Week 12

PHY 304 Quantum Mechanics-II
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11 (Glimpse at) Relativistic quantum mechanics

Further reading: For this section, refer to Shankar, section 20 (SH), and Sakurai, chapter 8 (SA)

What we have done so far was exclusively non-relativistic quantum mechanics. The formalism shown is incompatible with special relativity in three essential ways: (i) Space and time are clearly treated in a very different way, which they should not since they can transform among each other using the Lorentz transformation. (ii) We used non-relativistic formulae for energy and momentum, these have to be changed into the relativistic version. (iii) We usually dealt with one particle, where we mentioned multiple particles, their number was conserved. However due to $E = mc^2$, we can convert energy into particles and the reverse, hence a relativistic theory must also accommodate changing particle numbers. Ultimately both objectives are fulfilled in the framework of **quantum field theory**, which replaces the concept of particles with the concept of (quantum) fields. As a first step in that direction, we shall show here how one can at least replace the TDSE with a relativistically invariant equation of motion for the electron, called the Dirac equation. This already provides us with two important concepts, **spin** and **anti-matter**.

Note that the *general* theory of relativity has **not yet** been successfully quantized, despite a century of trying (Nobel prices for you).

11.1 The Dirac equation

The simplest attempt to reach an equation of motion that adheres to special-relativity, would be to replace the Hamiltonian for the non-relativistic free particle $\hat{H} = \hat{p}^2/(2m)$ with its relativistic counter-parts:

$$\hat{H} = \sqrt{c^2\hat{p}^2 + m^2c^4}, \tag{11.1}$$

where m is the rest mass of the particle and c the speed of light. But inserting this into the TDSE (and expanding the squareroot into a power series) gives

$$i\hbar \frac{d}{dt}\phi(x,t) = mc^2 \left(1 + \frac{\hat{p}^2}{2m^2c^2} - \frac{\hat{p}^4}{8m^4c^4} + \cdots\right)\phi(x,t), \tag{11.2}$$

which, when converting $\hat{p} \to -i\hbar d/dx$, treats the space and time variables even more differently (first order derivatives in time, infinite order in space) than our non-relativstic TDSE, so it fails in our quest to find a more elegant, obviously Lorentz invariant, theory.

As slightly better approach is to not use the squareroot, and encode $E^2 = c^2\hat{p}^2 + m^2c^4$ into a waveequation (using the same replacements for $E = i\hbar d/dt$ and $\hat{p} \to -i\hbar d/dx$ that you had seen in e.g. PHY106 to motivate the TDSE. This provides us with the

Klein-Gordon equation

$$\left[\frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \boldsymbol{\nabla}^2 + \left(\frac{mc^2}{\hbar}\right)^2\right]\phi(x,t) = 0, \tag{11.3}$$

which is already a relativistic wave equation for a spinless particle

- This is now symmetric in the order of space and time derivatives, and you could proof, if you wanted to, that the equation remains form invariant under a Lorentz transformation.
- An unsatisfactory feature is that it is second order in time, while we know the non-relativistic TDSE is first order in time, such that knowledge of $\phi(x, t = 0)$ dictates the entire future of the wavefunction. We would want to preserve this feature also in relativistic theory.
- Let us take it as an experimental fact that the electron is a spin-1/2 particle and has anti-particles. The equation fails to provide either, so we cannot use it to describe electrons. It can however be used to describe particles that actually have spin $s = 0$, such as some pions.

To try to finally reach a relativistic quantum wave equation that is first order in time, we follow a brute force approach due to Dirac: From (11.1) we would reach our objective of first order equations in time AND space, if the argument of the squareroot could be written as the square of a function that is linear in the momentum. Let us just demand this:

$$\begin{aligned} c^2\hat{\mathbf{p}}^2 + m^2c^4 &= c^2\left(\hat{p}_x^2 + \hat{p}_y^2 + \hat{p}_z^2\right) + m^2c^4 \\ &\overset{!}{=} (c\alpha_x\hat{p}_x + c\alpha_y\hat{p}_y + c\alpha_z\hat{p}_z + \beta mc^2)^2. \end{aligned} \tag{11.4}$$

Here $\boldsymbol{\alpha} = [\alpha_x, \alpha_y, \alpha_z]^T$ and β are "coefficient objects", that we now want to fix by equating the left hand side and right hand side. We obtain the requirement (see Shankar for one more line of math):

$$\begin{aligned} \alpha_k^2 &= \beta^2 = 1, \\ \alpha_i\alpha_j + \alpha_j\alpha_i &= \{\alpha_i, \alpha_j\} = 0, \text{ for } i \neq j \\ \alpha_i\beta + \beta\alpha_i &= \{\alpha_i, \beta\} = 0. \end{aligned} \tag{11.5}$$

The conditions are called Clifford algebra. Clearly the coefficient objects cannot be real or complex numbers. We can however make the above algebraic rules work out, if we choose them as matrices.

Anti-commutator: In (11.5) and the following, the symbol

$$\{\hat{O}_1, \hat{O}_2\} = \hat{O}_1\hat{O}_2 + \hat{O}_2\hat{O}_1, \tag{11.6}$$

is called the anti-commutator of two operators (matrices).

These matrices have to be Hermitian, so that the Hamiltonian is Hermitian. They also must be traceless and have eigenvalues ± 1 (See Shankar for reasons), such that in the end one finds they must be 4×4 matrices. The exact choice is not unique, but usually one takes the

Dirac matrices: as

$$\boldsymbol{\alpha} = \begin{bmatrix} 0 & \boldsymbol{\sigma} \\ \boldsymbol{\sigma} & 0 \end{bmatrix}, \qquad \beta = \begin{bmatrix} \mathbb{1} & 0 \\ 0 & -\mathbb{1} \end{bmatrix}, \tag{11.7}$$

where each panel in the matrix is itself a 2×2 matrix, such that $\boldsymbol{\sigma}$ is the vector of Pauli matrices defined in Eq. (4.112).

Using these matrices we can now write the

Dirac equation for a relativistic spin-1/2 particle as

$$i\hbar \frac{\partial}{\partial t}\phi(x,t) = \left(c\boldsymbol{\alpha} \cdot \hat{\mathbf{p}} + \beta mc^2\right)\phi(x,t), \tag{11.8}$$

where the wavefunction $\phi(x,t)$ must be a four-component vector (composed of spinors, see section 4.7.2), for it to make sense to apply the 4×4 matrices $\boldsymbol{\alpha}$, β onto it.

- Roughly speaking, we got ourselves into a 4 components wavefunction because it turns out the equation describes not only the electron (which would need only two components, being spin-1/2) but also the positron (another spin-1/2 particle).
- By adding to the Dirac equation the interaction with electromagnetic fields as in (10.1), we can now derive all of the terms that give rise to Finestructure that we had used in section 7.3.1, without having to make the handwaving arguments we did there. See e.g section "Hydrogen finestructure" from page 569 in Shankar.
- When looking at the free-particle at rest $\mathbf{p}$ one finds solutions with energy $E = mc^2$ and $E = -mc^2$. The negative energy solutions are of course very irritating. See Shankar and Sakurai for the discussion of the early historical ideas on how to resolve this, Dirac's "electron sea", just filling the negative energy states up with Fermions thus making them inaccessible, and Feynmans "negative energy particles travel backwards in time". All these concepts are now more satisfactorily replaced in QFT (quantum field theory), where we no longer start

with a certain number of electrons or positrons, but instead start with a Lorentz invariant spin-1/2, spinor quantum field, which then contains electrons and positrons as excitations of varying number (see QFT lectures).

- While we show the Dirac equations here mainly as an appetiser for QED/QFT lectures, it has its applications also in e.g. atomic physics, for example when you look at electronic states of massively ionized heavy atoms (i.e. U^{+91}). In these the "outer electron" then sees so strong fields, and thus becomes so fast, that it becomes highly relativistic.