INTRODUCTION TO RELATIVISTIC QUANTUM MECHANICS AND THE DIRAC EQUATION

JACOB E. SONE

Abstract. The development of quantum mechanics is presented from a historical perspective. The principles of special relativity are reviewed. Relativistic quantum mechanics is developed, including the Klein-Gordon equation and up to the Dirac equation.

1. Introduction

Near the end of the 19th century, physicists were confident in their view of the world. Newton's mechanics had explained the dynamics of everything from the heavenly bodies down to rubber balls. Maxwell's equations of electromagnetism had successfully unified the seemingly different phenomena of electricity, magnetism, and light. Although there remained some unresolved questions, most physicists were confident that these would soon be solved, within the well-understood framework of the time. They were wrong.

In the early twentieth century, the development of two new theories drastically altered the way that physicists view the universe and everything in it. Quantum mechanics and relativity theory changed the fundamental framework of all future physical theories, putting the lie to previous notions of absolute velocity or length, and precise knowledge of momentum or position.

Supported by countless experiments, and verified under widely ranging conditions, special relativity (SR) and quantum mechanics (QM) have proven very useful theories for predicting physical phenomena. Unfortunately, as it was first understood, quantum mechanics was incompatible with special relativity. In this paper I intend to summarize the development of non-relativistic QM, review the relevant features of SR, and document two attempts to consolidate QM to the framework of SR.

I assume the reader is comfortable with non-relativistic QM, and has been exposed to the basics of SR. I hope the reader will come away with a basic understanding of the development of relativistic quantum mechanics, up to and including the Dirac equation. In order to maintain the flow of the narrative, I have relegated the proofs of certain results to Appendix A.

Throughout this article I will employ the Einstein summation convention, whereby repeated indices in a term are summed over all their values. Greek letters (e.g. μ, ν) are summed over $\mu = 0, 1, 2, 3$, and Latin letters (e.g. i, j, k) are summed over $i = 1, 2, 3$.

Date: April 12, 2002.

2. Non-Relativistic Quantum Mechanics

In 1900, constrained by a classical framework, physicists had been unable to explain the observed blackbody spectrum. Max Planck recognized that he could do away with the problem by assuming that atoms emit radiation only in discrete packets with specific energies. If the energy E of each packet was related to the angular frequency of the radiation ω by

$$E = \hbar\omega \tag{1}$$

then the observed spectrum could be explained. Equation (1) is known as Planck's relation, and $h = 2\pi\hbar$ is Planck's constant, $h \approx 6.626 \times 10^{-34} J \cdot s$.

In 1905, Albert Einstein used Planck's ideas to explain the puzzling photoelectric effect, when he made the further assumption that *all* electromagnetic radiation comes in packets (or "photons"), obeying the Planck relation (1). In the same year, Einstein would revolutionize physical thinking about time and space with his special theory of relativity, to be discussed later.

In 1923, Louis de Broglie proposed that a material particle should have some sort of wave associated with it. Using (1) in the context of special relativity, he derived his relation

$$\vec{p} = \hbar\vec{k}, \tag{2}$$

where $\vec{p}$ is the momentum of the particle and $\vec{k}$ is the wave vector of the associated wave. The dual particle-wave nature of light and matter were slowly becoming clear: Planck associated particle-like properties to light waves, and de Broglie associated wave-like properties to matter.

Erwin Schrödinger discovered the differential equation governing de Broglie's "matter waves", and laid down the framework for the extremely successful theory of quantum mechanics. Schrödinger postulated that the state of a particle of mass m ought to be described by a complex-valued function $\psi(t, \vec{x})$, varying in time and space.

Following de Broglie, Schrödinger considered a plane wave function,

$$\psi(\vec{x}, t) = e^{-i(\omega t - \vec{k}\cdot\vec{x})}. \tag{3}$$

He noted that, differentiating with respect to time,

$$\frac{\partial\psi}{\partial t} = -i\omega e^{-i(\omega t - \vec{k}\cdot\vec{x})}.$$

Upon multiplying both sides by $i\hbar$ and applying Planck's relation (1),

$$i\hbar\frac{\partial\psi}{\partial t} = \hbar\omega\psi = E\psi.$$

This motivated Schrödinger to consider the energy operator on wave functions,

$$E_{op} = i\hbar\frac{\partial}{\partial t} \tag{4}$$

whose value on a plane wave is the energy of the photon, as given by Planck.

Similarly, taking the gradient of both sides of (3), multiplying both sides by $-i\hbar$, and using the de Broglie relation (2), we have

$$-i\hbar\nabla\psi = \hbar\vec{k}\psi = \vec{p}\psi,$$

which leads us to define the momentum operator

$$\vec{P}_{op} = -i\hbar\nabla, \tag{5}$$

whose value on a plane wave is its momentum, as given by de Broglie.

The classical energy of an unconstrained particle of mass m is

$$E = \frac{|\vec{p}|^2}{2m}. \tag{6}$$

Schrödinger replaced the classical energy E and momentum $\vec{p}$ in (6) by the wave operators introduced above in (4) and (5), to obtain

$$E_{op} = \frac{\left|\vec{P}_{op}\right|^2}{2m}. \tag{7}$$

If we substitute the definitions of the wave operators, and apply both sides to the matter wave function ψ, we obtain

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

This is the *free particle Schrödinger equation*, and it is the basis of non-relativistic quantum mechanics. Its solutions $\psi(\vec{x}, t)$ describe the states of matter.

A plethora of experiments in many diverse contexts have validated (SE), and much of modern technology is based on the quantum mechanical theory of which it is the basis. However, as we will later see, Schrödinger's formulation of QM is inconsistent with Einstein's special relativity, and we must seek a relativistically covariant equation to reconcile the problem.

3. Special Relativity

In 1905, Albert Einstein proposed the theory of special relativity (SR), revolutionizing the field of physics. Motivated by the observation of Michelson and Morley in 1887 that the speed of light in vacuum c is independent of any motion of an observer, Einstein postulated the following axiom:

Axiom 1. *(Relativity Principle) All inertial observers observe the same laws of physics. In particular, all inertial observers observe the same speed of light c, with* $c \approx 3.00 \times 10^8 m/s$.

Minkowski reformulated Einstein's ideas in a geometric way, and this is the approach that I will follow.

The set of all events is called *spacetime*, and is denoted M. In special relativity, we assume that M has the manifold structure of $\mathbb{R}^4$. We further assume that there exists a class of preferred observers in spacetime, called *inertial observers*, and that inertial observers can label each event $x \in M$ by cartesian coordinates: $x = (x^0, x^1, x^2, x^3)$, with the "time" component of x being $t = x^0/c$, and the "position" is $\vec{x} = (x^1, x^2, x^3)$. Such a labelling of spacetime is called an *inertial coordinate system.* The coordinate systems of different observers are related by the elements of the 10-parameter Poincaré group, consisting of the Lorentz transformations and the translations.

We define the *metric of spacetime* η, a 2-form, by

$$\eta_{ab} = \eta_{\mu\nu}(dx^\mu)_a(dx^\nu)_b, \tag{8}$$

where $\eta_{\mu\nu} = diag(1, -1, -1, -1)$, and $\{x^\mu\}$ is any inertial coordinate system. It is a consequence of Axiom 1 that η is a tensor, i.e. is independent of the choice of coordinates. If we write out the action of η on two vectors $x^a, y^b \in M$, we have

$$\eta(x, y) = \eta_{ab}x^a y^b = x^0y^0 - x^1y^1 - x^2y^2 - x^3y^3 = x^0y^0 - \vec{x} \cdot \vec{y}.$$

We can view particles in spacetime as tracing out a curve in M as time varies. Special relativity asserts that the paths of material particles are *timelike* curves, that is

$$\eta_{ab}T^aT^b > 0, \tag{9}$$

where T^a is the tangent vector to the curve. We can parametrize timelike curves by the *proper time* τ, defined so that $\eta_{ab}T^aT^b = c^2$ everywhere along the curve. τ measures the time elapsed on a clock carried along the given curve in M.

The *4-velocity* of a timelike curve, denoted U^a, is the tangent vector to the curve when it is parametrized by proper time. In particular,

$$\eta_{ab}U^aU^b = c^2. \tag{10}$$

Material particles have an invariant quantity called the *rest mass*, m, which is the mass of the particle as measured by an observer at rest with respect to the particle.

The *4-momentum* of a particle with mass m is defined as

$$p^a = mU^a, \tag{11}$$

a relativistically covariant vector. Direct substitution and (10) yields the following relation:

$$\eta(p, p) = \eta_{ab}p^ap^b = \eta_{ab}(mU^a)(mU^b) = m^2(\eta_{ab}U^aU^b) = m^2c^2. \tag{12}$$

The energy of a particle in special relativity depends on the motion of the observer who measures the energy. If a particle with 4-momentum p^a is measured by an observer with 4-velocity V^a, the *energy* of the particle is defined as

$$E = \eta(p, V) = \eta_{ab}p^aV^b. \tag{13}$$

For a 'static' observer with 4-velocity $V = (c, 0, 0, 0)$, the energy is $E = \eta(V, p) = cp^0$. Now, (12) gives

$$\eta(p, p) = (p^0)^2 - |\vec{p}|^2 = m^2c^2.$$

Isolating cp^0, we obtain

$$E = cp^0 = c(|\vec{p}|^2 + m^2c^2)^{1/2}, \tag{14}$$

the important equation relating relativistic momentum and energy.

4. The Klein-Gordon Equation

Now that we have some understanding of the principles of special relativity, it is clear that the Schrödinger equation (SE) is not suitable for the new relativistic context. Indeed, it is manifest that (SE) is not relativistically covariant; the derivative in the time coordinate is first order, while the derivatives with respect to the spacial coordinates are all second order. In relativity, there can be no distinction between time and space coordinates, because these are mixed together by Lorentz transformations. It is not difficult to show that (SE) is not fixed by a general

Lorentz transformation, so a theory based upon it will certainly violate Axiom 1 of special relativity.

Erwin Schrödinger was certainly aware of this difficulty, but he found it useful to work with the non-relativistic equation (SE) that he discovered, which is valid for particles with small velocities, relative to c.

The first successful attempt to find a relativistic wave equation that could describe the quantum mechanical states of matter was published by Klein and Gordon. To derive his equation, Schrödinger had started with the non-relativistic equation for kinetic energy, $E = |\vec{p}|^2/2m$, and changed the physical quantities E, $\vec{p}$ to wave function operators. Klein and Gordon followed a similar procedure, but they used as a starting point the relativistic relation between energy and momentum (14). Upon squaring, and making the substitutions motivated earlier, (4) and (5), we get

$$-\hbar^2 \frac{\partial^2}{\partial t^2} = c^2(m^2c^2 + \hbar^2\nabla^2),$$

or

$$\boxed{\text{(KGE)} \qquad \hbar^2\left(\frac{1}{c^2}\frac{\partial^2\psi}{\partial t^2} - \nabla^2\psi\right) + m^2c^2\psi = 0}$$

which is the *Klein-Gordon equation.* If we rewrite (KGE) with $x^0 = ct$, we have

$$\partial_a\partial_b\eta^{ab} = -\frac{m^2c^2}{\hbar^2},$$

where I have written $\partial_a = \partial/\partial x^a$. When the equation is written in this form, it is clear that (KGE) is relativistically covariant, as both sides are clearly (scalar) tensors on M.

The Klein-Gordon equation was the first relativistic quantum mechanical wave equation, and it had some degree of success. It is immediate that if the mass m vanishes, as in the case of a photon, (KGE) reduces to the standard electromagnetic wave equation

$$\frac{1}{c^2}\frac{\partial^2\psi}{\partial t^2} - \nabla^2\psi = 0, \tag{15}$$

which is usually derived from Maxwell's equations. Further, Yukawa managed to use (KGE) to predict the form of the strong nuclear force that holds nuclei together.

Although the Klein-Gordon equation was appealing because it fit into the SR framework and did have some predictive power, physicists were not satisfied with it. While the Schrödinger equation (SE) is first order in time and so the solution is specified by the initial condition $\psi_0(\vec{x}) = \psi(\vec{x}, t_0)$, (KGE) is second order in time, and so solutions are *not* uniquely specified by a single initial condition; we need both ψ_0 and $(\partial\psi/\partial t)_0$ to determine a solution for all time.

This suggests that (KGE) may not be fundamental, but perhaps a consequence of some first order equation. This would parallel the case in electrodynamics, where the EM wave equation (15), a second order system, is a consequence of the first order Maxwell's equations, which are the fundamental equations.

5. The Dirac Equation

With the goal of discovering a relativistically covariant first order differential equation governing the matter wave, we seek a linear constraint on the momentum of the particle, of the form $\gamma(p) = \mu I$, where I is an identity operator of some dimension. In addition, we have the quadratic constraint (12), $\eta(p,p) = m^2c^2$. We can rescale γ so that $\mu = mc$, and then we have $\gamma(p)^2 = m^2c^2 I = \eta(p,p)I$. So, to be consistent we need

$$\gamma(p)^2 = \eta(p,p)I. \tag{16}$$

The simplest solution for $\gamma(p)$ in (16) lies in the 4×4 matrices, but to write the solution down in a concise form we must first consider another important set of matrices. The *Pauli spin matrices* are 2×2 matrices that arise in considerations of angular momentum in QM. They are:

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{17}$$

Notice that

$$\sigma_j p^j = \sigma_1 p^1 + \sigma_2 p^2 + \sigma_3 p^3 = \begin{pmatrix} p_3 & p_1 - ip_2 \\ p_1 + ip_2 & -p_3 \end{pmatrix}. \tag{18}$$

From this point forward, all matrices appear in 2×2 *block form*, i.e. each entry in a matrix is considered to be multiplied by $I_{2\times 2}$, to form a 2×2 block. Now we are ready to present the solution to (16).

Theorem 1. *In 2×2 block form, the matrices*

$$\gamma(p) = \begin{pmatrix} p^0 & -\sigma_j p^j \\ \sigma_j p^j & -p^0 \end{pmatrix}$$

satisfy the equation $\gamma(p)^2 = \eta(p,p)$ for all $p \in M$.

Proof. First, a direct calculation using (18) shows that $(\sigma_j p^j)^2 = |\vec{p}|^2 I_{2\times 2}$. Now,

$$\begin{aligned}
\gamma(p)^2 &= \begin{pmatrix} p^0 & -\sigma_j p^j \\ \sigma_j p^j & -p^0 \end{pmatrix} \begin{pmatrix} p^0 & -\sigma_j p^j \\ \sigma_j p^j & -p^0 \end{pmatrix} \\
&= \begin{pmatrix} (p^0)^2 - (\sigma_j p^j)^2 & 0 \\ 0 & (p^0)^2 - (\sigma_j p^j)^2 \end{pmatrix} \\
&= \begin{pmatrix} (p^0)^2 - |\vec{p}|^2 & 0 \\ 0 & (p^0)^2 - |\vec{p}|^2 \end{pmatrix} \\
&= \eta(p,p) \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \\
&= \eta(p,p) I_{2\times 2}
\end{aligned}$$

□

The matrices $\gamma(p)$ are called the *Dirac matrices*. These solutions to (16) are essentially unique, as any operators $\gamma(p)$ depending linearly on $p \in M$ and satisfying (16) are direct sums of operators equivalent to the Dirac matrices [1, page 295].

Being 4×4 matrices, the Dirac matrices act on column vectors of four complex numbers. The space of such column vectors is called the space of *Dirac spinors*.

We can gain further insight into the Dirac matrices by working in a chosen inertial reference frame. If $\{e_\mu\}$ is an orthonormal basis for M, then $\eta(e_\mu, e_\nu) = \eta_{\mu\nu}$. We write $\gamma_\mu = \gamma(e_\mu)$, so that $\gamma(p) = \gamma_\mu p^\mu$. With $\gamma(p)$ the Dirac matrices, direct substitutions for $\mu = 0, 1, 2, 3$ show

$$\gamma_0 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \qquad \gamma_j = \begin{pmatrix} 0 & -\sigma_j \\ \sigma_j & 0 \end{pmatrix}.$$

If we raise the indices on the γ_μ, we have $\gamma^0 = \eta^{\mu 0}\gamma_\mu = \gamma_0$, but $\gamma^j = -\gamma_j$.

So we have identified the essentially unique linear operators satisfying (16): the Dirac matrices. The constraint equation we have been seeking is thus expressed by $\gamma(p) = mcI$, or $\gamma_\mu p^\mu = mcI$ in coordinates. If we again use the operator forms (4) and (5) for the energy and momentum, together with (14), we obtain

$$\gamma_\mu p^\mu = \gamma^0 E - \gamma^j p_j \quad \rightarrow \quad \gamma^0 E_{op} - \vec{\gamma} \cdot \vec{P}_{op} = i\hbar\gamma^\mu \partial_\mu,$$

leading to the differential equation for the Dirac spinor-valued wave function ψ,

$$\boxed{\text{(DE)} \qquad i\hbar\gamma^\mu \partial_\mu \psi = mc\psi}$$

which is the *free Dirac equation.*

It is not difficult to show that the free Dirac equation is relativistically covariant. Moreover, it is clear that (DE) is first order in time, and so solutions $\psi(\vec{x}, t)$ are specified by a single initial condition $\psi_0(\vec{x})$, as desired. The free Dirac equation is the realization of our goal to bring quantum mechanics into the special relativity framework. Indeed, physicists currently believe that the free Dirac equation is the correct equation to describe elementary particles with spin $\frac{1}{2}$, such as the electron, the muon, and the tau particle.

Before concluding, I will give a brief sketch of one of the implications of the free Dirac equation (DE). Given the block form of the γ matrices, and hence of the Dirac equation, it appears useful to split each Dirac spinor into a pair of two-component vectors

$$\psi(x) = \begin{pmatrix} \psi_+ \\ \psi_- \end{pmatrix}.$$

We can interpret the two functions ψ_+ and ψ_- as representing electron-like solutions with positive and negative energies, respectively.

The presence of negative energy solutions was a great worry to Dirac, and he felt that it was a "great blemish" on his theory. However, not long after Dirac published his equation, Carl Anderson experimentally discovered a positively charged particle, identical to the electron except for conjugation of charge. This particle, called the *positron*, is the antiparticle to the electron, and it is thought that each elementary particle has an antiparticle. That Dirac's equation predicted the existence of the positron before its experimental discovery is quite remarkable, and is a triumph for the theory.

6. Concluding Remarks

The development of the theories of quantum mechanics and special relativity profoundly altered the basic way that we view the universe and the objects in it. These theories extend the knowledge of physics into the realm of the very small and the very fast, and so they are surely among the greatest achievements that humankind has accomplished in our history.

Appendix A. Proof of the de Broglie relation

Theorem 2. *(de Broglie law) If the Planck relation $E = \hbar\omega$ is true for one observer observing a plane wave, then the de Broglie relation*

$$\vec{p} = \hbar\vec{k}$$

holds.

Proof. Consider a plane wave, $\psi(t, \vec{x}) = exp[-i(\omega t - \vec{k} \cdot \vec{x})]$. We introduce the *frequency 4-vector* $\kappa = (\omega, c\vec{k})$. Then we can write the plane wave in relativistic form, $\psi(x) = exp\,(-i[\eta(\kappa, x)/c])$. It is now clear that the Planck and de Broglie relations are the temporal and spacial components of the equation $cp = \hbar\kappa$. If the Planck relation holds for one observer, i.e. $\eta(V, p) = \hbar\eta(V, \kappa)/c$, then the corresponding identity must be true for all inertial observers. That is, for any 4-velocity W, $\eta(W, p) = \hbar\eta(W, \kappa)/c$, which implies $\eta(W, cp - \hbar\kappa) = 0$, for any W. This implies that $cp - \hbar\kappa = 0$, the spacial component of which is de Broglie's law. $\square$

References

[1] Hannabuss, Kieth. *An Introduction to Quantum Theory*, New York: Oxford University Press, 1997.

[2] Kellogg, Brian C. *An Introduction to Relativistic Electronic Structure Theory in Quantum Chemistry*, http://www.adi.uam.es/Docs/Knowledge/Fundamental_Theory/rltvt/rltvt.html, 1996. Viewed March 2002

[3] Schutz, Bernard F. *A first course in general relativity*, Cambridge: Cambridge University Press, 1985.

[4] Wald, Robert M. *General Relativity*, Chicago: University of Chicago Press, 1984.