**Relativistic Hamiltonians**

Now let’s go ahead and solve a few problems. We’ll use the Dirac representation throughout.

**Eigenfunctions/values of free-particle Hamiltonian**

Let’s look at the eigenfunctions of the free particle Hamiltonian in the relativistic theory. We will recall that in the non-relativistic theory, they are solutions to the equation:



which are:



But in the relativistic theory, we have, putting the Dirac-equation in position/spin space:



Let’s solve this equation. We can write the wavefunction as a 4 dimensional column vector of the form,



where **χ** and **Φ** are themselves two-component column vectors which are not known a priori. Filling this in we have:



and so we get two coupled equations for **χ** and **Φ**, which are explicitly,



Let’s solve for the Φ and put everything in terms of χ,



and,



and we end up with:



[transforming the coupled eigenvalue equation into a decoupled eigenvalue equation by substitution is okay – see Math/Differential Equations/Coupled ODEs file] As we saw in the last file, we may write this as:



Now we know the eigenfunctions of the momentum squared operator. Those are just plane waves. So we have:



And the energies are, filling this expression into our equation:



So we have the energy eigenvalues, which as desired conform to the relativistic spectrum…except for the presence of negative energy solutions. Negative energy solutions are not good. Negative energy isn’t bad per se′ since potential energy can be negative, but we don’t have any potential energy here, and even worse is this spectrum is unbounded. An electron could indefinitely lower its energy down to -∞, and should then by energy conservation radiate an ∞ amount of energy as it does so. But this doesn’t happen in reality and so we must address this issue. We consider the resolution in a bit. For now let’s go on to get the Φ’s associated with our χ’s. So these are:



and so we have:



But the solutions are usually not presented like this exactly. Typically an explicit distinction is made between positive and negative energy solutions. For the positive energy solutions we ‘normalize’ it to make electron (χ) part of the solution take the unit values (1 0), (0 1). So we would say,



For the negative energy solutions, we ‘normalize’ it so that Φ comes out as (1 0), (0 1). These look like:



since it is the case that:



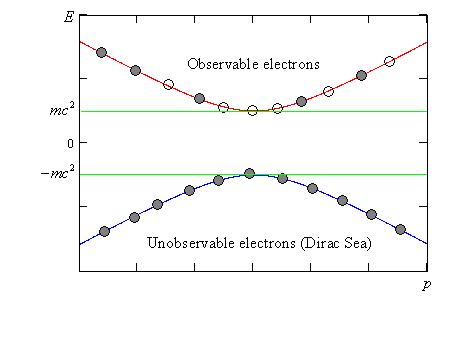
Let’s observe that for the positive energy solution, in the classical limit, when p2/2m << mc2, we have Φ → 0, and so this solution reduces to the usual spinor wavefunctions we obtained before.



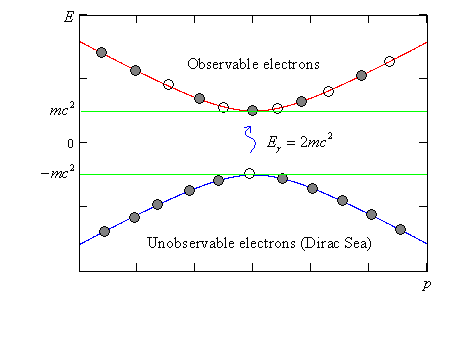
Thus these positive energy solutions should be thought of as the relativistic generalization to the usual electron wavefunction . And we’ll also observer that in the same limit, the negative energy solutions do the opposite thing: **χ** → 0. In that case we get:



What are these negative energy solutions to be interpreted as? This is the question that Dirac had to wrestle with in order to give this equation any validity. In order to avoid the problem of positive energy electrons making a cascading transition into negative energy states he proposed that all of these negative energy states were already filled by unobservable electrons which constituted what is now called the ‘Dirac sea’. And thus, by the Pauli-exclusion principle, positive energy electrons (which we can observe) cannot generally make those transitions into negative energy states.



This ad hoc device resolved the problem, but also made some interesting predictions. One is that a negative energy electron could absorb some energy (a photon I suppose) and make a transition into a positive energy state. Suppose a negative E electron at rest were to absorb a photon with energy Eγ = 2mc2. Then we would find this situation below.



What we would observe is the presence of another electron with p = 0. And we would also observe a hole in the Dirac Sea. This hole would appear to have a charge of +e since by assumption the Sea itself would be unobservable and all we would notice is the changes in the Sea. Additionally, the hole would have momentum of p = 0. This *hole* in the Dirac Sea is called a positron since it would behave just like an electron, accept with opposite charge.

So what we would *observe* is this: a photon of energy Eγ = 2mc2 disappears (is absorbed) and out pops an additional electron with momentum p = 0, and a positron (hole in the Dirac Sea) with momentum p = 0. In other words this is just a photon coalescing into an electron and positron (pair production).

The situation could easily reverse itself as well, an electron could drop into a hole in the Dirac sea, by giving off a photon of the requisite energy. This would be observed as an electron disappearing and a positron (hole in the Dirac Sea) disappearing and the release of a photon of energy Eγ. In other words this is just an electron and positron colliding and dissolving in a release of energy (pair annihilation).

So we see that Dirac’s equation, with the ancillary Dirac Sea hypothesis predicts the existence of a new type of particle – the positron. The positive energy solutions are basically electrons, and the negative energy solutions are basically the ‘unobservable electrons’, the absence of which corresponds to a positron. This prediction was confirmed in 1931 I believe, just a few years after Dirac published his theory! Note that electrons are now not independent, but are actually coupled to the unobservable ones. We can predict the behavior of the electron itself only by solving for the unobservable one too.

**Eigenfunctions of particle in magnetic field: Anomalous g-factor**

First a little review. Recall that when we have a macroscopic spinning object, with angular momentum **S**, and with its charge, q, uniformly distributed throughout its volume, then its magnetic moment is **μ** = γ**L**, where γ = q/2m. Furthermore, when placed in a magnetic field, its interaction energy is:



If this classical model is applied to the electron, then we would assume that its interaction energy was:



But in fact it was discovered to be:



The reason for the factor of 2 is so far unexplained. Dirac’s theory resolves this paradox though. So let’s write out the Hamiltonian for an otherwise free electron in a magnetic field. Recalling that to incorporate a magnetic field we must make the replacement **p** → **p** – e**A**, (where ) we have:



Now we’re going to go through the motions of solving for the positive energy eigenvalues of this Hamiltonian (which are those appropriate to electrons) in the classical limit and see that the ‘Schrodinger’ equation which results contains this anomalous g-factor in it already. So to start, let



and plug this into the Dirac equation. I’m going to leave off the **r**-dependences since it looks a lot better that way.



Now we want an equation for the electrons themselves (the **χ** part of the wavefunction), so we’ll solve for positron part (the **Φ** part of the wavefunction) and plug it back into the equation for **χ**. Solving for **Φ** we get:



And then plugging this into the **χ** equation we get:



Now let’s work out the expression in the numerator,



The last two terms can be worked out using our identity:



We get:



Now the **p** in the second term acts on both the **A** and the **χ** (not present explicitly). Using the product rule for the derivative, when **p** acts on χ it will cancel out the third term, leaving just its action on **A** alone. Using the fact that , and ****we get:



Filling this into our equation for **χ** we get:



This is the Dirac equation for an electron in a magnetic field. Note we can explicitly solve this equation, just like we did the classical counterpart, because it’s conveniently separable. But all we want to do is tease out the g-factor. So let’s take the classical limit, where pc << mc2. In that case our equation reads,



Filling in that **S** =(ћ/2)**σ** we have our ‘Schrodinger’ equation for an electron in a magnetic field.



Comparing with the classical Hamiltonian,



we see that the Dirac equation predicts a g-factor of 2, in exquisite agreement with known results. I think we can interpret the doubling of this factor as having to do with the fact that the electrons and unobservable electrons are coupled. So if in an electron precesses in the field, then the unobservable one must too. And so we actually have twice the energy we’d expect. In any event, it turns out that g is *really* given by ~ 2.002…and so evidently, the Dirac equation isn’t the last word on this subject).

**Fine Structure of the Hydrogen atom (sort of)**

Now let’s look at another achievement of the Dirac equation. We will recall that there are fine structure corrections to the Hydrogen atom spectrum, which we were able to account for to some degree by using the relativistic expression for the kinetic energy, and by including the spin-orbit interaction term. We will see how these ad-hoc corrections emerge naturally from the Dirac equation. Let’s look at the Dirac equation for an electron in a hydrogen atom:



Solving for **Φ** in the bottom equation:



The latter expression is just shorthand for the former. It’s not literally the same because V(r) is an operator, not a scalar. We must be careful about keeping the order of the operators correct. And now plugging into the top equation to get **χ**…



This would be our Dirac equation for the Hydrogen atom. Interestingly, it has been solved and the energy level spectrum conforms with experimental observations quite well. It’s a little awkward to solve since we have V(r) in the denominator – and note it is an *operator*. One thing we can do is multiple both sides by the denominator.



Then we can commute the [ ]**σ**·**p** at the expense of the commutator:



Then we may presume that mc2 + E >> V(**r**), which would allow us to neglect the commutator, and write:



Anyway, going back to:



We could we take the classical limit here, where E ≈ mc2 >> V(r) then we get our customary Schrodinger equation…



In order to obtain the spin-orbit correction and other relativistic corrections we would simply take the Dirac equation and do a Taylor series expansion for small E. This would generate extra terms which we could, through a little bit of simplification, equate to the spin-orbit term, and the relativistic kinetic energy correction, etc.

**Conservation of Total Angular Momentum**

We’ll recall that operators which commute with H are conserved in a time-development sense. Let’s examine the conservation of angular momentum in the relativistic theory. Let’s look at the free-particle Hamiltonian for simplicity.



Classically, the angular momentum of a free particle is conserved. And this is reflected in the fact that:



But observe that it is not conserved by the relativistic Hamiltonian. Consider the component Li.



The important thing about this result is that it isn’t 0. This means that the orbital angular momentum of a particle is not conserved in reality. Neither is the spin angular momentum, the 4D spinor matrix S = (ℏ/2)diag(σ,σ), as we can verify by checking the commutator of **S** with H.



Now this is:



so spin angular momentum is not conserved – even for the free particle solution. But observe that what is conserved is the total angular momentum, **J** = **L** + **S**. If we form the total angular momentum, and check the commutation relation we find that it is equal to 0, as is clear from the relations above. This indicates that **J** is the fundamental quantity here, that **L** and **S** are kind of like space and time, that they are just facets of the same fundamental thing. I suppose **S** comes about from Thomas precession or something?