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Relativistic Wave Equations: Dirac

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Relativistic Wave Equations

Reference

L. I. Schiff, *Quantum mechanics* (McGraw-Hill, 1968), Chapter 13 (Chem QC174.1 S34 1955).

Classical Mechanics

The special ("restricted") theory of relativity starts by defining *Galilean frames* (to follow Einstein's nomenclature). These are coordinate systems in which a particle initially at rest remains at rest. If a frame is Galilean, any other frame that is moving at a constant velocity $\boldsymbol{V}$ relative to it will also be Galilean. Newtonian dynamics was built under the assumption that there would be a *universal* time t. That is, if $\boldsymbol{r}, t$ characterized an *event* in one Galilean frame and $\boldsymbol{r}', t'$ characterized the same event in another Galilean frame, then $t' = t$ for all events. If the origins of the coordinate systems coincide at $t = 0$, then $\boldsymbol{r}' = \boldsymbol{r} + \boldsymbol{V}t$ for all events.

Einstein postulated that the speed of light c is the same for all Galilean observers. This is inconsistent with there being a universal time, with the transformation rule $\boldsymbol{r}' = \boldsymbol{r} + \boldsymbol{V}t$ relating two different frames. The correct transformation rule can be constructed by defining the *interval between two events* as

$$\Delta s = s_2 - s_1 = \sqrt{c^2(t_2 - t_1)^2 - (x_2 - x_1)^2 - (y_2 - y_1)^2 - (z_2 - z_1)^2}$$

$\Delta s = 0$ if light travels from $\boldsymbol{r}_1, t_1$ to $\boldsymbol{r}_2, t_2$, no matter which Galilean frame is used to make the observation. For small Δs, $\Delta s'$ will also be small. Since $\Delta s = 0 \Rightarrow \Delta s' = 0$, expanding $\Delta s'$ in Δs gives

$$\Delta s' = \text{constant} * \Delta s + \text{higher order terms}$$

We can make the higher order terms negligible by taking $\Delta s \to 0$. Since the labeling of the primed and unprimed frames could be reversed, the "constant" can only be ± 1. We may define a "handedness" which makes this always $+1$. Knowing the result for small Δs enables us to obtain the result for large Δs by integration. Thus the line integral over s connecting two *events* is the same, no matter what frame is used. In symbols,

$$\int ds = \int ds'$$

We can construct a (Euclidean) geometrical view of this by replacing the time coordinate t by $\tau = i\,c\,t$, with $i = \sqrt{-1}$.
The *interval* then becomes

$$-(\Delta s)^2 = (\tau_2 - \tau_1)^2 + (x_2 - x_1)^2 + (y_2 - y_1)^2 + (z_2 - z_1)^2,$$

with the right hand side just the square of the distance between two points (events) in the four dimensional x, y, z, τ space. The transformation rule, that the distance between two events appears the same to all Galilean observers, means that the transformation between two different frames can only look like a rotation in the four dimensional r, τ space.

As an example, consider a rotation in the x, τ plane,

$$\begin{aligned}\Delta x' =& \Delta x \cos\theta + \Delta\tau \sin\theta \\ \Delta\tau' =& -\Delta x \sin\theta + \Delta\tau \cos\theta\end{aligned} \tag{1}$$

If a particle is stationary in the r', τ' coordinate system, $\Delta x' = 0$ whence

$$\frac{\Delta x}{\Delta\tau} = -\tan\theta \qquad \text{or} \qquad \frac{\Delta x}{\Delta t} = -i\,c\,\tan\theta$$

That is, the primed frame is moving with respect to the unprimed frame with a speed

$$V = -i\,c\,\tan\theta \tag{2}$$

in the x-direction. Using (2) to replace θ in (1) with V gives

$$\begin{aligned}\Delta x' =& \frac{\Delta x - V\Delta t}{\sqrt{1 - \frac{V^2}{c^2}}} \\ \Delta t' =& \frac{-\frac{V}{c^2}\Delta x + \Delta t}{\sqrt{1 - \frac{V^2}{c^2}}}\end{aligned} \tag{3}$$

This is an example of a *Lorentz transformation*.

If *events* are described by $\boldsymbol{r}, t$ or $\boldsymbol{r}, \tau$ – that is, by a *four vector* – the corresponding momentum in Hamiltonian mechanics must also be a four vector. The corresponding components are

$$\boldsymbol{r} \to \boldsymbol{p}$$
$$\tau \to \frac{iE}{c}$$

That is, the energy E of the particle is just the fourth component of the momentum four vector. The Hamiltonian for the system is

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

Quantum Mechanics

The function

$$f(\boldsymbol{r}, t) = A\cos[\boldsymbol{k} \cdot \boldsymbol{r} - \omega t]$$

describes a plane wave that (i) propagates in the direction of the *wave vector* $\boldsymbol{k}$, (ii) has frequency $\omega/2\pi$, (iii) has wavelength $2\pi/k$, (iv) and moves with the speed $c = \omega/k$. The argument of the cosine function can be written as the dot product of two four vectors,

$$\boldsymbol{k} \cdot \boldsymbol{r} - \omega t = xk_x + yk_y + zk_z + (ict)(i\omega/c)$$

The relativistic interpretation is thus that $\boldsymbol{k}, i\omega/c$ must be a four vector.

DeBroglie's argument was that Planck's rule $E = h\nu$ just says that the fourth component of the momentum vector is $\hbar$ times the fourth component of the wave vector. Applying the same rule to the first three components gives $\boldsymbol{p} = \hbar\boldsymbol{k}$ (or $\lambda = h/p$ in one-dimension). DeBroglie suggested that the "quantization" of the Bohr orbits in the hydrogen atom could be explained by the rule that only orbits with circumference = some multiple of λ would be possible – as if some "wave interference" prevented other motions. Implicit, then was the picture of some wave. Further, the operator rules for such a wave were clear,

$$\begin{aligned} E &\to i\hbar\frac{\partial}{\partial t} \\ \boldsymbol{p} &\to -i\hbar\nabla \end{aligned} \tag{5}$$

E. Schrödinger (1926)

The square root in (4) is awkward, so Schrödinger applied the rules (5) to the square of (4),

$$H^2 = c^2\boldsymbol{p}^2 + m^2c^4$$

getting

$$-\hbar^2\frac{\partial^2\Psi}{\partial t^2} = -\hbar^2 c^2\nabla^2\Psi + m^2c^4\Psi,$$

an equation usually referred to as the *Klein-Gordon equation*. If

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

then

$$\left(E^2 - m^2c^4\right)\psi(\boldsymbol{r}) = -\hbar^2c^2\nabla^2\psi(\boldsymbol{r}) \tag{6}$$

The addition of a potential energy is not trivial, for the invariance under Lorentz transformations must be maintained, but Schrödinger was able to solve the extension of (6) that describes the motion of an electron in the electromagnetic field of a proton. The energy eigenvalues are close to those predicted by the Bohr theory, but the differences were large enough to conclude that this dynamical equation did not describe the electron in the hydrogen atom.

The errors are of the order of typical relativistic corrections to non-relativistic mechanics, however, so Schrödinger backed up and examined the non-relativistic description associated with

$$H = \frac{\boldsymbol{p}^2}{2m} + V(\boldsymbol{r})$$

and found that the energy levels of the hydrogen atom were precisely those predicted by the Bohr theory.

How is the Klein-Gordon equation viewed today? First, if one prescribes a wave vector $\boldsymbol{k}$, it turns out that both positive and negative energy states can be constructed since

$$E = \pm c\sqrt{\hbar^2\boldsymbol{k}^2 + m^2c^2}$$

A particle with a high momentum could have a very low energy! Second, it turns out that (and this is related to the problem of negative energies or the fact that the equation is *second order* in time) it is not possible to construct a "density" function that both satisfies conservation of probability and is non-negative. Third, the construction of the equation presumed from the outset that the particle was *structureless*. So a particle like the electron that has a spin-1/2 could not be naturally described with a soltution to this equation. In fact the equation is considered correct, but with these two changes in interpretation: (i) it can only describe a spin-0 particles such as π or $\boldsymbol{K}$ mesons; (ii) Ψ cannot be interpreted as a probability density. Rather it is a *quantum field*, an operator that varies with $\boldsymbol{r}, t$. While the Klein-Gordon equation describes the time evolution of this field operator, there are other constraints associated with *commutation* rules on the field. This added complexity is required to allow the processes that actually occur at relativistic energies, the creation and destruction of mesons.

P. A. M. Dirac (1928)

While the square root in (4) is awkward, it is not impossible. Dirac proposed writing (4) as

$$H = c\sqrt{p^2 + m^2c^2} = c\boldsymbol{\alpha}\cdot\boldsymbol{p} + \beta mc^2 \tag{7}$$

with $\boldsymbol{\alpha} = \{\alpha_x, \alpha_y, \alpha_z\}$ and β quantities that would make H^2 calculated from (4) and (7) agree. Eq(7), with the identifications in (5), leads to an equation of motion for a state function Ψ of an electron moving in free space,

$$i\hbar\frac{\partial}{\partial ct}\Psi = \left[\frac{\hbar}{i}\left(\alpha_x\frac{\partial}{\partial x} + \alpha_y\frac{\partial}{\partial y} + \alpha_z\frac{\partial}{\partial z}\right) + \beta\right]\Psi \tag{8}$$

The squares of (4) and (7) will agree if

$$\begin{aligned} \alpha_r^2 &= 1, & \alpha_r\alpha_s + \alpha_s\alpha_r &= 0 \quad (r \neq s) \\ \beta^2 &= m^2c^2, & \alpha_r\beta + \beta\alpha_r &= 0 \end{aligned}$$

for $r, s = 1, 2, 3$. While there are no *numbers* that satisfy these constraints, Dirac identified 4×4 *matrices* that do. This means, of course, that the wave function itself must be a four component vector,

$$\Psi = \begin{bmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{bmatrix}$$

To simplify the set of constraints, Dirac set $\beta = mc\alpha_0$. The set of constraints then becomes

$$\alpha_r\alpha_s + \alpha_s\alpha_r = 2\delta_{rs}, \qquad r, s = 0, 1, \ldots, 3$$

When the spectroscopists suggested that the electron had an intrinsic angular momentum corresponding to $\ell = 1/2$, Pauli introduced four matrices to characterize this spin in atomic Hamiltonians. If $\boldsymbol{L} = \hbar\{\sigma_x, \sigma_y, \sigma_z\}/2$,

$$\sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \sigma_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \quad \sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}, \quad \mathbb{1} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

Since these satisfy the relations

$$\sigma_r \sigma_s + \sigma_s \sigma_r = 2\delta_{rs}, \quad r, s = 1, 2, 3$$

they provide a model for the α_i. Explicitly, describing the 4×4 matrices in terms of 2×2 arrays of 2×2 matrices, the matrices

$$\alpha_x = \begin{bmatrix} 0 & \sigma_x \\ \sigma_x & 0 \end{bmatrix}, \quad \alpha_y = \begin{bmatrix} 0 & \sigma_y \\ \sigma_y & 0 \end{bmatrix}, \quad \alpha_z = \begin{bmatrix} 0 & \sigma_z \\ \sigma_z & 0 \end{bmatrix}, \quad \alpha_0 = \begin{bmatrix} \mathbb{1} & 0 \\ 0 & -\mathbb{1} \end{bmatrix}$$

satisfy the required anti-commutation behavior.

The four components of Ψ are now interpreted as corresponding to an electron with spin-up, an electron with spin-down (the two states with $E > 0$), a positron with spin-up and an positron with spin-down (the two states with $E < 0$).

The natural emergence of the intrinsic spin was a fantastic success, but the difficulties of constructing a probabilistic interpretation from the theory remained and it was not clear why an electron in a positive energy state wouldn't turn into a positron in a negative energy state. That is, the basic difficulties of the Klein-Gordon equation remained. The modern interpretation is that Dirac's dynamical equation describes the time evolution of quantum fields associated with spin-1/2 particles. The associated commutation constraints are different from those associated with the Klein-Gordon equation, but one can successfully describe the creation and destruction of electron-positron pairs.

Chemists' have been quite successful thinking about wave functions in terms of a probability interpretation, $|\Psi(r,t)|^2 \sim$ the probability density of finding an electron at r, t. While discussing relativistic wave equations is interesting from an historical perspective, a much more elaborate structure is required to explain modern "relativistic" quantum theories. Advanced courses spend weeks introducing this structure before any practical problem is encountered. Quantum field theory represents one more layer of *constructionist* thinking and the conceptual shift from wave mechanics $\rightarrow$ quantum field theory is the same order as that from classical mechanics $\rightarrow$ wave mechanics.