From the photoelectric effect to the Dirac equation

It is strange to start a discussion of the origin of quantum mechanics talking about special relativity, but I think it is just fair. As you know, within special relativity, time and space get mixed. Events are characterized by 4-vectors, (t, x, y, z), which have special transformation rules when you change the reference frame. In the same fashion, energy and momentum behave in the same way: (E, p_x, p_y, p_z).

The real breakthrough in quantum mechanics was the idea put forward by Einstein that energy and frequency of light was related: $E = h\omega$. The motivation for this relation was the photoelectric effect. But ω gives the time periodicity of a wave, right? What is it that gives the space periodicity? The wavenumber k_x, k_y and k_z. Then, following the reasoning of special relativity, we can associate them to momenta, right? $p_x = hk_x$, and so on.

What was good for light, why not for massive particles? This question was put forward by de Broglie, and motivated by the neutron diffraction experiments of Davisson and Germer. We can associate for them also, frequency with energy, wavenumber with momentum.

Schrödinger wanted to find out the wave equation for these matter waves. The standard wave equation

$$\partial_x^2\psi - \frac{1}{c^2}\partial_t^2 = 0\psi$$

worked for light, but it need not work for matter waves... How to find a criterion for it?

First of all, let us consider a plane wave in 1D: $\exp(i(kx - \omega t))$. If you derivate with respect to x, you get an extra ik in front. If you derivate with respect to t, you get $-i\omega$. Right? Then, you can see that the previous wave equation is equivalent to:

$$k^2 - \frac{1}{c^2}\omega^2 = 0$$

Or $E = pc$, the relativistic relation for photons! So far, the idea is promising!

So, Schrödinger thought: the wave equation, as applied to a plane wave, should give us the relation between energy and momentum. For photons, it is $E = pc$. For nonrelativistic massive particles it is $E = p^2/2m$. What happens if I write the equivalent? Remember: derivative with respect to space yields ik, and with respect to time, $-i\omega$. Then, the equation might read

$$-\frac{\hbar^2}{2m}\partial_x^2\psi = i\hbar\partial_t\psi$$

If you put the plane wave inside, you get $p^2/2m = E$! So, it seems to be alright. Here you are, Schrödinger's equation. First success.

((You may wonder about the addition of a potential $V(x)$. You'll find without difficulty that you have to add the $V(x)\psi$ term in order to obtain the relation $E = p^2/2m + V$.))

Schrödinger himself thought, before he came to write his equation, of another one which was relativistically invariant. With this I mean that it followed the relativistic relation between energy and momentum for a massive particle. In units where $c = 1$, $E^2 = p^2 + m^2$. Then, using the same trick, one gets:

$$-\partial_t^2\psi = -\partial_x^2\psi + m^2\psi$$

which is known today as Klein-Gordon equation. As a matter of fact, it seems that Schrödinger himself didn't quite like it, and made some simplifying assumptions which led him to the Schrödinger equation. I am not aware of what he didn't like precisely, but I can tell you the reasons for which the equation is not satisfactory nowadays. First of all, the equation is of second order in time. This means that you need to know both the value of ψ and of $\partial_t\psi$ at some initial time $t = 0$, unlike Schrödinger's equation, where if you know ψ at $t = 0$, you can find it out for any future time. But another thing was strange there: it is impossible to interpret $|\psi|^2$ as a probability, because it is not necessarily conserved. The final reason for it is that, if you hit a potential barrier with a particle at energy which is high enough, there may appear *new* particles! But let's not go too fast!

Dirac thought of a different way to make Schrödinger's equation relativistic. He disliked a lot it being second order: to know the wavefunction now should be enough to know the future! So, he decided to use the alternative relativistic expression for the energy: $E = \sqrt{p^2 + m^2}$. If the equation has to be relativistic, it should have a similar behaviour in the time and space variables, right? So, if the time derivative is first order, so should be the spatial ones! Let's bet for that and try to write down an equation:

$$-i\partial_t \psi = \alpha_x \partial_x \psi + \alpha_y \partial_y \psi + \alpha_z \partial_z \psi + \alpha_0 m \psi$$

Now the problem is to identify α_x, α_y, α_z and α_0 so as the condition $E = \sqrt{p^2 + m^2}$ is fulfilled in a plane wave. The condition, in the end, is equivalent to the old one, $E^2 = p^2 + m^2$, which led to Klein-Gordon equation. Therefore, the right-hand side of the previous equation must be the same as Klein-Gordon's:

$$(\alpha_x \partial_x + \alpha_y \partial_y + \alpha_z \partial_z + \alpha_0 m)^2 \psi = \left(-\hbar^2 \nabla^2 \psi + m^2\right) \psi$$

In other terms, the new "operator" $(\alpha_x \partial_x + \alpha_y \partial_y + \alpha_z \partial_z + \alpha_0 m)$ should be the "square root" of $p^2 + m^2$. If we try to find α_i, developing the square, we get:

$$\alpha^2_{\{x,y,z\}} = -\hbar^2, \qquad \alpha_0^2 = 1$$

this is easy! Just make $\alpha_{\{x,y,z\}} = i\hbar$, $\alpha_0 = 1$. Is that all? No! We have the "crossed" terms, which give

$$\alpha_i \alpha_j + \alpha_j \alpha_i = 0$$

for any pair i and j. How to make it? Impossible for any set of numbers!!

Wait, who said that they *had* to be numbers? What about *matrices*? Then, they could simply *not commute*! This is what Dirac thought. He found the following solution:

$$\alpha_i = i\hbar \begin{bmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{bmatrix}$$

for $i \in \{i, j, k\}$, and

$$\alpha_0 = \begin{bmatrix} I_2 & 0 \\ 0 & -I_2 \end{bmatrix}$$

where σ_i are the Pauli σ-matrices, and I_2 is the 2×2 identity matrix. You can check the identities...

Finally, the Dirac equation reads:

$$\left(\sum_{i=0}^{3} \gamma_i \partial_i + m \right) \psi = 0$$

where the Dirac's γ-matrices are defined as:

$$\gamma_0 = \alpha_0, \qquad \gamma_i = -i\alpha_0 \alpha_i$$

with $i \in \{1, 2, 3\}$.

OK, the equation is nice. It was a great idea to jump from numbers to matrices. But, what is the meaning of that? The physical meaning of this equation starts when we notice that the wavefunction becomes "vector-like". Now it has as many components as the γ matrices, right? So, 4. What are the meanings? Now we'll give some statements without proof, another piece of this course will fill in the gaps!

– The equation $E^2 = p^2 + m^2$ has two possible solutions for E, one is positive the other is negative. Therefore, there are states with "negative" total energy... which is unbounded from below. Why don't the electrons fall into those states? Because, Dirac proposed, they are fully occupied from the beginning. This is Dirac's sea of particles. When one of this electrons in the sea jumps into the positive energy region, it leaves a "hole" in it.

– These hole states couple to the electromagnetic field as if they had opposed electric charge. Their equation of motion is the same as the one for the electron if you change dt into $-dt$. Somehow, it is as if they traveled backwards in time. They are the "antiparticles".

– Dirac proposed that the "antiparticle" of the electron was the proton... but Pauli proved that, if this was true, the electron and proton of a nucleus would annihilate each other in a very short fraction of a second. It was then when he proposed the second moral law of the physicists, according to which any theory should apply immediately to the body of the beholder, thus allowing us to get rid of stupid proposals... Tough guy, Pauli!

– Then, Dirac proposed that his antiparticle was a new particle, not yet discovered. This was in 1928. A few years later, in 1932, Anderson discovered the positrons in the cosmic rays, proving right the conjecture of Pauli. Conclusions: do not rush into destroying somebody's body, perhaps he was right after all...

Dirac had a very peculiar personality himself. Among the fathers of quantum mechanics, he was the only one to have some modesty. He said once that he did his discoveries because he was at the correct place in the correct time. According to him, "it was easy for any second rate physicist to do first rate research".