20

The Dirac Equation

Nonrelativistic quantum mechanics, which was developed in the previous chapters, is very successful when applied to problems like the hydrogen atom, where the typical velocity (speaking semiclassically) is small compared to c. (Recall $v/c = \beta = \alpha \cong 1/137$ in the ground state.) But even in this case, there are measurable (fine-structure) corrections of the order of $(v/c)^4$ which have to be put in by hand. If these corrections are to emerge naturally and if relativistic systems (high-Z atoms, for example) are to be described well, it is clear that we need an equation for the electron that has relativity built into it from the start. Such an equation was discovered by Dirac. We study it here with the *main goal* of seeing the coherent emergence of several concepts that were introduced disjointly at various stages—the spin of the electron, its magnetic moment ($g=2$), the spin–orbit, and other fine-structure corrections.

In the last section we address some general questions that accompany Dirac's formulation and indicate the need for quantum field theory.

20.1. The Free-Particle Dirac Equation

Let us consider the simplest case, of a free particle. We start by stating the relation between classical mechanics and the free-particle Schrödinger equation in a way that facilitates generalization. If we start with the nonrelativistic relation

$$\mathscr{H} = \frac{|\mathbf{p}|^2}{2m} = \frac{p^2}{2m} \tag{20.1.1}$$

and make the substitution

$$\begin{aligned} \mathbf{p} &\to \mathbf{P} \\ \mathscr{H} &\to i\hbar \frac{\partial}{\partial t} \end{aligned} \tag{20.1.2}$$

and let both sides act on a state vector $|\psi\rangle$, we get Schrödinger's equation

$$i\hbar \frac{\partial |\psi\rangle}{\partial t} = \frac{P^2}{2m} |\psi\rangle \tag{20.1.3}$$

A natural starting point for the relativistic equation is the corresponding relation due to Einstein

$$\mathscr{H} = (c^2 p^2 + m^2 c^4)^{1/2} \tag{20.1.4}$$

If we make the substitution mentioned above, we get

$$i\hbar \frac{\partial |\psi\rangle}{\partial t} = (c^2 P^2 + m^2 c^4)^{1/2} |\psi\rangle \tag{20.1.5}$$

This equation is undesirable because it treats space and time asymmetrically. To see this, we first go to the momentum basis, where $\mathbf{P}$ is just $\mathbf{p}$ and the square root may be expanded in a series:

$$i\hbar \frac{\partial \psi(\mathbf{p}, t)}{\partial t} = mc^2 \left(1 + \frac{p^2}{2m^2 c^2} - \frac{p^4}{8m^4 c^4} + \cdots\right) \psi(\mathbf{p}, t) \tag{20.1.6}$$

If we now transform to the coordinate basis, each p^2 becomes $(-\hbar^2 \nabla^2)$ and the asymmetry between space and time is manifest. What we want is an equation that is of the same order in both space and time.

There are two ways out. One is to replace Eq. (20.1.4) by

$$\mathscr{H}^2 = c^2 p^2 + m^2 c^4 \tag{20.1.7}$$

and obtain, upon making the operator substitution,

$$\frac{\partial^2 |\psi\rangle}{\partial t^2} = \left(-\frac{c^2 P^2}{\hbar^2} - \frac{m^2 c^4}{\hbar^2}\right) |\psi\rangle \tag{20.1.8a}$$

In the coordinate basis this becomes

$$\left[\frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \nabla^2 + \left(\frac{mc^2}{\hbar}\right)^2\right] \psi = 0 \tag{20.1.8b}$$

This is called the *Klein-Gordon equation* and has the desired symmetry between space and time. But we move along, since ψ here is a scalar and cannot describe the electron. It is, however, a good candidate for pions, kaons, etc., which are spinless.

The second alternative, due to Dirac, is the following. Let us suppose that the quantity in the square root in Eq. (20.1.5) can be written as a perfect square of a quantity that is linear in $\mathbf{P}$. We can then take the square root (which will give us

our Hamiltonian) and obtain an equation that is of the first order in time and space. So let us write

$$\begin{aligned} c^2P^2+m^2c^4 &= (c\alpha_x P_x + c\alpha_y P_y + c\alpha_z P_z + \beta mc^2)^2 \\ &= (c\boldsymbol{\alpha}\cdot\mathbf{P}+\beta mc^2)^2 \end{aligned} \tag{20.1.9}$$

where $\boldsymbol{\alpha}$ and β are to be determined by matching both sides of

$$\begin{aligned} &c^2(P_x^2+P_y^2+P_z^2)+m^2c^4 \\ &\quad = [c^2(\alpha_x^2P_x^2+\alpha_y^2P_y^2+\alpha_z^2P_z^2)+\beta^2m^2c^4] \\ &\qquad + [c^2P_xP_y(\alpha_x\alpha_y+\alpha_y\alpha_x)+ \text{ and cyclic permutations}] \\ &\qquad + [mc^3P_x(\alpha_x\beta+\beta\alpha_x)+x\to y+x\to z] \end{aligned} \tag{20.1.10}$$

(We have assumed that $\boldsymbol{\alpha}$ and β are space independent, which is a reasonable assumption for a free particle.) These equations tell us that

$$\begin{aligned} \alpha_i^2=\beta^2=1 \qquad & (i=x,y,z) \\ \alpha_i\alpha_j+\alpha_j\alpha_i=[\alpha_i,\alpha_j]_+=0 \qquad & (i\neq j) \\ \alpha_i\beta+\beta\alpha_i=[\alpha_i,\beta]_+=0 & \end{aligned} \tag{20.1.11}$$

It is evident that $\boldsymbol{\alpha}$ and β are not c numbers. They are matrices and furthermore Hermitian (so that the Hamiltonian $H=c\boldsymbol{\alpha}\cdot\mathbf{P}+\beta mc^2$ is Hermitian), traceless, and have eigenvalues ±1. (Recall the results of Exercise 1.8.8). They must also be even dimensional if the last two properties are to be compatible. They cannot be 2×2 matrices, since, as we saw in Exercise 14.3.8, the set of three Pauli matrices with these properties cannot be enlarged to include a fourth. So they must be 4×4 matrices. They are not unique (since $\alpha\to S^\dagger\alpha S$, $\beta\to S^\dagger\beta S$ preserves the desired properties if S is unitary.) The following four are frequently used and will be used by us:

$$\boldsymbol{\alpha}=\begin{bmatrix}0 & \boldsymbol{\sigma}\\ \boldsymbol{\sigma} & 0\end{bmatrix}, \qquad \beta=\begin{bmatrix}I & 0\\ 0 & -I\end{bmatrix} \tag{20.1.12}$$

In the above, $\boldsymbol{\sigma}$ and I are 2×2 matrices.‡ We now have the *Dirac equation*:

$$i\hbar\frac{\partial|\psi\rangle}{\partial t}=(c\boldsymbol{\alpha}\cdot\mathbf{P}+\beta mc^2)|\psi\rangle \tag{20.1.13}$$

with $\boldsymbol{\alpha}$ and β known. Hereafter we work exclusively in the coordinate basis. However, we depart from our convention and use the symbol $\mathbf{P}$, reserved for the momentum operator in the abstract, to represent it in the coordinate basis (instead of using $-i\hbar\boldsymbol{\nabla}$). This is done to simplify the notation in what follows.

‡ For example, β is a 4×4 diagonal matrix with the first two entries $+1$ and the next two entries -1.

The fact that $\boldsymbol{\alpha}$ and β in

$$i\hbar \frac{\partial \psi}{\partial t} = (c\boldsymbol{\alpha} \cdot \mathbf{P} + \beta mc^2)\psi \tag{20.1.14}$$

are 4×4 matrices implies that ψ is a four-component object. It is called a *Lorentz spinor*. Our reaction is mixed. We are happy that relativity, plus the requirement that the equation be first order in time and space, have led naturally to a multicomponent wave function. But we are distressed that ψ has four components instead of two. In the next two sections we will see how, despite this apparent problem, the Dirac equation describes electrons.

For later use, let us note that since the Hamiltonian is Hermitian, the norm of the state is conserved. In the coordinate basis this means

$$\int \psi^\dagger \psi \, d^3\mathbf{r} = \text{const} \tag{20.1.15}$$

Just as in the nonrelativistic case, this global conservation law has a local version also. (See exercise below.)

*Exercise 20.1.1.** Derive the continuity equation

$$\frac{\partial P}{\partial t} + \nabla \cdot \mathbf{j} = 0$$

where $P = \psi^\dagger \psi$ and $\mathbf{j} = c\psi^\dagger \boldsymbol{\alpha} \psi$.

20.2. Electromagnetic Interaction of the Dirac Particle

In this central section, we see how several properties of the electron emerge naturally from the Dirac equation. As a first step, we couple the particle to the potential $(\mathbf{A}, \phi)$. We then consider the equation to order $(v/c)^2$ and show that the particle can be described by a two-component wave function and that it has $g = 2$. Finally we consider the equation to order $(v/c)^4$ and see the fine-structure emerge.

The coupling of the electromagnetic potentials is suggested by the classical Hamiltonian for a particle of charge q:

$$\mathscr{H} = [(\mathbf{p} - q\mathbf{A}/c)^2 c^2 + m^2 c^4]^{1/2} + q\phi \tag{20.2.1}$$

which leads us to

$$i\hbar \frac{\partial \psi}{\partial t} = [c\boldsymbol{\alpha} \cdot (\mathbf{P} - q\mathbf{A}/c) + \beta mc^2 + q\phi]\psi \tag{20.2.2}$$

To see just these two features emerge, we can set $\phi = 0$ and work to order $(v/c)^2$. If we look for energy eigenstates

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

of Eq. (20.2.2), we get

$$E\psi = (c\boldsymbol{\alpha}\cdot\boldsymbol{\pi} + \beta mc^2)\psi \tag{20.2.3}$$

where

$$\boldsymbol{\pi} = \mathbf{P} - q\mathbf{A}/c \tag{20.2.4}$$

is the kinetic ($m\mathbf{v}$) momentum operator. We now write ψ as

$$\psi = \begin{bmatrix} \chi \\ \Phi \end{bmatrix} \tag{20.2.5}$$

where χ *and* Φ *are two-component spinors*. Equation (20.2.3), with $\boldsymbol{\alpha}$ and β explicitly written, becomes

$$\begin{bmatrix} E - mc^2 & -c\boldsymbol{\sigma}\cdot\boldsymbol{\pi} \\ -c\boldsymbol{\sigma}\cdot\boldsymbol{\pi} & E + mc^2 \end{bmatrix} \begin{bmatrix} \chi \\ \Phi \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \tag{20.2.6}$$

which means

$$(E - mc^2)\chi - c\boldsymbol{\sigma}\cdot\boldsymbol{\pi}\Phi = 0 \tag{20.2.7}$$

and

$$(E + mc^2)\Phi - c\boldsymbol{\sigma}\cdot\boldsymbol{\pi}\chi = 0 \tag{20.2.8}$$

The second equation tells us that

$$\Phi = \left(\frac{c\boldsymbol{\sigma}\cdot\boldsymbol{\pi}}{E + mc^2}\right)\chi \tag{20.2.9}$$

Let us examine the term in brackets at low velocities. The denominator is

$$E + mc^2 = E_S + 2mc^2 \tag{20.2.10}$$

where $E_S = E - mc^2$ is the energy that appears in Schrödinger's equation. At low velocities, since $E_S \ll mc^2$‡

$$E + mc^2 \cong 2mc^2 \tag{20.2.11}$$

The numerator is of the order mvc, where mv is the typical momentum of the state. So

$$\left|\frac{\Phi}{\chi}\right| \cong \frac{1}{2}\left(\frac{v}{c}\right) \ll 1 \tag{20.2.12}$$

For this reason χ and Φ are called the *large and small components*, respectively. The terminology is of course appropriate only in the nonrelativistic domain. In this domain

$$\Phi \cong \frac{\boldsymbol{\sigma}\cdot\boldsymbol{\pi}}{2mc}\chi \tag{20.2.13}$$

and Eq. (20.2.7) becomes

$$E_S\chi = c\boldsymbol{\sigma}\cdot\boldsymbol{\pi}\Phi = \frac{(\boldsymbol{\sigma}\cdot\boldsymbol{\pi})(\boldsymbol{\sigma}\cdot\boldsymbol{\pi})}{2m}\chi \tag{20.2.14}$$

This is called the *Pauli equation*.§ If we use the identity

$$\boldsymbol{\sigma}\cdot\mathbf{A}\boldsymbol{\sigma}\cdot\mathbf{B} = \mathbf{A}\cdot\mathbf{B} + i\boldsymbol{\sigma}\cdot\mathbf{A}\times\mathbf{B} \tag{20.2.15}$$

and

$$\boldsymbol{\pi}\times\boldsymbol{\pi} = \frac{iq\hbar}{c}\mathbf{B} \tag{20.2.16}$$

we get

$$\left[\frac{(\mathbf{P} - q\mathbf{A}/c)^2}{2m} - \frac{q\hbar}{2mc}\boldsymbol{\sigma}\cdot\mathbf{B}\right]\chi = E_S\chi \tag{20.2.17}$$

It is evident that this equation describes a spin-$\frac{1}{2}$ particle *with* $g = 2$. It is therefore appropriate to electrons. {Although $g = 2$ emerges so naturally from Dirac theory,

‡ $E_S = T + V = \dfrac{\pi^2}{2m} + V \underset{\text{(virial theorem)}}{\cong} O\left(\dfrac{\pi^2}{m}\right) = mv^2, \qquad \dfrac{E_S}{mc^2} \cong \left(\dfrac{v}{c}\right)^2 \ll 1$

§ Actually the Pauli equation is the time-dependent version, with $i\hbar\dot{\chi}$ on the left-hand side.

it is incorrect to say that we need relativity to get this result. If we write the free-particle Schrödinger equation as

$$\frac{(\boldsymbol{\sigma}\cdot\mathbf{P})^2}{2m}\chi = E_S\chi$$

[since $(\boldsymbol{\sigma}\cdot\mathbf{P})^2 = P^2$] and then couple the vector potential $\mathbf{A}$ as prescribed by *nonrelativistic* mechanics ($\mathbf{P}\to\mathbf{P}-q\mathbf{A}/c$), we get $g=2$. Of course spin is introduced artificially here, but $g=2$ is not.}

*Exercise 20.2.1.** Derive Eq. (20.2.16).

*Exercise 20.2.2.** Solve for the exact levels of the Dirac particle in a uniform magnetic field $\mathbf{B}=B_0\mathbf{k}$. Assume $\mathbf{A}=(B_0/2)(-y\mathbf{i}+x\mathbf{j})$. Consult Exercise 12.3.8. (Write the equation for χ.)

Hydrogen Fine Structure

We now apply the Dirac equation to the case

$$V = e\phi = -e^2/r \tag{20.2.18}$$

that is to say, the electron in the hydrogen atom. (The proton is assumed to be fixed, i.e., infinitely massive.) The small and big components obey the following coupled equations:

$$(E - V - mc^2)\chi - c\boldsymbol{\sigma}\cdot\mathbf{P}\Phi = 0 \tag{20.2.19}$$

$$(E - V + mc^2)\Phi - c\boldsymbol{\sigma}\cdot\mathbf{P}\chi = 0 \tag{20.2.20}$$

The second one tells us that

$$\Phi = (E - V + mc^2)^{-1}c\boldsymbol{\sigma}\cdot\mathbf{P}\chi \tag{20.2.21}$$

(Since $\mathbf{P}$ can differentiate V, the order of the factors is important.) If we feed this into the first, we get

$$(E - V - mc^2)\chi = c\boldsymbol{\sigma}\cdot\mathbf{P}\left[\frac{1}{E - V + mc^2}\right]c\boldsymbol{\sigma}\cdot\mathbf{P}\chi \tag{20.2.22}$$

If we approximate $E - V + mc^2$ on the right-hand side as $2mc^2$, we get

$$\begin{aligned} E_S\chi &= \left[\frac{(\boldsymbol{\sigma}\cdot\mathbf{P})^2}{2m} + V\right]\chi \\ &= \left[\frac{P^2}{2m} + V\right]\chi \end{aligned} \tag{20.2.23}$$

This is just the nonrelativistic Schrödinger equation we solved in Chapter 13. Notice that the Hamiltonian is order $(v/c)^2$ since it is quadratic in the momentum. To see the fine structure, we must go to order $(v/c)^4$. We do this by expanding $(E-V+mc^2)^{-1}$ on the right-hand side to one more order in v^2/c^2:

$$\frac{1}{E-V+mc^2}=\frac{1}{2mc^2+E_S-V}=\frac{1}{2mc^2}\left(1+\frac{E_S-V}{2mc^2}\right)^{-1}$$
$$\cong\frac{1}{2mc^2}\left(1-\frac{E_S-V}{2mc^2}\right)=\frac{1}{2mc^2}-\frac{E_S-V}{4m^2c^4} \tag{20.2.24}$$

Equation (20.2.22) now becomes

$$E_S\chi=\left[\frac{P^2}{2m}+V-\frac{\boldsymbol{\sigma}\cdot\mathbf{P}(E_S-V)\boldsymbol{\sigma}\cdot\mathbf{P}}{4m^2c^2}\right]\chi \tag{20.2.25}$$

We cannot view this as the time-independent Schrödinger equation (i.e., as $E_S\chi=H\chi$) since E_S appears on *both sides*. By now even our spinal column knows how to respond to such a crisis. The right-hand side is a power series in v^2/c^2. The first two terms are of the order v^2/c^2, and the third is expected to be of order v^4/c^4. Now the two $\boldsymbol{\sigma}\cdot\mathbf{P}$ factors in the third form use up a factor v^2/c^2. So we need E_S-V only to order v^2/c^2. This we get from the same equation truncated to this order:

$$(E_S-V)\chi=\frac{P^2}{2m}\chi \tag{20.2.26}$$

We cannot use this result directly in Eq. (20.2.25) since E_S-V there does not act on χ directly; there is $\boldsymbol{\sigma}\cdot\mathbf{P}$ in the way. So we do the following:

$$(E_S-V)\boldsymbol{\sigma}\cdot\mathbf{P}\chi=\boldsymbol{\sigma}\cdot\mathbf{P}(E_S-V)\chi+\boldsymbol{\sigma}\cdot[E_S-V,\mathbf{P}]\chi$$
$$=(\boldsymbol{\sigma}\cdot\mathbf{P})\frac{P^2}{2m}\chi+\boldsymbol{\sigma}\cdot[\mathbf{P},V]\chi \tag{20.2.27}$$

Feeding this into Eq. (20.2.25) we get

$$E_S\chi=\left\{\frac{P^2}{2m}+V-\frac{P^4}{8m^3c^2}-\frac{(\boldsymbol{\sigma}\cdot\mathbf{P})(\boldsymbol{\sigma}\cdot[\mathbf{P},V])}{4m^2c^2}\right\}\chi$$
$$=\left\{\frac{P^2}{2m}+V-\frac{P^4}{8m^3c^2}-\frac{i\boldsymbol{\sigma}\cdot\mathbf{P}\times[\mathbf{P},V]}{4m^2c^2}-\frac{\mathbf{P}\cdot[\mathbf{P},V]}{4m^2c^2}\right\}\chi$$
$$=H\chi \tag{20.2.28}$$

using once again the identity (20.2.15). We recognize the third term to be just the relativistic correction to the kinetic energy. It is just [recall Eq. (17.3.6)]

$$H_T = -\frac{P^4}{8m^3c^2} \tag{20.2 29}$$

The fourth term is the spin–orbit interaction, $H_{\text{s.o.}}$ of Eq. (17.3.16):

$$\begin{aligned}
&\frac{-i\boldsymbol{\sigma}\cdot\mathbf{P}\times[\mathbf{P}, V]}{4m^2c^2} \\
&= \frac{-i\boldsymbol{\sigma}\cdot\mathbf{P}\times[-i\hbar\nabla(-e^2/r)]}{4m^2c^2} \qquad \left\{\text{using} \quad [P, f(x)] = -i\hbar\frac{df}{dx}\right\} \\
&= \frac{-\hbar e^2\boldsymbol{\sigma}\cdot\mathbf{P}\times\mathbf{r}}{4m^2c^2r^3} = \frac{\hbar e^2}{4m^2c^2r^3}\boldsymbol{\sigma}\cdot\mathbf{r}\times\mathbf{P}\ddagger \\
&= \frac{e^2}{2m^2c^2r^3}\mathbf{S}\cdot\mathbf{L} = H_{\text{s.o.}}
\end{aligned} \tag{20.2.30}$$

Notice that the Thomas factor is built in.

Consider now the fifth and last term. It upsets the whole interpretation because *it is not Hermitian* (check this). So if the quantity in brackets in Eq. (20.2.28) is used as a Hamiltonian we will find

$$\int |\chi|^2 d^3\mathbf{r} \neq \text{const in time}$$

But this is not surprising, since the conservation law that comes from the Dirac equation is

$$\int \psi^\dagger\psi \, d^3\mathbf{r} = \int [|\chi|^2 + |\Phi|^2] \, d^3\mathbf{r} = \text{const} \tag{20.2.31}$$

It follows that χ is not a good candidate for the Schrödinger wave function to this order in v/c. [It was all right when we worked to order $(v/c)^2$.] We find the right one as follows. Note that

$$\Phi = \frac{c\boldsymbol{\sigma}\cdot\mathbf{P}}{E - V + mc^2}\chi = \frac{c\boldsymbol{\sigma}\cdot\mathbf{P}}{2mc^2 + E_S - V}\chi \cong \frac{\boldsymbol{\sigma}\cdot\mathbf{P}}{2mc}\chi \tag{20.2.32}$$

‡ Although $\mathbf{P}$ is a differential operator, $\mathbf{P}\times\mathbf{r} = -\mathbf{r}\times\mathbf{P}$, just as if $\mathbf{P}$ and $\mathbf{r}$ were c numbers, because the cross product never involves the product of a given coordinate and its conjugate momentum. This point was made earlier in the book when it was stated that there was no ordering ambiguity in passing from $\mathbf{l} = \mathbf{r}\times\mathbf{p}$ to $\mathbf{L}$.

(The neglected terms makes corrections of order v^6/c^6 in the end.) Consequently

$$|\Phi|^2 = \frac{\chi^\dagger(\boldsymbol{\sigma}\cdot\mathbf{P})(\boldsymbol{\sigma}\cdot\mathbf{P})\chi}{(2mc)^2} = \chi^\dagger \frac{P^2}{4m^2c^2}\chi$$

and so, from Eq. (20.2.31),

$$\int \chi^\dagger\left(1+\frac{P^2}{4m^2c^2}\right)\chi\, d^3\mathbf{r} = \int \left[\left(1+\frac{P^2}{8m^2c^2}\right)\chi\right]^\dagger \cdot \left(1+\frac{P^2}{8m^2c^2}\right)\chi\, d^3\mathbf{r}$$
$$= \text{const} \tag{20.2.33}$$

using $(1+x)=(1+x/2)(1+x/2)+O(x^2)$ and the Hermiticity of P^2. Consequently, the candidate for the Schrödinger wave function is

$$\chi_S = \left(1+\frac{P^2}{8m^2c^2}\right)\chi \tag{20.2.34}$$

for it will have a time-independent norm. (To the present accuracy, that is. If we go to higher and higher orders in v^2/c^2, Φ will creep in more and more.)

The equation for χ_S is obtained by eliminating χ in Eq. (20.2.28):

$$E_S\left(1+\frac{P^2}{8m^2c^2}\right)^{-1}\chi_S = H\left(1+\frac{P^2}{8m^2c^2}\right)^{-1}\chi_S$$

$$E_S\chi_S = \left(1+\frac{P^2}{8m^2c^2}\right)H\left(1-\frac{P^2}{8m^2c^2}\right)\chi_S$$
$$= \left(H+\left[\frac{P^2}{8m^2c^2}, H\right]\right)\chi_S \qquad \text{(to this order in } v/c\text{)}$$
$$= H_S\chi_S \tag{20.2.35}$$

In evaluating the commutator, we need consider just the v^2/c^2 part of H, since $P^2/8m^2c^2$ is $O(v^2/c^2)$ and we are working to order v^4/c^4. So

$$H_S = H+\left[\frac{\mathbf{P}\cdot\mathbf{P}}{8m^2c^2}, V\right]$$

is the desired Schrödinger Hamiltonian. The extra piece the above analysis yields combines with the non-Hermitian piece in Eq. (20.2.28) to form the *Darwin*

term H_D:

$$H_D = \frac{1}{8m^2c^2}\left(-2\mathbf{P}\cdot[\mathbf{P}, V]+[\mathbf{P}\cdot\mathbf{P}, V]\right)$$

$$= \frac{-1}{8m^2c^2}[\mathbf{P}\cdot[\mathbf{P}, V]] \quad \text{(using the chain rule for commutators of products)}$$

$$= \frac{\hbar^2}{8m^2c^2}\nabla^2 V \quad \{\text{using } [P, f(x)] = -i\hbar\, df/dx \text{ twice}\}$$

$$= \frac{e^2\hbar^2\pi}{2m^2c^2}\delta^3(\mathbf{r}) \tag{20.2.37}$$

Thus the Darwin term affects only the *s states.*‡ In the ground state, for example,

$$\langle 100|H_D|100\rangle = \frac{e^2\hbar^2\pi}{2m^2c^2}\frac{1}{\pi a_0^3} = \frac{1}{2}mc^2\alpha^4$$

and in general

$$\langle n00|H_D|n00\rangle = \frac{1}{2}\frac{mc^2\alpha^4}{n^3} \tag{20.2.38}$$

Recall that in our previous treatment of fine structure we obtained a spin–orbit shift valid only for $l\neq 0$ and then applied it to $l=0$ as well, without any real justification. The result we got for $l=0$ is just what H_D generated above, which was our reason for doing what we did then. Thus $H_{\text{s.o.}}$ (relevant for $l\neq 0$) and H_D (relevant only for $l=0$) *together* conspire to produce a fine-structure shift that is smooth in l. The physics behind the Darwin term has nothing to do with spin–orbit coupling (for there is no such thing for $l=0$). Rather, it reflects the fact that in a relativistic theory, the particle cannot be localized to better than its Compton wavelength $\hbar/mc$. Thus the potential that is relevant is not $V(\mathbf{r})$ but some smeared average around the point $\mathbf{r}$:

$$\overline{V(\mathbf{r})} = V(\mathbf{r}) + \sum_i \overline{\frac{\partial V}{\partial r_i}\delta r_i} + \frac{1}{2!}\sum_i\sum_j \overline{\frac{\partial^2 V}{\partial r_i \partial r_j}\delta r_i \delta r_j} + O(\delta r^3)$$

$$= V(\mathbf{r}) + \tfrac{1}{6}(\delta r)^2\nabla^2 V + O(\delta r^3)^3 \tag{20.2.39}$$

where, in the averaging, we have assumed that fluctuations in the various directions are uncorrelated and spherically symmetric. If we now feed in $\delta r \simeq \hbar/mc$, we get the right sign and almost the right magnitude for the Darwin term [see Eq. (20.2.37)].

‡ Recall that only in these states is ψ nonzero at the origin.

Although we chose to work to order v^4/c^4, the Dirac equation can be solved exactly in the Coulomb case, $V=-e^2/r$. The resulting energy spectrum is

$$E_{nj}=mc^2\left[1+\left(\frac{\alpha}{n-(j+\frac{1}{2})+[(j+\frac{1}{2})^2-\alpha^2]^{1/2}}\right)^2\right]^{-1/2} \tag{20.2.40}$$

If we expand this in powers of α, we get the rest energy, the Schrödinger energy, the fine-structure energy, and so on. Notice that the states of a given n and j are degenerate to all orders in α.

Whereas the above formula is in fantastic agreement with experiment,‡ it is not the last word. For example, very precise measurements show that the $2S_{1/2}$ level is above the $2P_{1/2}$ level. This phenomenon, called the *Lamb shift*, can be understood only if the electromagnetic field is treated quantum mechanically.

20.3. More on Relativistic Quantum Mechanics

With the principal goal of this chapter achieved in the last section, we direct our attention to certain phenomena that come out of Dirac theory but were not apparent in the last few pages. Let us first note that the union of relativity and quantum mechanics produces the following problem: relativity allows particle production given enough energy, and quantum mechanics allows arbitrarily large energy violations over short times. Consequently the degrees of freedom of a relativistic system are neither fixed nor finite; a system that initially has one particle can evolve into a state with 15 of them. Why doesn't this problem appear in the Dirac theory, which seems like a single-particle theory? The answer is that it does appear, but in the guise of *negative-energy solutions*. Let us see what these are and how they lead to proliferation of the degrees of freedom.

Consider the free-particle Dirac equation (with $\hbar=c=1$)

$$i\frac{\partial\psi}{\partial t}=(\boldsymbol{\alpha}\cdot\mathbf{P}+\beta m)\psi \tag{20.3.1}$$

Let us look for plane wave solutions

$$\psi=w(\mathbf{p})\,e^{i(\mathbf{p}\cdot\mathbf{r}-Et)} \tag{20.3.2}$$

where $w(\mathbf{p})$ is a spinor that has no space-time dependence. It satisfies

$$Ew=(\boldsymbol{\alpha}\cdot\mathbf{p}+\beta m)w \tag{20.3.3}$$

‡ After hyperfine interactions are taken into account.

Figure 20.1. In the Dirac theory there are two continuous bands of energy available to the free particle; one goes from $+m$ up to ∞ and the other goes from $-m$ down to $-\infty$.

or in terms of χ and Φ,

$$\begin{bmatrix} E-m & -\boldsymbol{\sigma}\cdot\mathbf{p} \\ -\boldsymbol{\sigma}\cdot\mathbf{p} & E+m \end{bmatrix}\begin{bmatrix} \chi \\ \Phi \end{bmatrix}=\begin{bmatrix} 0 \\ 0 \end{bmatrix} \tag{20.3.4}$$

If $\mathbf{p}=0$, χ and Φ decouple. The equation for χ is

$$(E-m)\chi=0\rightarrow E=m \tag{20.3.5}$$

which is fine. It says a particle at rest has energy $E=m$ and is described by an arbitrary two-component spinor which we identify as the spin degree of freedom.

The equation for Φ is

$$(E+m)\Phi=0\rightarrow E=-m \tag{20.3.6}$$

Now even a layperson will tell you that E is supposed to be mc^2 not $-mc^2$. The significance of the four components of ψ are evident in the rest frame: there are two possible spin orientations and two signs of the energy. The problem persists for $\mathbf{p}\neq 0$ as well. Here we find

$$\chi=\frac{\boldsymbol{\sigma}\cdot\mathbf{p}}{E-m}\Phi \tag{20.3.37}$$

$$\Phi=\frac{\boldsymbol{\sigma}\cdot\mathbf{p}}{E+m}\chi \tag{20.3.8}$$

These are consistent only if

$$\frac{p^2}{E^2-m^2}=1$$

or

$$E^2=p^2+m^2$$

or

$$E=\pm(p^2+m^2)^{1/2} \tag{20.3.9}$$

The energy levels corresponding to these two options are shown in Fig. 20.1. What do we do with the negative-energy solutions? If there are no interactions, positive-energy electrons will stay where they are and we can postulate that there

are no negative-energy electrons. But there are always some perturbations acting on all electrons and these can induce all positive-energy electrons to cascade down to the negative-energy states. How do we understand the stability of positive-energy electrons?

There are two ways out, one due to Dirac and one due to Feynman.‡ Dirac postulated that the negative-energy states are all occupied—that what we call the vacuum is really the occupied (but *unobservable*) sea of negative-energy electrons. If we accept this, the stability problem is solved by the exclusion principle, which prevents the positive-energy electrons from decaying to the occupied negative-energy states. This picture has some profound consequences. Suppose we give a negative-energy electron enough energy (at least $2m$) for it to come to a positive-energy state. Now we have a positive-energy, charge $-e$ object. But we also have created a hole in the "Dirac sea." Since the filled Dirac sea was postulated to be unobservable, the hole is observable; it represents an increase in charge by $+e$ (the disappearance of $-e$ = appearance of $+e$), and an increase in energy by $|E|$, if $-|E|$ was the energy of the electron ejected from the sea.§ Thus the hole, which has charge $+e$ and *positive* energy, is created along with the electron. It is called a *positron*. Its mass can easily be shown to be m. Positrons were observed a few years after Dirac's theory of holes was published.

When an electron meets a positron, i.e., a hole in the sea, it jumps in and we lose both particles, though some energy (at least equal to $2m$) will be liberated in the form of photons. (Hereafter we will occasionally refer to these particles as e^-, e^+, and γ, respectively.)

The trouble with Dirac's solution is that it doesn't apply to spinless particles, which don't obey the Pauli principle but which do have the same problem of negative-energy solutions, as one can see by plugging a plane wave solution into the Klein-Gordon equation. (In fact this was the reason the Klein-Gordon equation was rejected in the early days and Dirac sought a first-order equation.) So let us turn to Feynman's resolution, which applies to bosons *and* fermions.

Feynman's idea is the following: *negative-energy particles can only travel backward in time*. Let us see first how this resolves the problem and then how the statement is actually implemented in quantum theory. Consider a negative-energy particle that is created at the space-time point c and travels backward to d, where it is destroyed (Fig. 20.2a). To us, who move forward in time and see space-time in equal-time slices, this is what will seem to be happening:

(1) $t < t_d$ Nothing anywhere.
(2) $t = t_d$ Negative energy $-|E|$ and charge $-e$ are destroyed, i.e., world energy goes up by $|E|$ and charge goes up by e relative to the past. A positron is born.
(3) $t = t_c$ Negative energy is created, charge $-e$ is created. This wipes out the positron.
(4) $t > t_c$ Nothing anywhere.

‡ In its basic form, the idea exploited by Feynman was pointed out by Stueckelberg.

§ Recall the story of the fellow who got so used to the midnight express going past his house that one day when it failed to show up, we woke up screaming "What's that noise?"

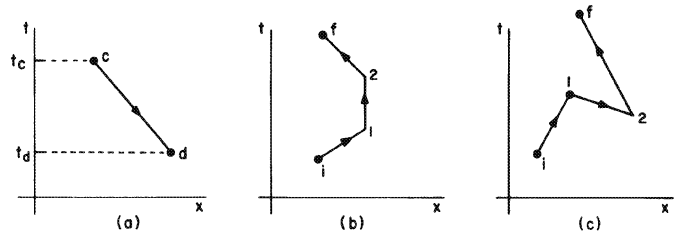

Figure 20.2. (a) A negative-energy particle is created at c, travels back in time to d, where it is destroyed. To us, who move forward in time, it will seem as though an antiparticle of positive energy is created at d and destroyed at c. (b) A normal second order scattering process. (c) A second-order process that involves back-scattering in time. Between times 2 and 1 we will see a particle–antiparticle pair in addition to the original particle.

Thus the process makes perfect sense and represents a positron *created at d* and *destroyed at c*.

How does Feynman ensure that negative-energy states propagate backward? Here is a sketchy description. Recall that the Schrödinger propagator we have used so far is (in the coordinate basis)

$$U_S(\mathbf{r}, t; \mathbf{r}', t') = \sum_n \psi_n(\mathbf{r}) \psi_n^*(\mathbf{r}')\, e^{-iE_n(t-t')} \tag{20.3.10}$$

where ψ_n is an energy eigenfunction labeled by a generic quantum number n.

Since every term in the sum satisfies the Schrödinger equation, it is clear that

$$\left(i\frac{\partial}{\partial t} - H\right) U_S = 0 \tag{20.3.11}$$

given this U_S and $\psi(t')$ at some initial time, we can get $\psi(t)$ at a later time $(t > t')$:

$$\psi(t) = U_S \psi(t') \quad \text{(schematic)} \tag{20.3.12}$$

Now note that although we use U_S to propagate ψ forward in time, it can also propagate it backward, since $U_S \neq 0$ for $t < t'$. To avoid this possibility explicitly, let us work with

$$G_S(\mathbf{r}t, \mathbf{r}'t') = \theta(t-t') U_S(\mathbf{r}t, \mathbf{r}'t') \tag{20.3.13}$$

which simply cannot propagate ψ backward. The equation satisfied by G_S is

$$\begin{aligned}\left(i\frac{\partial}{\partial t} - H\right) G_S &= \left[i\frac{\partial}{\partial t}\theta(t-t')\right] \sum_n \psi_n(\mathbf{r})\, \psi_n^*(\mathbf{r}')\, e^{-iE_n(t-t')} \\ &= i\delta(t-t')\delta^3(\mathbf{r}-\mathbf{r}') \\ &= i\delta^4(x-x') \qquad [x = (t, \mathbf{r})]\end{aligned} \tag{20.3.14}$$

[We have used the completeness of the eigenfunctions, and $\dot{\theta}(t-t')=\delta(t-t')$.]

The propagator in Dirac theory, G_D, obeys a similar equation. Consider the *free-particle case*. Here

$$\left(i\frac{\partial}{\partial t}-H^0\right)G_D^0=i\delta^4(x-x') \tag{20.3.15}$$

with H^0 the free-particle Dirac Hamiltonian. The solution is

$$G_D^0(x,x')=\theta(t-t')\left(\sum_{n+}+\sum_{n-}\right) \tag{20.3.16}$$

where $\sum_{n\pm}$ denote sums over *positive- and negative*-energy eigenfunctions, respectively. [If we throw away $\sum_{n-}$ we lose completeness and won't get $i\delta^4$ on the right-hand side of Eq. (20.3.15).] Although G_D^0 satisfies the requisite equation, it has the negative-energy solutions propagating forward in time. Now here is the trick. G_D^0 is not a unique solution to Eq. (20.3.15); we can add or subtract any solution to the free-Dirac equation, provided we subtract it for all times. (If we subtract it only for $t>0$, say, we are subtracting a θ function times the solution, which doesn't obey the homogeneous equation.) Let us subtract all negative-energy solutions for all times. This gives us *Feynman's propagator*

$$G_F^0(x,x')=\theta(t-t')\sum_{n+}-\theta(t'-t)\sum_{n-} \tag{20.3.17}$$

Consider now some initial state $\psi_i(t')$ which is composed of just positive-energy solutions. G_F^0 will propagate it forward in time, since $\psi_i(t')$ is orthogonal to every term in $\sum_{n-}$. Thus $G_F^0\psi_i(t')=\psi_f(t)$ contains only positive-energy components and keeps moving forward. On the other hand if $\psi_i(t')$ is built out of negative-energy components only, it is orthogonal to every term in $\sum_{n+}$ and gets propagated backwards from t' to t. We will see it as a positron propagating from t to t'.

Consider now the electron in some external potential V. The exact propagation of the electron can be described by a perturbation series based on G_F^0; and in schematic form,

$$\psi_f(t)=G_F^0(t,t')\psi_i(t')+\sum_{t''}G_F^0(t,t'')V(t'')G_F^0(t'',t')\psi_i(t')+\cdots$$

We can represent these multiple scattering events by diagrams very much like the ones in Section 18.3. There is just one difference. Consider a second-order process. There is of course the usual double scattering in which the electron just gets scattered forward in time (Fig. 20.2b). But now there is also the possibility that the potential scatters it backward in time at 1 and then forward at 2 (Fig. 20.2c). As we move forward in time, we first see the electron, then an e^+e^- pair created at 2, then the annihilation of the e^+ with the original e^- at 1 and finally the arrival of the created e^- at f. Since the electron can wiggle and jiggle any number of times (as we go to higher orders in the expansion) the intermediate stages can contain any number of

e^+e^- pairs. This is how the degrees of freedom proliferate in a relativistic theory. Even though we started with a one-particle equation, particle production creeps in through the negative-energy solutions—either because the latter imply an infinite sea of sleeping particles which can be awakened or because they allow a single electron to go back and forth in time, thereby becoming many particles at a given time. Although particle production (at least pair production) can be handled in the present formulation, it is time to learn quantum field theory, which provides a natural framework for handling the creation and destruction of particles. We have already seen one example, namely, the quantized electromagnetic field, whose quanta, the photons, can be created and destroyed by operators $a^\dagger$ and a. We need a theory in which particles like electrons and positrons can also be created and destroyed. You are ready for that subject.‡

‡ See for example J. D. Bjorken and S. D. Drell, *Relativistic Quantum Mechanics* and *Relativistic Quantum Fields*, McGraw-Hill, New York (1964), or C. Itzykson and J. B. Zuber, *Quantum Field Theory*, McGraw-Hill, New York (1980).