to energies of 300GeV (1GeV= 10^9eV) which is considerably larger than their rest mass energy, 0.94 GeV. Electrons at LEP are accelerated to even larger multiples of their energy (30GeV compared to 5×10^{-4}GeV for their rest mass energy). In fact we do not have to appeal to such exotic machines to see relativistic effects – high resolution electron microscopes use relativistic electrons. More mundanely, photons have zero rest mass and always travel at the speed of light – they are never non-relativistic.

What new phenomena occur? To mention a few:

▷ **Particle production**: One of the most striking new phenomena to emerge is that of particle production – for example, the production of electron-positron pairs by energetic γ-rays in matter. Obviously one needs collisions involving energies of order twice the rest mass energy of the electron to observe production.

Astrophysics presents us with several examples of pair production. Neutrinos have provided some of the most interesting data on the 1987 supernova. They are believed to be massless, and hence inherently relativistic; moreover the method of their production is the annihilation of electron-positron pairs in the hot plasma at the core of the supernova. High temperatures, of the order of 10^{12}K are also inferred to exist in the nuclei of some galaxies (i.e. $k_B T \gg 2mc^2$). Thus electrons and positrons

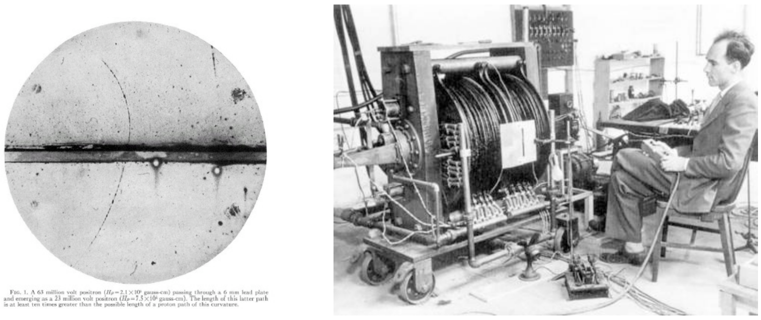


Figure 15.1: Anderson's cloud chamber picture of cosmic radiation from 1932 showing for the first time the existence of the positron. A cloud chamber contains a gas supersaturated with water vapour (left). In the presence of a charged particle (such as the positron), the water vapour condenses into droplets – these droplets mark out the path of the particle. In the picture a charged particle is seen entering from the bottom at high energy. It then looses some of the energy in passing through the 6 mm thick lead plate in the middle. The cloud chamber is placed in a magnetic field and from the curvature of the track one can deduce that it is a positively charged particle. From the energy loss in the lead and the length of the tracks after passing though the lead, an upper limit of the mass of the particle can be made. In this case Anderson deduces that the mass is less that two times the mass of the electron. Carl Anderson (right) won the 1936 Nobel Prize for Physics for this discovery. (The cloud chamber track is taken from C. D. Anderson, *The positive electron*, Phys. Rev. **43**, 491 (1933).

are produced in thermal equilibrium like photons in a black-body cavity. Again a relativistic analysis is required.

▷ **Vacuum instability**: Neglecting relativistic effects, we have shown that the binding energy of the innermost electronic state of a nucleus of charge Z is given by,

$$E = -\left(\frac{Ze^2}{4\pi\epsilon_0}\right)^2 \frac{m}{2\hbar^2}\,.$$

If such a nucleus is created without electrons around it, a peculiar phenomenon occurs if $|E| > 2mc^2$. In that case, the total change in energy of producing an electron-positron pair, subsequently binding the electron in the lowest state and letting the positron escape to infinity (it is repelled by the nucleus), is negative. There is an instability! The attractive electrostatic energy of binding the electron pays the price of producing the pair. Nuclei with very high atomic mass spontaneously "screen" themselves by polarising the vacuum via electron-positron production until the they lower their charge below a critical value Z_c. This implies that objects with a charge greater than Z_c are unobservable due to screening.

▷ INFO. An estimate based on the non-relativistic formula above gives $Z_c \simeq 270$. Taking into account relativistic effects, the result is renormalised downwards to 137, while taking into account the finite size of the nucleus one finally obtains $Z_c \sim 165$. Of course, no such nuclei exist in nature, but they can be manufactured, fleetingly, in uranium ion collisions where $Z = 2 \times 92 = 184$. Indeed, the production rate of positrons escaping from the nucleus is seen to increase dramatically as the total Z of the pair of ions passes 160.

▷ **Spin**: Finally, while the phenomenon of electron spin has to be grafted artificially onto the non-relativistic Schrödinger equation, it emerges naturally from a relativistic treatment of quantum mechanics.

When do we expect relativity to intrude into quantum mechanics? According to the uncertainty relation, $\Delta x \Delta p \geq \hbar/2$, the length scale at which the kinetic energy is comparable to the rest mass energy is set by the **Compton wavelength**

$$\Delta x \geq \frac{h}{mc} \equiv \lambda_c.$$

We may expect relativistic effects to be important if we examine the motion of particles on length scales which are less than λ_c. Note that for particles of zero mass, $\lambda_c = \infty$! Thus for photons, and neutrinos, relativity intrudes at any length scale.

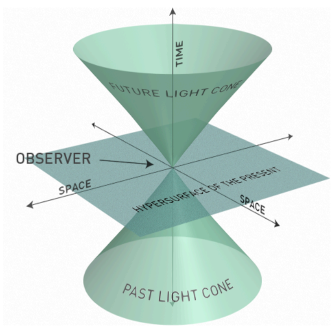
What is the relativistic analogue of the Schrödinger equation? Non-relativistic quantum mechanics is based on the time-dependent Schrödinger equation $\hat{H}\psi = i\hbar\partial_t\psi$, where the wavefunction ψ contains all information about a given system. In particular, $|\psi(x,t)|^2$ represents the probability density to observe a particle at position x and time t. Our aim will be to seek a relativistic version of this equation which has an analogous form. The first goal, therefore, is to find the relativistic Hamiltonian. To do so, we first need to revise results from Einstein's theory of **special relativity**:

▷ Info. **Lorentz Transformations and the Lorentz Group**: In the special theory of relativity, a coordinate in space-time is specified by a 4-vector. A **contravariant 4-vector** $x = (x^\mu) \equiv (x^0, x^1, x^2, x^3) \equiv (ct, \mathbf{x})$ is transformed into the **covariant** 4-vector $x_\mu = g_{\mu\nu}x^\nu$ by the **Minkowskii metric**

$$(g_{\mu\nu}) = \begin{pmatrix} 1 & & & \\ & -1 & & \\ & & -1 & \\ & & & -1 \end{pmatrix}, \qquad g_\mu{}^\nu g_{\nu\lambda} = \delta_{\mu\lambda}\,,$$

Here, by convention, summation is assumed over repeated indicies. Indeed, summation covention will be assumed throughout this chapter. The scalar product of 4-vectors is defined by

$$x \cdot y = x_\mu y^\mu = x^\mu y^\nu g_{\mu\nu} = x^\mu y_\mu\,.$$



The **Lorentz group** consists of linear **Lorentz transformations**, Λ, preserving $x\cdot y$, i.e. for $x^\mu \mapsto x'^\mu = \Lambda^\mu{}_\nu x^\nu$, we have the condition

$$\boxed{g_{\mu\nu}\Lambda^\mu{}_\alpha\Lambda^\nu{}_\beta = g_{\alpha\beta}\,.} \tag{15.1}$$

Specifically, a Lorentz transformation along the x_1 direction can be expressed in the form

$$\Lambda^\mu{}_\nu = \begin{pmatrix} \gamma & -\gamma v/c & & \\ -\gamma v/c & \gamma & & \\ & & 1 & 0 \\ & & 0 & 1 \end{pmatrix}$$

where $\gamma = (1 - v^2/c^2)^{-1/2}$.[1] With this definition, the **Lorentz group** splits up into four components. Every Lorentz transformation maps time-like vectors ($x^2 > 0$) into

[1]Equivalently the Lorentz transformation can be represented in the form

$$\Lambda = \exp[\omega K_1], \qquad [K_1]^\mu{}_\nu = \begin{pmatrix} 0 & -1 & & \\ -1 & 0 & & \\ & & 0 & 0 \\ & & 0 & 0 \end{pmatrix},$$

where $\omega = \tanh^{-1}(v/c)$ is known as the **rapidity**, and K_1 is the generator of velocity transformations along the x_1-axis.

time-like vectors. Time-like vectors can be divided into those pointing forwards in time ($x^0 > 0$) and those pointing backwards ($x^0 < 0$). Lorentz transformations do not always map forward time-like vectors into forward time-like vectors; indeed Λ does so if and only if $\Lambda^0{}_0 > 0$. Such transformations are called **orthochronous**. (Since $\Lambda^\mu{}_0 \Lambda_{\mu 0} = 1$, $(\Lambda^0{}_0)^2 - (\Lambda^j{}_0)^2 = 1$, and so $\Lambda^0{}_0 \neq 0$.) Thus the group splits into two according to whether $\Lambda^0{}_0 > 0$ or $\Lambda^0{}_0 < 0$. Each of these two components may be subdivided into two by considering those Λ for which $\det \Lambda = \pm 1$. Those transformations Λ for which $\det \Lambda = 1$ are called **proper**.

Thus the **subgroup** of the Lorentz group for which $\det \Lambda = 1$ and $\Lambda^0{}_0 > 0$ is called the **proper orthochronous Lorentz group**, sometimes denoted by $\mathcal{L}_+^\uparrow$. It contains neither the time-reversal nor parity transformation,

$$T = \begin{pmatrix} -1 & & & \\ & 1 & & \\ & & 1 & \\ & & & 1 \end{pmatrix}, \qquad P = \begin{pmatrix} 1 & & & \\ & -1 & & \\ & & -1 & \\ & & & -1 \end{pmatrix}. \tag{15.2}$$

We shall call it the Lorentz group for short and specify when we are including T or P. In particular, $\mathcal{L}_+^\uparrow$, $\mathcal{L}^\uparrow = \mathcal{L}_+^\uparrow \cup \mathcal{L}_-^\uparrow$ (the orthochronous Lorentz group), $\mathcal{L}_+ = \mathcal{L}_+^\uparrow \cup \mathcal{L}_+^\downarrow$ (the proper Lorentz group), and $\mathcal{L}_0 = \mathcal{L}_+^\uparrow \cup \mathcal{L}_-^\downarrow$ are subgroups, while $\mathcal{L}_-^\downarrow = P\mathcal{L}_+^\uparrow$, $\mathcal{L}_-^\uparrow = T\mathcal{L}_+^\uparrow$ and $\mathcal{L}_+^\downarrow = TP\mathcal{L}_+^\uparrow$ are not.

Special relativity requires that theories should be invariant under Lorentz transformations $x^\mu \longmapsto \Lambda^\mu{}_\nu x^\nu$, and, more generally, **Poincaré transformations** $x^\mu \to \Lambda^\mu{}_\nu x^\nu + a^\mu$. The proper orthochronous Lorentz transformations can be reached continuously from identity.[2] Loosely speaking, we can form them by putting together infinitesimal Lorentz transformations $\Lambda^\mu{}_\nu = \delta^\mu{}_\nu + \omega^\mu{}_\nu$, where the elements of $\omega^\mu{}_\nu \ll 1$. Applying the identity $g_{\alpha\beta} = \Lambda^\mu{}_\alpha \Lambda_{\mu\beta} = g_{\alpha\beta} + \omega_{\alpha\beta} + \omega_{\beta\alpha} + O(\omega^2)$, we obtain the relation $\omega_{\alpha\beta} = -\omega_{\beta\alpha}$. $\omega_{\alpha\beta}$ has six independent components: $\mathcal{L}_+^\uparrow$ is a six-dimensional (Lie) group, i.e. it has six independent generators: three rotations and three boosts.

Finally, according to the definition of the 4-vectors, the covariant and contravariant derivative are respectively defined by $\partial_\mu = \frac{\partial}{\partial x^\mu} = (\frac{1}{c}\frac{\partial}{\partial t}, \nabla)$, $\partial^\mu = \frac{\partial}{\partial x_\mu} = (\frac{1}{c}\frac{\partial}{\partial t}, -\nabla)$. Applying the scalar product to the derivative we obtain the d'Alembertian operator (sometimes denoted as $\Box$), $\partial^2 = \partial_\mu \partial^\mu = \frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \nabla^2$.

15.1 Klein-Gordon equation

Historically, the first attempt to construct a relativistic version of the Schrödinger equation began by applying the familiar quantization rules to the relativistic energy-momentum invariant. In non-relativistic quantum mechanics the correspondence principle dictates that the momentum operator is associated with the spatial gradient, $\hat{\mathbf{p}} = -i\hbar\nabla$, and the energy operator with the time derivative, $\hat{E} = i\hbar\partial_t$. Since $(p^\mu \equiv (E/c, \mathbf{p})$ transforms like a 4-vector under Lorentz transformations, the operator $\hat{p}^\mu = i\hbar\partial^\mu$ is relativistically covariant.

Oskar Benjamin Klein 1894-1977
A Swedish theoretical physicist, Klein is credited for inventing the idea, part of Kaluza-Klein theory, that extra dimensions may be physically real but curled up and very small, an idea essential to string theory/M-theory.

Non-relativistically, the Schrödinger equation is obtained by quantizing the classical Hamiltonian. To obtain a relativistic version of this equation, one might apply the quantization relation to the dispersion relation obtained from the energy-momentum invariant $p^2 = (E/c)^2 - \mathbf{p}^2 = (mc)^2$, i.e.

$$E(p) = +\left(m^2c^4 + \mathbf{p}^2c^2\right)^{1/2} \quad \Rightarrow \quad i\hbar\partial_t\psi = \left[m^2c^4 - \hbar^2c^2\nabla^2\right]^{1/2}\psi$$

where m denotes the rest mass of the particle. However, this proposal poses a dilemma: how can one make sense of the square root of an operator? Interpreting the square root as the Taylor expansion,

$$i\hbar\partial_t = mc^2\psi - \frac{\hbar^2\nabla^2}{2m}\psi - \frac{\hbar^4(\nabla^2)^2}{8m^3c^2}\psi + \cdots$$

[2] They are said to form the *path component* of the identity.

we find that an infinite number of boundary conditions are required to specify the time evolution of ψ.[3] It is this effective "non-locality" together with the asymmetry (with respect to space and time) that suggests this equation may be a poor starting point.

A second approach, and one which circumvents these difficulties, is to apply the quantization procedure directly to the energy-momentum invariant:

$$E^2 = \mathbf{p}^2 c^2 + m^2 c^4, \qquad -\hbar^2 \partial_t^2 \psi = \left(-\hbar^2 c^2 \nabla^2 + m^2 c^4\right) \psi.$$

Recast in the Lorentz invariant form of the d'Alembertian operator, we obtain the **Klein-Gordon equation**

$$\boxed{\left(\partial^2 + k_c^2\right) \psi = 0\,,} \tag{15.3}$$

where $k_c = 2\pi/\lambda_c = mc/\hbar$. Thus, at the expense of keeping terms of second order in the time derivative, we have obtained a *local* and manifestly covariant equation. However, invariance of ψ under global spatial rotations implies that, if applicable at all, the Klein-Gordon equation is limited to the consideration of spin-zero particles. Moreover, if ψ is the wavefunction, can $|\psi|^2$ be interpreted as a probability density?

To associate $|\psi|^2$ with the probability density, we can draw intuition from the consideration of the non-relativistic Schrödinger equation. Applying the identity $\psi^*(i\hbar\partial_t\psi + \frac{\hbar^2\nabla^2}{2m}\psi) = 0$, together with the complex conjugate of this equation, we obtain

$$\partial_t |\psi|^2 - i\frac{\hbar}{2m}\nabla \cdot (\psi^* \nabla\psi - \psi\nabla\psi^*) = 0\,.$$

Conservation of probability means that density ρ and current $\mathbf{j}$ must satisfy the continuity relation, $\partial_t \rho + \nabla \cdot \mathbf{j} = 0$, which states simply that the rate of decrease of density in any volume element is equal to the net current flowing out of that element. Thus, for the Schrödinger equation, we can consistently define $\rho = |\psi|^2$, and $\mathbf{j} = -i\frac{\hbar}{2m}(\psi^*\nabla\psi - \psi\nabla\psi^*)$.

Applied to the Klein-Gordon equation (15.3), the same consideration implies

$$\hbar^2 \partial_t \left(\psi^* \partial_t \psi - \psi \partial_t \psi^*\right) - \hbar^2 c^2 \nabla \cdot \left(\psi^* \nabla \psi - \psi \nabla \psi^*\right) = 0\,,$$

from which we deduce the correspondence,

$$\rho = i\frac{\hbar}{2mc^2}\left(\psi^* \partial_t \psi - \psi \partial_t \psi^*\right), \qquad \mathbf{j} = -i\frac{\hbar}{2m}\left(\psi^* \nabla \psi - \psi \nabla \psi^*\right)\,.$$

The continuity equation associated with the conservation of probability can be expressed covariantly in the form

$$\partial_\mu j^\mu = 0\,, \tag{15.4}$$

where $j^\mu = (\rho c, \mathbf{j})$ is the 4-current. Thus, the Klein-Gordon density is the time-like component of a 4-vector.

From this association it is possible to identify three aspects which (at least initially) eliminate the Klein-Gordon equation as a wholey suitable candidate for the relativistic version of the wave equation:

[3] You may recognize that the leading correction to the free particle Schrödinger equation is precisely the relativistic correction to the kinetic energy that we considered in chapter 9.

- ▷ The first disturbing feature of the Klein-Gordon equation is that the density ρ is not a positive definite quantity, so it can not represent a probability. Indeed, this led to the rejection of the equation in the early years of relativistic quantum mechanics, 1926 to 1934.

- ▷ Secondly, the Klein-Gordon equation is not first order in time; it is necessary to specify ψ *and* $\partial_t \psi$ everywhere at $t = 0$ to solve for later times. Thus, there is an extra constraint absent in the Schrödinger formulation.

- ▷ Finally, the equation on which the Klein-Gordon equation is based, $E^2 = m^2c^4 + \mathbf{p}^2c^2$, has both positive and negative solutions. In fact the apparently unphysical negative energy solutions are the origin of the preceding two problems.

To circumvent these difficulties one might consider dropping the negative energy solutions altogether. For a free particle, whose energy is thereby constant, we can simply supplement the Klein-Gordon equation with the condition $p^0 > 0$. However, such a definition becomes inconsistent in the presence of local interactions, e.g.

$$\begin{aligned} \left(\partial^2 + k_c^2\right)\psi = F(\psi) & \qquad \text{self} - \text{interaction} \\ \left[(\partial + iqA/\hbar c)^2 + k_c^2\right]\psi = 0 & \qquad \text{interaction with EM field.} \end{aligned}$$

The latter generate transitions between positive and negative energy states. Thus, merely excluding the negative energy states does not solve the problem. Later we will see that the interpretation of ψ as a quantum field leads to a resolution of the problems raised above. Historically, the intrinsic problems confronting the Klein-Gordon equation led Dirac to introduce another equation.[4] However, as we will see, although the new formulation implied a positive norm, it did not circumvent the need to interpret negative energy solutions.

15.2 Dirac Equation

Dirac attached great significance to the fact that Schrödinger's equation of motion was first order in the time derivative. If this holds true in relativistic quantum mechanics, it must also be linear in ∂. On the other hand, for free particles, the equation must imply $\hat{p}^2 = (mc)^2$, i.e. the wave equation must be consistent with the Klein-Gordon equation (15.3). At the expense of introducing vector wavefunctions, Dirac's approach was to try to factorise this equation:

$$\boxed{(\gamma^\mu \hat{p}_\mu - m)\,\psi = 0\,.} \qquad (15.5)$$

(Following the usual convention we have, and will henceforth, adopt the short-hand convention and set $\hbar = c = 1$.) For this equation to be admissible, the following conditions must be enforced:

- ▷ The components of ψ must satisfy the Klein-Gordon equation.

Paul A. M. Dirac 1902-1984

Dirac was born on 8th August, 1902, at Bristol, England, his father being Swiss and his mother English. He was educated at the Merchant Venturer's Secondary School, Bristol, then went on to Bristol University. Here, he studied electrical engineering, obtaining the B.Sc. (Engineering) degree in 1921. He then studied mathematics for two years at Bristol University, later going on to St. John's College, Cambridge, as a research student in mathematics. He received his Ph.D. degree in 1926. The following year he became a Fellow of St.John's College and, in 1932, Lucasian Professor of Mathematics at Cambridge. Dirac's work was concerned with the mathematical and theoretical aspects of quantum mechanics. He began work on the new quantum mechanics as soon as it was introduced by Heisenberg in 1928 – independently producing a mathematical equivalent which consisted essentially of a non-commutative algebra for calculating atomic properties – and wrote a series of papers on the subject, leading up to his relativistic theory of the electron (1928) and the theory of holes (1930). This latter theory required the existence of a positive particle having the same mass and charge as the known (negative) electron. This, the positron was discovered experimentally at a later date (1932) by C. D. Anderson, while its existence was likewise proved by Blackett and Occhialini (1933) in the phenomena of "pair production" and "annihilation". Dirac was made the 1933 Nobel Laureate in Physics (with Erwin Schrödinger) for the discovery of new productive forms of atomic theory.

[4] The original references are P. A. M. Dirac, *The Quantum theory of the electron*, Proc. R. Soc. A**117**, 610 (1928); *Quantum theory of the electron, Part II*, Proc. R. Soc. A**118**, 351 (1928). Further historical insights can be obtained from Dirac's book on *Principles of Quantum mechanics*, 4th edition, Oxford University Press, 1982.

- ▷ There must exist a 4-vector current density which is conserved and whose time-like component is a positive density.
- ▷ The components of ψ do not have to satisfy any auxiliary condition. At any given time they are independent functions of $\mathbf{x}$.

Beginning with the first of these requirements, by imposing the condition $[\gamma^\mu, \hat{p}_\nu] = \gamma^\mu \hat{p}_\nu - \hat{p}_\nu \gamma^\mu = 0$, (and symmetrizing)

$$(\gamma^\nu \hat{p}_\nu + m)(\gamma^\mu \hat{p}_\mu - m)\psi = \left(\frac{1}{2}\{\gamma^\nu, \gamma^\mu\}\hat{p}_\nu \hat{p}_\mu - m^2\right)\psi = 0\,,$$

the latter recovers the Klein-Gordon equation if we define the elements γ^μ such that they obey the *anticommutation* relation,[5] $\{\gamma^\nu, \gamma^\mu\} \equiv \gamma^\nu\gamma^\mu + \gamma^\mu\gamma^\nu = 2g^{\mu\nu}$ – thus γ^μ, and therefore ψ, can not be scalar. Then, from the expansion of Eq. (15.5), $\gamma^0(\gamma^0\hat{p}_0 - \gamma\cdot\hat{\mathbf{p}} - m)\psi = i\partial_t\psi - \gamma^0\gamma\cdot\hat{\mathbf{p}}\psi - m\gamma^0\psi = 0$, the Dirac equation can be brought to the form

$$\boxed{i\partial_t\psi = \hat{H}\psi, \qquad \hat{H} = \boldsymbol{\alpha}\cdot\hat{\mathbf{p}} + \beta m\,,} \tag{15.6}$$

where the elements of the vector $\boldsymbol{\alpha} = \gamma^0\boldsymbol{\gamma}$ and $\beta = \gamma^0$ obey the commutation relations,

$$\{\alpha_i, \alpha_j\} = 2\delta_{ij}, \qquad \beta^2 = \mathbf{1}, \qquad \{\alpha_i, \beta\} = 0\,. \tag{15.7}$$

$\hat{H}$ is Hermitian if, and only if, $\boldsymbol{\alpha}^\dagger = \boldsymbol{\alpha}$, and $\beta^\dagger = \beta$. Expressed in terms of $\boldsymbol{\gamma}$, this requirement translates to the condition $(\gamma^0\boldsymbol{\gamma})^\dagger \equiv \boldsymbol{\gamma}^\dagger\gamma^{0\dagger} = \gamma^0\boldsymbol{\gamma}$, and $\gamma^{0\dagger} = \gamma^0$. Altogether, we thus obtain the defining properties of Dirac's γ matrices,

$$\boxed{\gamma^{\mu\dagger} = \gamma^0\gamma^\mu\gamma^0, \qquad \{\gamma^\mu, \gamma^\nu\} = 2g^{\mu\nu}\,.} \tag{15.8}$$

Given that space-time is four-dimensional, the matrices γ must have dimension of at least 4×4, which means that ψ has at least four components. It is not, however, a 4-vector; it does not transform like x^μ under Lorentz transformations. It is called a **spinor**, or more correctly, a **bispinor** with special Lorentz transformations which we will shall discuss presently.

▷ INFO. An explicit representation of the γ matrices which most easily captures the non-relativistic limit is the following,

$$\gamma^0 = \begin{pmatrix} \mathbb{I}_2 & 0 \\ 0 & -\mathbb{I}_2 \end{pmatrix}, \qquad \boldsymbol{\gamma} = \begin{pmatrix} 0 & \boldsymbol{\sigma} \\ -\boldsymbol{\sigma} & 0 \end{pmatrix}, \tag{15.9}$$

where $\boldsymbol{\sigma}$ denote the familiar 2×2 Pauli spin matrices which satisfy the relations, $\sigma_i\sigma_j = \delta_{ij} + i\epsilon_{ijk}\sigma_k$, $\boldsymbol{\sigma}^\dagger = \boldsymbol{\sigma}$. The latter is known in the literature as the **Dirac-Pauli representation**. We will adopt the particular representation,

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Note that with this definition, the matrices $\boldsymbol{\alpha}$ and β take the form,

$$\boldsymbol{\alpha} = \begin{pmatrix} 0 & \boldsymbol{\sigma} \\ \boldsymbol{\sigma} & 0 \end{pmatrix}, \qquad \beta = \begin{pmatrix} \mathbb{I}_2 & 0 \\ 0 & -\mathbb{I}_2 \end{pmatrix}.$$

[5] Note that, in some of the literature, you will see the convention $[\ ,\ ]_+$ for the anticommutator.

15.2.1 Density and Current

Turning to the second of the requirements placed on the Dirac equation, we now seek the probability density $\rho = j^0$. Since ψ is a complex spinor, ρ has to be of the form $\psi^\dagger M\psi$ in order to be real and positive. Applying hermitian conjugation to the Dirac equation, we obtain

$$[(\gamma^\mu \hat{p}_\mu - m)\psi]^\dagger = \psi^\dagger(-i\gamma^{\dagger\mu}\overleftarrow{\partial}_\mu - m) = 0\,,$$

where $\psi^\dagger\overleftarrow{\partial}_\mu \equiv (\partial_\mu\psi)^\dagger$. Making use of (15.8), and defining $\bar{\psi} \equiv \psi^\dagger\gamma^0$, the Dirac equation takes the form $\bar{\psi}(i\overleftarrow{\not\partial} + m) = 0$, where we have introduced the **Feynman 'slash' notation** $\not a \equiv a_\mu\gamma^\mu$. Combined with Eq. (15.5) (i.e. $(i\overrightarrow{\not\partial} - m)\psi = 0$), we obtain

$$\bar{\psi}\left(\overleftarrow{\not\partial} + \overrightarrow{\not\partial}\right)\psi = \partial_\mu\left(\bar{\psi}\gamma^\mu\psi\right) = 0\,.$$

From this result and the continuity relation (15.4) we can identify

$$\boxed{j^\mu = \bar{\psi}\gamma^\mu\psi\,,} \tag{15.10}$$

(or, equivalently, $(\rho, \mathbf{j}) = (\psi^\dagger\psi, \psi^\dagger\boldsymbol{\alpha}\psi))$ as the 4-current. In particular, the density $\rho = j^0 = \psi^\dagger\psi$ is, as required, positive definite.

15.2.2 Relativistic Covariance

To complete our derivation, we must verify that the Dirac equation remains invariant under Lorentz transformations. More precisely, if a wavefunction $\psi(x)$ obeys the Dirac equation in one frame, its counterpart $\psi'(x')$ in a Lorentz transformed frame $x' = \Lambda x$, must obey the Dirac equation,

$$\left(i\gamma^\mu\partial'_\mu - m\right)\psi'(x') = 0\,. \tag{15.11}$$

In order that an observer in the second frame can reconstruct ψ' from ψ there must exist a local transformation between the wavefunctions. Taking this relation to be linear, we therefore must have,

$$\boxed{\psi'(x') = S(\Lambda)\psi(x)\,,}$$

where $S(\Lambda)$ represents a non-singular 4×4 matrix. Now, using the identity, $\partial'_\mu \equiv \frac{\partial}{\partial x'^\mu} = \frac{\partial x^\nu}{\partial x'^\mu}\frac{\partial}{\partial x^\nu} = (\Lambda^{-1})^\nu{}_\mu\frac{\partial}{\partial x^\nu} = (\Lambda^{-1})^\nu{}_\mu\partial_\nu$, the Dirac equation (15.11) in the transformed frame takes the form,

$$\left(i\gamma^\mu(\Lambda^{-1})^\nu{}_\mu\partial_\nu - m\right)S(\Lambda)\psi(x) = 0\,.$$

The latter is compatible with the Dirac equation in the original frame if

$$\boxed{S(\Lambda)\gamma^\nu S^{-1}(\Lambda) = \gamma^\mu(\Lambda^{-1})^\nu{}_\mu\,.} \tag{15.12}$$

To define an explicit form for $S(\Lambda)$ we must now draw upon some of the defining properties of the Lorentz group discussed earlier. For an infinitesimal proper Lorentz transformation we have $\Lambda^\nu{}_\mu = g^\nu{}_\mu + \omega^\nu{}_\mu$ and $(\Lambda^{-1})^\nu{}_\mu = g^\nu{}_\mu - \omega^\nu{}_\mu + \cdots$, where the matrix $\omega_{\mu\nu}$ is antisymmetric and $g^\nu{}_\mu \equiv \delta^\nu{}_\mu$. Correspondingly, by Taylor expansion in ω, we can define

$$S(\Lambda) = \mathbb{I} - \frac{i}{4}\Sigma_{\mu\nu}\omega^{\mu\nu} + \cdots\,, \qquad S^{-1}(\Lambda) = \mathbb{I} + \frac{i}{4}\Sigma_{\mu\nu}\omega^{\mu\nu} + \cdots\,,$$

where the matrices $\Sigma_{\mu\nu}$ are also antisymmetric in $\mu\nu$. To first order in ω, Eq. (15.12) yields (a somewhat unrewarding exercise!)

$$[\gamma^\nu, \Sigma_{\alpha\beta}] = 2i \left(g^\nu{}_\alpha \gamma_\beta - g^\nu{}_\beta \gamma_\alpha\right) . \tag{15.13}$$

The latter is satisfied by the set of matrices (another exercise!)[6]

$$\boxed{\Sigma_{\alpha\beta} = \frac{i}{2} [\gamma_\alpha, \gamma_\beta] .} \tag{15.14}$$

In summary, if $\psi(x)$ obeys the Dirac equation in one frame, the wavefunction can be obtained in the Lorentz transformed frame by applying the transformation $\psi'(x') = S(\Lambda)\psi(\Lambda^{-1}x')$. Let us now consider the physical consequences of this Lorentz covariance.

15.2.3 Angular momentum and spin

To explore the physical manifestations of Lorentz covariance, it is instructive to consider the class of spatial rotations. For an anticlockwise spatial rotation by an infinitesimal angle θ about a fixed axis $\mathbf{n}$, $\mathbf{x} \mapsto \mathbf{x}' = \mathbf{x} - \theta\mathbf{x} \times \mathbf{n}$. In terms of the "Lorentz transformation", Λ, one has

$$x'_i = [\Lambda x]_i \equiv x_i - \omega_{ij} x_j$$

where $\omega_{ij} = \epsilon_{ijk} n_k \theta$, and the remaining elements $\Lambda^\mu{}_0 = \Lambda^0{}_\mu = 0$. Applied to the argument of the wavefunction we obtain a familiar result,[7]

$$\begin{aligned}\psi(x) = \psi(\Lambda^{-1}x') = \psi(x'_0, \mathbf{x}' + \mathbf{x}' \times \mathbf{n}\theta) &= (1 - \theta\mathbf{n} \cdot \mathbf{x}' \times \nabla + \cdots)\psi(x') \\ &= (1 - i\theta\mathbf{n} \cdot \hat{\mathbf{L}} + \cdots)\psi(x'),\end{aligned}$$

where $\hat{\mathbf{L}} = \hat{\mathbf{x}} \times \hat{\mathbf{p}}$ represents the non-relativistic angular momentum operator. Formally, the angular momentum operators represent the generators of spatial rotations.[8]

However, we have seen above that Lorentz covariance demands that the transformed wavefunction be multiplied by $S(\Lambda)$. Using the definition of ω_{ij} above, one finds that

$$S(\Lambda) \equiv S(\mathbb{I} + \omega) = \mathbb{I} - \frac{i}{4} \epsilon_{ijk} n_k \Sigma_{ij} \theta + \cdots$$

Then drawing on the Dirac/Pauli representation,

$$\Sigma_{ij} = \frac{i}{2} [\gamma_i, \gamma_j] = \frac{i}{2} \left[\begin{pmatrix} 0 & \sigma_i \\ -\sigma_i & 0 \end{pmatrix}, \begin{pmatrix} 0 & \sigma_j \\ -\sigma_j & 0 \end{pmatrix} \right] = -\frac{i}{2} [\sigma_i, \sigma_j] \otimes \mathbb{I}_2 = \epsilon_{ijk} \sigma_k \otimes \mathbb{I}_2,$$

one obtains

$$S(\Lambda) = \mathbb{I} - i\mathbf{n} \cdot \mathbf{S}\theta + \cdots, \qquad \boxed{\mathbf{S} = \frac{1}{2} \begin{pmatrix} \boldsymbol{\sigma} & 0 \\ 0 & \boldsymbol{\sigma} \end{pmatrix} .}$$

Combining both contributions, we thus obtain

$$\boxed{\psi'(x') = S(\Lambda)\psi(\Lambda^{-1}x') = (1 - i\theta\mathbf{n} \cdot \hat{\mathbf{J}} + \cdots)\psi(x') ,}$$

[6] Since finite transformations are of the form $S(\Lambda) = \exp[-(i/4)\Sigma_{\alpha\beta}\omega^{\alpha\beta}]$, one may show that $S(\Lambda)$ is unitary for spatial rotations, while it is Hermitian for Lorentz boosts.

[7] Recall that spatial rotataions are generated by the unitary operator, $\hat{U}(\theta) = \exp(-i\theta\mathbf{n} \cdot \hat{\mathbf{L}})$.

[8] For finite transformations, the generator takes the form $\exp[-i\theta\mathbf{n} \cdot \hat{\mathbf{L}}]$.

where $\hat{\mathbf{J}} = \hat{\mathbf{L}} + \mathbf{S}$ can be identified as a *total* effective angular momentum of the particle being made up of the orbital component, together with an intrinsic contribution known as **spin**. The latter is characterised by the defining condition:

$$\boxed{[S_i, S_j] = i\epsilon_{ijk} S_k, \qquad (S_i)^2 = \frac{1}{4} \qquad \text{for each } i\,.} \tag{15.15}$$

Therefore, in contrast to non-relativistic quantum mechanics, the concept of spin does not need to be grafted onto the Schrödinger equation, but emerges naturally from the fundamental invariance of the Dirac equation under Lorentz transformations. As a corollary, we can say that the Dirac equation is a relativistic wave equation for particles of spin 1/2.

15.2.4 Parity

So far, our discussion of the covariance properties of the Dirac equation have only dealt with the subgroup of proper orthochronous Lorentz transformations, $\mathcal{L}_+^\uparrow$ – i.e. those that can be reached from $\Lambda = \mathbb{I}$ by a sequence of infinitesimal transformations. Taking the parity operation into account, relativistic covariance demands

$$S^{-1}(P)\gamma^0 S(P) = \gamma^0, \qquad S^{-1}(P)\gamma^i S(P) = -\gamma^i.$$

This is achieved if $S(P) = \gamma^0 e^{i\phi}$, where ϕ denotes some arbitrary phase. Taking into account the fact that $P^2 = \mathbb{I}$, $\phi = 0$ or π, and we find

$$\boxed{\psi'(x') = S(P)\psi(x) = \eta\gamma^0\psi(P^{-1}x') = \eta\gamma^0\psi(ct', -\mathbf{x}')\,,} \tag{15.16}$$

where $\eta = \pm 1$ represents the **intrinsic parity** of the particle.

15.3 Free Particle Solution of the Dirac Equation

Having laid the foundation we will now apply the Dirac equation to the problem of a free relativistic quantum particle. For a free particle, the plane wave

$$\psi(x) = \exp[-ip\cdot x]u(p)\,,$$

with energy $E \equiv p^0 = \pm\sqrt{\mathbf{p}^2 + m^2}$ will be a solution of the Dirac equation if the components of the spinor $u(p)$ are chosen to satisfy the equation $(\not{p} - m)u(p) = 0$. Evidently, as with the Klein-Gordon equation, we see that the Dirac equation therefore admits negative as well as positive energy solutions! Soon, having attached a physical significance to the former, we will see that it is convenient to reverse the sign of p for the negative energy solutions. However, for now, let us continue without worrying about the dilemma posed by the negative energy states.

In the Dirac-Pauli block representation,

$$\gamma^\mu p_\mu - m = \begin{pmatrix} p^0 - m & -\boldsymbol{\sigma}\cdot\mathbf{p} \\ \boldsymbol{\sigma}\cdot\mathbf{p} & -p^0 - m \end{pmatrix}.$$

Thus, defining the spin elements $u(p) = (\xi, \eta)$, where ξ and η represent two-component spinors, we find the conditions, $(p^0 - m)\xi = \boldsymbol{\sigma}\cdot\mathbf{p}\,\eta$ and $\boldsymbol{\sigma}\cdot\mathbf{p}\,\xi =$

$(p^0+m)\eta$. With $(p^0)^2 = \mathbf{p}^2+m^2$, these equations are consistent if $\eta = \frac{\boldsymbol{\sigma}\cdot\mathbf{p}}{p^0+m}\xi$. We therefore obtain the bispinor solution

$$u^{(r)}(p) = N(p)\begin{pmatrix} \chi^{(r)} \\ \dfrac{\boldsymbol{\sigma}\cdot\mathbf{p}}{p^0+m}\chi^{(r)} \end{pmatrix},$$

where $\chi^{(r)}$ represents any pair of orthogonal two-component vectors, and $N(p)$ is the normalisation.

Concerning the choice of $\chi^{(r)}$, in many situations, the most convenient basis is the eigenbasis of **helicity** – eigenstates of the component of spin resolved in the direction of motion,

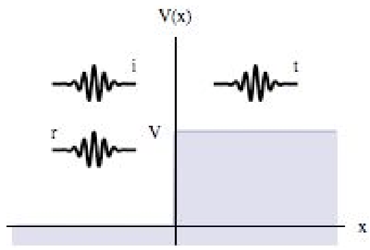
$$\mathbf{S}\cdot\frac{\mathbf{p}}{|\mathbf{p}|}\chi^{(\pm)} \equiv \frac{\boldsymbol{\sigma}}{2}\cdot\frac{\mathbf{p}}{|\mathbf{p}|}\chi^{(\pm)} = \pm\frac{1}{2}\chi^{(\pm)},$$

e.g., for $\mathbf{p} = p_3\hat{\mathbf{e}}_3$, $\chi^{(+)} = (1,0)$ and $\chi^{(-)} = (0,1)$. Then, for the positive energy states, the two spinor plane wave solutions can be written in the form

$$\boxed{\psi_p^{(\pm)}(x) = N(p)e^{-ip\cdot x}\begin{pmatrix} \chi^{(\pm)} \\ \pm\dfrac{|\mathbf{p}|}{p^0+m}\chi^{(\pm)} \end{pmatrix}}$$

Thus, according to the discussion above, the Dirac equation for a free particle admits four solutions, two states with positive energy, and two with negative.

15.3.1 Klein paradox: anti-particles



While the Dirac equation has been shown to have positive definite density, as with the Klein-Gordon equation, it still exhibits negative energy states! To make sense of these states it is illuminating to consider the scattering of a plane wave from a potential step. To be precise, consider a beam of relativistic particles with unit amplitude, energy E, momentum $p\hat{\mathbf{e}}_3$, and spin $\uparrow$ (i.e. $\chi = (1,0)$), incident upon a potential $V(\mathbf{x}) = V\theta(x_3)$ (see figure). At the potential barrier, spin is conserved, while a component of the beam with amplitude r is reflected (with energy E and momentum $-p\hat{\mathbf{e}}_3$), and a component t is transmitted with energy $E' = E - V$ and momentum $p'\hat{\mathbf{e}}_3$. According to the energy-momentum invariant, conservation of energy across the interface dictates that $E^2 = p^2+m^2$ and $E'^2 = p'^2+m^2$.

Being first order, the boundary conditions on the Dirac equation require only continuity of ψ (cf. the Schrödinger equation). Therefore, matching ψ at the step, we obtain the relations

$$\begin{pmatrix} 1 \\ 0 \\ \frac{p}{E+m} \\ 0 \end{pmatrix} + r\begin{pmatrix} 1 \\ 0 \\ -\frac{p}{E+m} \\ 0 \end{pmatrix} = t\begin{pmatrix} 1 \\ 0 \\ \frac{p'}{E'+m} \\ 0 \end{pmatrix},$$

from which we find $1+r = t$, and $\frac{p}{p^0+m}(1-r) = \frac{p'}{p'^0+m}t$. Setting $\zeta = \frac{p'}{p}\frac{(E+m)}{(E'+m)}$, these equations lead to

$$t = \frac{2}{1+\zeta}, \qquad \frac{1+r}{1-r} = \frac{1}{\zeta}, \qquad r = \frac{1-\zeta}{1+\zeta}.$$

To interpret these solutions, let us consider the current associated with the reflected and transmitted components. Making use of the equation for the current density, $\mathbf{j} = \psi^\dagger\boldsymbol{\alpha}\psi$, and using the Dirac/Pauli representation wherein

$$\alpha_3 = \gamma_0\gamma_3 = \begin{pmatrix} \mathbb{I}_2 & \\ & -\mathbb{I}_2 \end{pmatrix}\begin{pmatrix} & \sigma_3 \\ -\sigma_3 & \end{pmatrix} = \begin{pmatrix} & \sigma_3 \\ \sigma_3 & \end{pmatrix},$$

the current along $\hat{\mathbf{e}}_3$-direction is given by

$$j_3 = \psi^\dagger \begin{pmatrix} & \sigma_3 \\ \sigma_3 & \end{pmatrix} \psi, \qquad j_1 = j_2 = 0\,.$$

Therefore, up to an overall constant of normalisation, the current densities are given by

$$j_3^{(i)} = \frac{2p}{p^0+m}, \qquad j_3^{(t)} = \frac{2(p'+p'^*)}{p'^0+m}|t|^2, \qquad j_3^{(r)} = -\frac{2p}{p^0+m}|r|^2.$$

From these relations we obtain

$$\begin{aligned} \frac{j_3^{(t)}}{j_3^{(i)}} &= |t|^2 \frac{(p'+p'^*)}{2p}\frac{p^0+m}{p'^0+m} = \frac{4}{|1+\zeta|^2}\frac{1}{2}(\zeta+\zeta^*) \\ \frac{j_3^{(r)}}{j_3^{(i)}} &= -|r|^2 = -\left|\frac{1-\zeta}{1+\zeta}\right|^2 \end{aligned}$$

from which current conservation can be confirmed:

$$1 + \frac{j_3^{(r)}}{j_3^{(i)}} = \frac{|1+\zeta|^2 - |1-\zeta|^2}{|1+\zeta|^2} = \frac{2(\zeta+\zeta^*)}{|1+\zeta|^2} = \frac{j_3^{(t)}}{j_3^{(i)}}.$$

Interpreting these results, it is convenient to separate our consideration into three distinct regimes of energy:

▷ $E' \equiv (E - V) > m$: In this case, from the Klein-Gordon condition (the energy-momentum invariant) $p'^2 \equiv E'^2 - m^2 > 0$, and (taking $p' > 0$ – i.e. beam propagates to the right) $\zeta > 0$ and real. From this result we find $|j_3^{(r)}| < |j_3^{(i)}|$ – as expected, within this interval of energy, a component of the beam is transmitted and the remainder is reflected (cf. non-relativistic quantum mechanics).

▷ $-m < E' < m$: In this case $p'^2 \equiv E'^2 - m^2 < 0$ and p' is purely imaginary. From this result it follows that ζ is also pure imaginary and $|j_3^{(r)}| = |j_3^{(i)}|$. In this regime the under barrier solutions are evanescent and quickly decay to the right of the barrier. All of the beam is reflected (cf. non-relativistic quantum mechanics).

▷ $E' < -m$: Finally, in this case $p'^2 \equiv E'^2 - m^2 > 0$ and, depending on the sign of p', $j_3^{(r)}$ can be greater or less than $j_3^{(i)}$. But the solution has the form $e^{-i(p'x - E't)}$. Since we presume the beam to be propagating to the right, we require $E' < 0$ and $p' > 0$. From this result it follows that $\zeta < 0$ and we are drawn to the surprising conclusion that $|j_3^{(r)}| > |j_3^{(i)}|$ – more current is reflected that is incident! Since we have already confirmed current conservation, we can deduce that $j_3^{(t)} < 0$. It is as if a beam of particles were incident from the right.

The resolution of this last seeming unphysical result, known as the **Klein paradox**,[9] in fact gives a natural interpretation of the negative energy solutions that plague both the Dirac and Klein-Gordon equations: Dirac particles are fermionic in nature. If we regard the vacuum as comprised of a filled Fermi sea of negative energy states or **antiparticles** (of negative charge), the Klein Paradox can be resolved as the stimulated emission of particle/antiparticle

[9] Indeed one would reach the same conclusion were one to examine the Klein-Gordon equation.

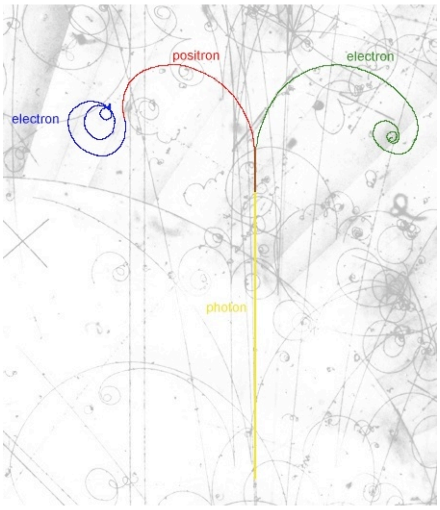


Figure 15.2: The photograph shows a small part of a complicated high energy neutrino event produced in the Fermilab bubble chamber filled with a neon hydrogen mixture. A positron (red) emerging from an electron-positron pair, produced by a gamma ray, curves round through about 180 degrees. Then it seems to change charge: it begins to curve in the opposite direction (blue). What has happened is that the positron has run head-on into a (more-or-less from the point of view of particle physics) stationary electron – transferring all its momentum. This tells us that the mass of the positron equals the mass of the electron.

pairs, the particles moving off towards $x_3 = -\infty$ and the antiparticles towards $x_3 = \infty$. What about energy conservation? One might worry that the energy for these pairs is coming from nowhere. However, the electrostatic energy recovered by the antiparticle when its created is sufficient to outweigh the rest mass energy of the particle and antiparticle pair (remember that a repulsive potential for particles is attractive for antiparticles). Taking into account the fact that the minimum energy to create a particle/antiparticle pair is twice the rest mass energy $2 \times m$, the regime where stimulated emission is seen to occur can be understood.

Negative energy states: With this conclusion, it is appropriate to revisit the definition of the free particle plane wave state. In particular, for energies $E < 0$, it is more sensible to set $p^0 = +\sqrt{(\mathbf{p}^2 + m^2)}$, and redefine the plane wave solution as $\psi(x) = v(p)e^{ip\cdot x}$, where the spinor satisfies the condition $(\not{p} + m)v(p) = 0$. Accordingly we find,

$$v^{(r)}(p) = N(p) \begin{pmatrix} \frac{\boldsymbol{\sigma} \cdot \mathbf{p}}{p^0 + m} \chi^{(r)} \\ \chi^{(r)} \end{pmatrix} .$$

So, to conclude, two relativistic wave equations have been proposed. The first of these, the Klein-Gordon equation was dismissed on the grounds that it exhibited negative probability densities and negative energy states. By contrast, the states of the Dirac equation were found to exhibit a positive definite probability density, and the negative energy states were argued to have a natural interpretation in terms of antiparticles: the vacuum state does not correspond to all states unoccupied but to a state in which all the negative energy states are occupied – the negative energy states are filled up by a Fermi sea of negative energy Fermi particles. For electron degrees of freedom, if a positive energy state is occupied we observe it as a (positive energy) electron of charge $q = -e$. If a negative energy state is unoccupied we observe it as a (positive energy) antiparticle of charge $q = +e$, a **positron**, the antiparticle of the electron. If a very energetic electron interacts with the sea causing a transition from a negative energy state to positive one (by communicating an energy of at least $2m$) this is observed as the production of a pair of particles, an electron and a positron from the vacuum (**pair production**) (see Fig. 15.2).

However, the interpretation attached to the negative energy states provides grounds to reconsider the status of the Klein-Gordon equation. Evidently, the

Dirac equation is not a relativistic wave equation for a single particle. If it were, pair production would not appear. Instead, the interpretation above forces us to consider the wavefunction of the Dirac equation as a **quantum field** able to host any number of particles – cf. the continuum theory of the quantum harmonic chain. In the next section, we will find that the consideration of the wavefunction as a field revives the Klein-Gordon equation as a theory of scalar (interger spin) particles.

15.4 Quantization of relativistic fields

15.4.1 Info: Scalar field: Klein-Gordon equation revisited

Previously, the Klein-Gordon equation was abandoned as a candidate for a relativistic theory on the basis that (i) it admitted negative energy solutions, and (ii) that the probability density associated with the wavefunction was not positive definite. Yet, having associated the negative energy solutions of the Dirac equation with antiparticles, and identified ψ as a quantum field, it is appropriate that we revisit the Klein-Gordon equation and attempt to revive it as a theory of relativistic particles of spin zero.

If ϕ were a classical field, the Klein-Gordon equation would represent the equation of motion associated with the Lagrangian density (exercise)

$$\boxed{\mathcal{L} = \frac{1}{2}\partial_\mu \phi\, \partial^\mu \phi - \frac{1}{2}m^2\phi^2\,,}$$

(cf. our discussion of the low energy modes of the classical harmonic chain and the Maxwell field of the waveguide in chapter 11). Defining the canonical momentum $\pi(x) = \partial_{\dot{\phi}}\mathcal{L}(x) = \dot{\phi}(x) \equiv \partial_0\phi(x)$, the corresponding Hamiltonian density takes the form

$$\mathcal{H} = \pi\dot{\phi} - \mathcal{L} = \frac{1}{2}\left[\pi^2 + (\nabla\phi)^2 + m^2\phi^2\right] .$$

Evidently, the Hamiltonian density is explicitly positive definite. Thus, the scalar field is not plagued by the negative energy problem which beset the single-particle theory. Similarly, the quantization of the classical field will lead to a theory in which the states have positive energy.

Following on from our discussion of the harmonic chain in chapter 11, we are already equipped to quantise the classical field theory. However, there we worked explicitly in the Schrödinger representation, in which the dynamics was contained within the time-dependent wavefunction $\psi(t)$, and the operators were time-independent. Alternatively, one may implement quantum mechanics in a representation where the time dependence is transferred to the operators instead of the wavefunction — the Heisenberg representation. In this representation, the Schrödinger state vector $\psi_S(t)$ is related to the Heisenberg state vector ψ_H by the relation,

$$\psi_S(t) = e^{-i\hat{H}t}\psi_H, \qquad \psi_H = \psi_S(0)\,.$$

Similarly, Schrödinger operators $\hat{O}_S$ are related to the Heisenberg operators $\hat{O}_H(t)$ by

$$\boxed{\hat{O}_H(t) = e^{i\hat{H}t}\hat{O}_S e^{-i\hat{H}t}\,.}$$

One can easily check that the matrix elements $\langle\psi'_S|\hat{O}_S|\psi_S\rangle$ and $\langle\psi'_H|\hat{O}_H|\psi_H\rangle$ are equivalent in the two representations, and which to use in non-relativistic quantum mechanics is largely a matter of taste and convenience. However, in relativistic quantum field theory, the Heisenberg representation is often preferable to the Schrödinger representation. The main reason for this is that by using the former, the Lorentz covariance of the field operators is made manifest.

In the Heisenberg representation, the quantisation of the fields is still enforced by promoting the classical fields to operators, $\pi \mapsto \hat{\pi}$ and $\phi \mapsto \hat{\phi}$, but in this case, we impose the equal time commutation relations,

$$\boxed{\left[\hat{\phi}(\mathbf{x},t),\hat{\pi}(\mathbf{x}',t)\right]=i\delta^3(\mathbf{x}-\mathbf{x}'),\qquad \left[\hat{\phi}(\mathbf{x},t),\hat{\phi}(\mathbf{x}',t)\right]=\left[\hat{\pi}(\mathbf{x},t),\hat{\pi}(\mathbf{x}',t)\right]=0\,,}$$

with $\hat{\pi}=\partial_0\hat{\phi}$. In doing so, the Hamiltonian density takes the form

$$\hat{\mathcal{H}}=\frac{1}{2}\left[\hat{\pi}^2+(\nabla\hat{\phi})^2+m^2\hat{\phi}^2\right]\,.$$

To see the connection between the quantized field and particles we need to Fourier transform the field operators to obtain the normal modes of the Hamiltonian,

$$\hat{\phi}(x)=\int\frac{d^4k}{(2\pi)^4}\hat{\phi}(k)e^{-ik\cdot x}\,.$$

However the form of the Fourier elements $\hat{\phi}(k)$ is constrained by the following conditions. Firstly to maintain Hermiticity of the field operator $\hat{\phi}(x)$ we must choose Fourier coefficients such that $\hat{\phi}^\dagger(k)=\hat{\phi}(-k)$. Secondly, to ensure that the field operator $\hat{\phi}(x)$ obeys the Klein-Gordon equation,[10] we require $\hat{\phi}(k)\sim 2\pi\delta(k^2-m^2)$. Taking these conditions together, we require

$$\hat{\phi}(k)=2\pi\delta(k^2-m^2)\left(\theta(k^0)a(\mathbf{k})+\theta(-k^0)a^\dagger(-\mathbf{k})\right)\,,$$

where $k^0\equiv\omega_k\equiv+\sqrt{\mathbf{k}^2+m^2}$, and $a(\mathbf{k})$ represent the operator valued Fourier coefficients. Rearranging the momentum integration, we obtain the Lorentz covariant expansion

$$\hat{\phi}(x)=\int\frac{d^4k}{(2\pi)^4}2\pi\delta(k^2-m^2)\theta(k^0)\left[a(\mathbf{k})e^{-ik\cdot x}+a^\dagger(\mathbf{k})e^{ik\cdot x}\right]\,.$$

Integrating over k^0, and making use of the identity

$$\begin{aligned}\int\frac{d^4k}{(2\pi)^4}2\pi\delta(k^2-m^2)\theta(k^0)&=\int\frac{d^4k}{(2\pi)^3}\delta(k_0^2-\omega_k^2)\theta(k^0)\\&=\int\frac{d^4k}{(2\pi)^3}\delta\left[(k_0-\omega_k)(k_0+\omega_k)\right]\theta(k^0)=\int\frac{d^4k}{(2\pi)^3}\frac{1}{2k_0}\left[\delta(k_0-\omega_k)+\delta(k_0+\omega_k)\right]\theta(k^0)\\&=\int\frac{d^3\mathbf{k}}{(2\pi)^3}\int\frac{dk_0}{2k_0}\delta(k_0-\omega_k)\theta(k^0)=\int\frac{d^3\mathbf{k}}{(2\pi)^3 2\omega_k},\end{aligned}$$

one obtains

$$\boxed{\hat{\phi}(x)=\int\frac{d^3\mathbf{k}}{(2\pi)^3 2\omega_k}\left(a(\mathbf{k})e^{-ik\cdot x}+a^\dagger(\mathbf{k})e^{ik\cdot x}\right)\,.}$$

More compactly, making use of the orthonormality of the basis

$$f_k=\frac{1}{\sqrt{(2\pi)^3 2\omega_k}}e^{-ik\cdot x},\qquad \int f_k^*(x)i\overleftrightarrow{\partial_0}f_{k'}(x)d^3\mathbf{x}=\delta^3(\mathbf{k}-\mathbf{k}'),$$

where $A\overleftrightarrow{\partial_0}B\equiv A\partial_t B-(\partial_t A)B$, we obtain

$$\hat{\phi}(x)=\int\frac{d^3\mathbf{k}}{\sqrt{(2\pi)^3 2\omega_k}}\left[a(\mathbf{k})f_k(x)+a^\dagger(\mathbf{k})f_k^*(x)\right]\,.$$

[10]Note that the field operators obey the equation of motion,

$$\dot{\pi}(\mathbf{x},t)=-\frac{\partial H}{\partial\phi(\mathbf{x},t)}=\nabla^2\phi-m^2\phi\,.$$

Together with the relation $\pi=\dot{\phi}$, one finds $(\partial^2+m^2)\phi=0$.

Similarly,

$$\hat{\pi}(x) \equiv \partial_0 \hat{\phi}(x) = \int \frac{d^3\mathbf{k}}{\sqrt{(2\pi)^3 2\omega_k}} i\omega_k \left[-a(\mathbf{k}) f_k(x) + a^\dagger(\mathbf{k}) f_k^*(x)\right] .$$

Making use of the orthogonality relations, the latter can be inverted to give

$$a(\mathbf{k}) = \sqrt{(2\pi)^3 2\omega_k} \int d^3\mathbf{x} f_k^*(x) i \overleftrightarrow{\partial_0} \hat{\phi}(x), \qquad a^\dagger(\mathbf{k}) = \sqrt{(2\pi)^3 2\omega_k} \int d^3\mathbf{x} \hat{\phi}(x) i \overleftrightarrow{\partial_0} f_k(x) ,$$

or, equivalently,

$$a(\mathbf{k}) = \int d^3\mathbf{x} \left(\omega_k \hat{\phi}(x) - i\hat{\pi}(x)\right) e^{-ik\cdot x}, \qquad a^\dagger(\mathbf{k}) = \int d^3\mathbf{x} \left(\omega_k \hat{\phi}(x) + i\hat{\pi}(x)\right) e^{ik\cdot x} .$$

With these definitions, it is left as an exercise to show

$$\boxed{\left[a(\mathbf{k}), a^\dagger(\mathbf{k}')\right] = (2\pi)^3 2\omega_k \delta^3(\mathbf{k} - \mathbf{k}'), \qquad [a(\mathbf{k}), a(\mathbf{k}')] = \left[a^\dagger(\mathbf{k}), a^\dagger(\mathbf{k}')\right] = 0 .}$$

The field operators $a^\dagger$ and a can therefore be identified as operators that create and annihilate bosonic particles. Although it would be tempting to adopt a different normalisation wherein $[a, a^\dagger] = 1$ (as is done in many texts), we chose to adopt the convention above where the covariance of the normalisation is manifest. Using this representation, the Hamiltonian is brought to the diagonal form

$$\hat{H} = \int \frac{d^3\mathbf{k}}{(2\pi)^3 2\omega_k} \frac{\omega_k}{2} \left[a^\dagger(\mathbf{k}) a(\mathbf{k}) + a(\mathbf{k}) a^\dagger(\mathbf{k})\right] ,$$

a result which can be confirmed by direct substitution.

Defining the vacuum state $|\Omega\rangle$ as the state which is annhiliated by $a(\mathbf{k})$, a single particle state is obtained by operating the creation operator on the vacuum,

$$|\mathbf{k}\rangle = a^\dagger(\mathbf{k})|\Omega\rangle .$$

Then $\langle \mathbf{k}'|\mathbf{k}\rangle = \langle \Omega | a(\mathbf{k}') a^\dagger(\mathbf{k}) |\Omega\rangle = \langle \Omega | [a(\mathbf{k}'), a^\dagger(\mathbf{k})] |\Omega\rangle = (2\pi)^3 2\omega_k \delta^3(\mathbf{k}' - \mathbf{k})$. Many-particle states are defined by $|\mathbf{k}_1 \cdots \mathbf{k}_n\rangle = a^\dagger(\mathbf{k}_1) \cdots a^\dagger(\mathbf{k}_n)|\Omega\rangle$ where the bosonic statistics of the particles is assured by the commutation relations.

Associated with these field operators, one can define the total particle number operator

$$\hat{N} = \int \frac{d^3\mathbf{k}}{\sqrt{(2\pi)^3 2\omega_k}} a^\dagger(\mathbf{k}) a(\mathbf{k}) .$$

Similarly, the total energy-momentum operator for the system is given by

$$\hat{P}^\mu = \int \frac{d^3\mathbf{k}}{\sqrt{(2\pi)^3 2\omega_k}} k^\mu a^\dagger(\mathbf{k}) a(\mathbf{k}) .$$

The time component $\hat{P}^0$ of this result can be compared with the Hamiltonian above. In fact, commuting the field operators, the latter is seen to differ from $\hat{P}^0$ by an infinite constant, $\int d^3\mathbf{k}\omega_k/2$. Yet, had we simply normal ordered[11] the operators from the outset, this problem would not have arisen. We therefore discard this infinite constant.

15.4.2 Info: Charged Scalar Field

A generalization of the analysis above to the complex scalar field leads to the Lagrangian,

$$\boxed{\mathcal{L} = \frac{1}{2} \partial_\mu \phi \partial^\mu \bar{\phi} - \frac{1}{2} m^2 |\phi|^2 .}$$

[11]Recall that normal ordering entails the construction of an operator with all the annihilation operators moved to the right and creation operators moved to the left.

The latter can be interpreted as the superposition of two independent scalar fields $\phi = (\phi_1 + i\phi_2)/\sqrt{2}$, where, for each (real) component $\phi_r^\dagger(x) = \phi_r(x)$. (In fact, we could as easily consider a field with n components.) In this case, the canonical quantisation of the classical fields is achieved by defining (exercise)

$$\hat{\phi}(x) = \int \frac{d^3\mathbf{k}}{\sqrt{(2\pi)^3 2\omega_k}} \left[a(\mathbf{k}) f_k(x) + b^\dagger(\mathbf{k}) f_k^*(x)\right] .$$

(similarly $\phi^\dagger(x)$) where both a and b obey bosonic commutation relations,

$$\begin{aligned} \left[a(\mathbf{k}), a^\dagger(\mathbf{k}')\right] &= \left[b(\mathbf{k}), b^\dagger(\mathbf{k}')\right] = (2\pi)^3 2\omega_k \delta^3(\mathbf{k}-\mathbf{k}'), \\ [a(\mathbf{k}), a(\mathbf{k}')] &= [b(\mathbf{k}), b(\mathbf{k}')] = \left[a(\mathbf{k}), b^\dagger(\mathbf{k}')\right] = [a(\mathbf{k}), b(\mathbf{k}')] = 0 . \end{aligned}$$

With this definition, the total number operator is given by

$$\hat{N} = \int \frac{d^3\mathbf{k}}{\sqrt{(2\pi)^3 2\omega_k}} \left[a^\dagger(\mathbf{k}) a(\mathbf{k}) + b^\dagger(\mathbf{k}) b(\mathbf{k})\right] \equiv \hat{N}_a + \hat{N}_b ,$$

while the energy-momentum operator is defined by

$$\hat{P}^\mu = \int \frac{d^3\mathbf{k}}{\sqrt{(2\pi)^3 2\omega_k}} k^\mu \left[a^\dagger(\mathbf{k}) a(\mathbf{k}) + b^\dagger(\mathbf{k}) b(\mathbf{k})\right] .$$

Thus the complex scalar field has the interpretation of creating different sorts of particles, corresponding to operators $a^\dagger$ and $b^\dagger$. To understand the physical interpretation of this difference, let us consider the corresponding charge density operator, $\hat{j}_0 = \hat{\phi}^\dagger(x) i \overleftrightarrow{\partial}_0 \phi(x)$. Once normal ordered, the total charge $Q = \int d^3\mathbf{x} j_0(x)$ is given by

$$\hat{Q} = \int \frac{d^3\mathbf{k}}{\sqrt{(2\pi)^3 2\omega_k}} \left[a^\dagger(\mathbf{k}) a(\mathbf{k}) - b^\dagger(\mathbf{k}) b(\mathbf{k})\right] = \hat{N}_a - \hat{N}_b .$$

From this result we can interpret the particles as carrying an electric charge, equal in magnitude, and opposite in sign. The complex scalar field is a theory of charged particles. The negative density that plagued the Klein-Gordon field is simply a manifestation of particles with negative charge.

15.4.3 INFO: Dirac Field

The quantisation of the Klein-Gordon field leads to a theory of relativistic spin zero particles which obey boson statistics. From the quantisation of the Dirac field, we expect a theory of Fermionic spin 1/2 particles. Following on from our consideration of the Klein-Gordon theory, we introduce the Lagrangian density associated with the Dirac equation (exercise)

$$\boxed{\mathcal{L} = \bar{\psi}\left(i\gamma^\mu \partial_\mu - m\right)\psi ,}$$

(or, equivalently, $\mathcal{L} = \bar{\psi}(\frac{1}{2} i\gamma^\mu \overleftrightarrow{\partial}_\mu - m)\psi)$. With this definition, the corresponding canonical momentum is given by $\partial_{\dot{\psi}}\mathcal{L} = i\bar{\psi}\gamma^0 = i\psi^\dagger$. From the Lagrangian density, we thus obtain the Hamiltonian density,

$$\mathcal{H} = \bar{\psi}\left(-i\gamma \cdot \nabla + m\right)\psi ,$$

which, making use of the Dirac equation, is equivalent to $\mathcal{H} = \bar{\psi} i\gamma^0 \partial_0 \psi = \psi^\dagger i\partial_t \psi$.

For the Dirac theory, we postulate the equal time anticommutation relations

$$\boxed{\left\{\psi_\alpha(\mathbf{x},t), i\psi_\beta^\dagger(\mathbf{x}',t)\right\} = i\delta^3(\mathbf{x}-\mathbf{x}')\delta_{\alpha\beta} ,}$$

(or, equivalently $\{\psi_\alpha(\mathbf{x},t), i\bar{\psi}_\beta(\mathbf{x}',t)\} = \gamma^0_{\alpha\beta}\delta^3(\mathbf{x}-\mathbf{x}')$), together with

$$\boxed{\{\psi_\alpha(\mathbf{x},t), \psi_\beta(\mathbf{x}',t)\} = \left\{\bar{\psi}_\alpha(\mathbf{x},t), \bar{\psi}_\beta(\mathbf{x}',t)\right\} = 0 .}$$

Using the general solution of the Dirac equation for a free particle as a basis set, together with the intuition drawn from the study of the complex scalar field, we may with no more ado, introduce the field operators which diagonalise the Hamiltonian density

$$\psi(x) = \sum_{r=1}^{2} \int \frac{d^3\mathbf{k}}{(2\pi)^3 2\omega_k} \left[a_r(\mathbf{k}) u^{(r)}(\mathbf{k}) e^{-ik\cdot x} + b_r^\dagger(\mathbf{k}) v^{(r)}(\mathbf{k}) e^{ik\cdot x} \right]$$
$$\bar{\psi}(x) = \sum_{r=1}^{2} \int \frac{d^3\mathbf{k}}{(2\pi)^3 2\omega_k} \left[a_r^\dagger(\mathbf{k}) \bar{u}^{(r)}(\mathbf{k}) e^{ik\cdot x} + b_r(\mathbf{k}) \bar{v}^{(r)}(\mathbf{k}) e^{-ik\cdot x} \right],$$

where the annihilation and creation operators also obey the anticommutation relations,

$$\left\{a_r(\mathbf{k}), a_s^\dagger(\mathbf{k}')\right\} = \left\{b_r(\mathbf{k}), b_s^\dagger(\mathbf{k}')\right\} = (2\pi)^3 2\omega_k \delta_{rs} \delta^3(\mathbf{k}-\mathbf{k}')$$
$$\{a_r(\mathbf{k}), a_s(\mathbf{k}')\} = \left\{a_r^\dagger(\mathbf{k}), a_s^\dagger(\mathbf{k}')\right\} = \{b_r(\mathbf{k}), b_s(\mathbf{k}')\} = \left\{b_r^\dagger(\mathbf{k}), b_s^\dagger(\mathbf{k}')\right\} = 0\,.$$

The latter condition implies the Pauli exclusion principle $a^\dagger(\mathbf{k})^2 = 0$. With this definition, $a(\mathbf{k})u(\mathbf{k})e^{-ik\cdot x}$ annilihates a postive energy electron, and $b^\dagger(\mathbf{k})v(\mathbf{k})e^{ik\cdot x}$ creates a positive energy positron.

From these results, making use of the expression for the Hamiltonian density operator, one obtains

$$\hat{H} = \sum_{r=1}^{2} \int \frac{d^3\mathbf{k}}{(2\pi)^3 2\omega_k} \omega_k \left[a_r^\dagger(\mathbf{k}) a_r(\mathbf{k}) - b_r(\mathbf{k}) b_r^\dagger(\mathbf{k}) \right].$$

Were the commutation relations chosen as bosonic, one would conclude the existence of negative energy solutions. However, making use of the anticommutation relations, and dropping the infinite constant (or, rather, normal ordering) one obtains a positive definite result. Expressed as one element of the total energy-momentum operator, one finds

$$\boxed{\hat{P}^\mu = \sum_{r=1}^{2} \int \frac{d^3\mathbf{k}}{(2\pi)^3 2\omega_k} k^\mu \left[a_r^\dagger(\mathbf{k}) a_r(\mathbf{k}) + b_r^\dagger(\mathbf{k}) b_r(\mathbf{k}) \right].}$$

Finally, the total charge is given by

$$\hat{Q} = \int \hat{j}^0 d^3\mathbf{x} = \int d^3\mathbf{x} \psi^\dagger \psi = \hat{N}_a - \hat{N}_b\,.$$

where $\hat{N}$ represents the total number operator. $N_a = \int d^3\mathbf{k}\, a^\dagger(\mathbf{k})a(\mathbf{k})$ is the number of the particles and $N_b = \int d^3\mathbf{k}\, b^\dagger(\mathbf{k})b(\mathbf{k})$ is the number of antiparticles with opposite charge.

15.5 The low energy limit of the Dirac equation

To conclude our abridged exploration of the foundations of relativistic quantum mechanics, we turn to the interaction of a relativistic spin 1/2 particle with an electromagnetic field. Suppose that ψ represents a particle of charge q ($q = -e$ for the electron). From non-relativistic quantum mechanics, we expect to obtain the equation describing its interaction with an EM field given by the potential A^μ by the **minimal substitution**

$$\boxed{p^\mu \longmapsto p^\mu - qA^\mu\,,}$$

where $A^0 \equiv \varphi$. Applied to the Dirac equation, we obtain for the interaction of a particle with a given (non-quantized) EM field, $[\gamma_\mu (p^\mu - qA^\mu) - m]\psi = 0$, or compactly

$$\boxed{(\not{p} - q\not{A} - m)\psi = 0\,.}$$

Previously, in chapter 9, we explored the relativistic (fine-structure) corrections to the hydrogen atom. At the time, we alluded to these as the leading relativistic contributions to the Dirac theory. In the following section, we will explore how these corrections are derived.

In the Dirac-Pauli representation,

$$\boldsymbol{\alpha} = \begin{pmatrix} 0 & \boldsymbol{\sigma} \\ \boldsymbol{\sigma} & 0 \end{pmatrix}, \qquad \beta = \begin{pmatrix} \mathbb{I}_2 & 0 \\ 0 & -\mathbb{I}_2 \end{pmatrix}.$$

we have seen that the plane-wave solution to the Dirac equation for particles can be written in the form

$$\psi_p(x) = N \begin{pmatrix} \chi \\ \frac{c\boldsymbol{\sigma}\cdot\hat{\mathbf{p}}}{mc^2+E}\chi \end{pmatrix} e^{i(px-Et)/\hbar},$$

where we have restored the parameters $\hbar$ and c. From this expression, we can see that, at low energies, where $|E - mc^2| \ll mc^2$, the second component of the bispinor is smaller than the first by a factor of order v/c. To obtain the non-relavistic limit, we can exploit this asymmetry to develop a perturbative expansion of the coefficients in v/c.

Consider then the Dirac equation for a particle moving in a potential $(\phi, \mathbf{A})$. Expressed in matrix form, the Dirac equation $H = c\boldsymbol{\alpha}\cdot(-i\hbar\nabla - \frac{e}{c}\mathbf{A}) + mc^2\beta + e\phi$ is expressed as

$$H = \begin{pmatrix} mc^2 + e\phi & c\boldsymbol{\sigma}\cdot(-i\hbar\nabla - \frac{e}{c}\mathbf{A}) \\ c\boldsymbol{\sigma}\cdot(\hat{\mathbf{p}} - \frac{q}{c}\mathbf{A}) & -mc^2 + q\phi \end{pmatrix}.$$

Defining the bispinor $\psi^T(x) = (\psi_a(x), \psi_b(x))$, the Dirac equation translates to the coupled equations,

$$(mc^2 + e\phi)\psi_a + c\boldsymbol{\sigma}\cdot(\hat{\mathbf{p}} - \frac{q}{c}\mathbf{A})\psi_b = E\psi_a$$
$$c\boldsymbol{\sigma}\cdot(\hat{\mathbf{p}} - \frac{q}{c}\mathbf{A})\psi_a - (mc^2 - q\phi)\psi_b = E\psi_b\,.$$

Then, if we define $W = E - mc^2$, a rearrangement of the second equation obtains

$$\psi_b = \frac{1}{2mc^2 + W - q\phi} c\boldsymbol{\sigma}\cdot(\hat{\mathbf{p}} - \frac{q}{c}\mathbf{A})\psi_a\,.$$

Then, **at zeroth order in** v/c, we have $\psi_b \simeq \frac{1}{2mc^2} c\boldsymbol{\sigma}\cdot(\hat{\mathbf{p}} - \frac{q}{c}\mathbf{A})\psi_a$. Substituted into the first equation, we thus obtain the **Pauli equation** $H_{\rm non-rel}\psi_a = W\psi_a$, where

$$H_{\rm non_rel} = \frac{1}{2m}\left[\boldsymbol{\sigma}\cdot(\hat{\mathbf{p}} - \frac{q}{c}\mathbf{A})\right]^2 + q\phi\,.$$

Making use of the Pauli matrix identity $\sigma_i\sigma_j = \delta_{ij} + i\epsilon_{ijk}\sigma_k$, we thus obtain the familiar non-relativistic Schrödinger Hamiltonian,

$$\boxed{H_{\rm non\_rel} = \frac{1}{2m}(\hat{\mathbf{p}} - \frac{q}{c}\mathbf{A})^2 - \frac{q\hbar}{2mc}\boldsymbol{\sigma}\cdot(\nabla\times\mathbf{A}) + q\phi\,.}$$

As a result, we can identify the spin magnetic moment

$$\boldsymbol{\mu}_S = \frac{q\hbar}{2mc}\boldsymbol{\sigma} = \frac{q\hbar}{mc}\hat{\mathbf{S}}\,,$$

with the **gyromagnetic ratio**, $g = 2$. This compares to the measured value of $g = 2 \times (1.0011596567 \pm 0.0000000035)$, the descrepency form 2 being attributed to small radiative corrections.

Let us now consider the expansion to **first order in** v/c. Here, for simplicity, let us suppose that $\mathbf{A} = 0$. In this case, taking into account the next order term, we obtain

$$\psi_b \simeq \frac{1}{2mc^2}\left(1 + \frac{V - W}{2mc^2}\right) c\boldsymbol{\sigma} \cdot \hat{\mathbf{p}}\psi_a$$

where $V = q\phi$. Then substituted into the second equation, we obtain

$$\left[\frac{1}{2m}(\boldsymbol{\sigma} \cdot \hat{\mathbf{p}})^2 + \frac{1}{4m^2c^2}(\boldsymbol{\sigma} \cdot \hat{\mathbf{p}})(V - W)(\boldsymbol{\sigma} \cdot \hat{\mathbf{p}}) + V\right]\psi_a = W\psi_a\,.$$

At this stage, we must be cautious in interpreting ψ_a as a complete non-relavistic wavefunction with leading relativistic corrections. To find the true wavefunction, we have to consider the normalization. If we suppose that the original wavefunction is normalized, we can conclude that,

$$\begin{aligned}\int d^3x \psi^\dagger(\mathbf{x}, t)\psi(\mathbf{x}, t) &= \int d^3x \left(\psi_a^\dagger(\mathbf{x}, t)\psi_a(\mathbf{x}, t) + \psi_b^\dagger(\mathbf{x}, t)\psi_b(\mathbf{x}, t)\right)\\ &\simeq \int d^3x \psi_a^\dagger(\mathbf{x}, t)\psi_a(\mathbf{x}, t) + \frac{1}{(2mc)^2}\int d^3x \psi_a^\dagger(\mathbf{x}, t)\hat{\mathbf{p}}^2\psi_a(\mathbf{x}, t)\,.\end{aligned}$$

Therefore, at this order, the normalized wavefunction is set by, $\psi_s = (1 + \frac{1}{8m^2c^2}\hat{\mathbf{p}}^2)\psi_a$ or, inverted,

$$\psi_a = \left(1 - \frac{1}{8m^2c^2}\hat{\mathbf{p}}^2\right)\psi_s\,.$$

Substituting, then rearranging the equation for ψ_s, and retaining terms of order $(v/c)^2$, one ontains (exercise) $\hat{H}_{\rm non-rel}\psi_s = W\psi_s$, where

$$\hat{H}_{\rm non-rel} = \frac{\hat{\mathbf{p}}^2}{2m} - \frac{\hat{\mathbf{p}}^4}{8m^3c^2} + \frac{1}{4m^2c^2}(\boldsymbol{\sigma} \cdot \hat{\mathbf{p}})V(\boldsymbol{\sigma} \cdot \hat{\mathbf{p}}) + V - \frac{1}{8m^2c^2}(V\hat{\mathbf{p}}^2 + \hat{\mathbf{p}}^2V)\,.$$

Then, making use of the identities,

$$\begin{aligned}&[V, \hat{\mathbf{p}}^2] = \hbar^2(\nabla^2 V) + 2i\hbar(\nabla V) \cdot \hat{\mathbf{p}}\\ &(\boldsymbol{\sigma} \cdot \hat{\mathbf{p}})V = V(\boldsymbol{\sigma} \cdot \hat{\mathbf{p}}) + \boldsymbol{\sigma} \cdot [\hat{\mathbf{p}}, V]\\ &(\boldsymbol{\sigma} \cdot \hat{\mathbf{p}})V(\boldsymbol{\sigma} \cdot \hat{\mathbf{p}}) = V\hat{\mathbf{p}}^2 - i\hbar(\nabla V) \cdot \hat{\mathbf{p}} + \hbar\boldsymbol{\sigma} \cdot (\nabla V) \times \hat{\mathbf{p}}\,,\end{aligned}$$

we obtain the final expression (exercise),

$$\boxed{\hat{H}_{\rm non-rel} = \frac{\hat{\mathbf{p}}^2}{2m} - \frac{\hat{\mathbf{p}}^4}{8m^3c^2} + \underbrace{\frac{\hbar}{4m^2c^2}\boldsymbol{\sigma} \cdot (\nabla V) \times \hat{\mathbf{p}}}_{\rm spin-orbit\ coupling} + \underbrace{\frac{\hbar^2}{8m^2c^2}(\nabla^2 V)}_{\rm Darwin\ term}\,.}$$

The second term on the right hand side represents the relativistic correction to the kinetic energy, the third term denotes the spin-orbit interaction and the final term is the Darwin term. For atoms, with a central potential, the spin-orbit term can be recast as

$$\hat{H}_{\rm S.O.} = \frac{\hbar^2}{4m^2c^2}\boldsymbol{\sigma} \cdot \frac{1}{r}(\partial_r V)\mathbf{r} \times \hat{\mathbf{p}} = \frac{\hbar^2}{4m^2c^2}\frac{1}{r}(\partial_r V)\boldsymbol{\sigma} \cdot \hat{\mathbf{L}}\,.$$

To address the effects of these relativistic contributions, we refer back to chapter 9.