The hydrogen atom and the Dirac equation – Part II: How the Dirac equation modifies the Schrodinger equation

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This accompanies the QM youtube lecture 4.4 by Burton Zwiebach, `https://www.youtube.com/watch?v=tl7q_VZ3eIQ`, which is also covered in online notes `https://ocw.mit.edu/courses/physics/8-06-quantum-physics-iii-spring-2018/lecture-notes/MIT8_06S18ch2.pdf`.

1 Where are we coming from and where are we heading?

- Previously on this program ...

  Following Zwiebach, we found the Schrodinger equation for an electron in a classical electromagnetic field. We found a term in the Hamiltonian proportional to the $\mathbf{L} \cdot \boldsymbol{\mu}$, the dot product of angular momentum and magnetic moment. Then – following Pauli – we hacked the Schrodinger equation to add spin and we got an extra term proportional to $\mathbf{S} \cdot \boldsymbol{\mu}$.

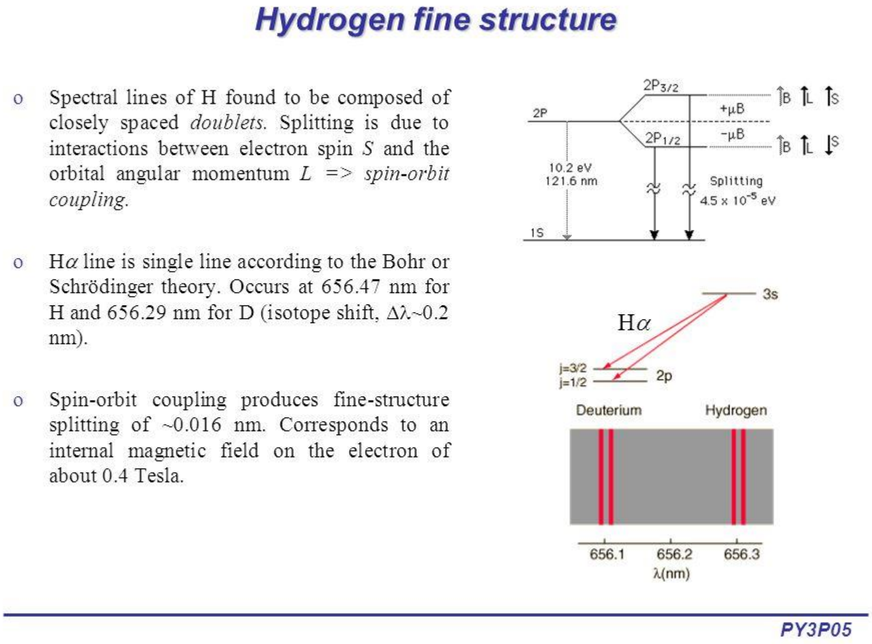
- Next we will modify the Schrodinger equation to make it consistent with relativity.
  - Zweibach follows the historical approach. He starts with a Schrodinger wavefunction equation, and looks for a Lorentz-invariant, first-order differential equation. This requires vectors. That's the Dirac equation **for wavefunctions** $\chi(t, \mathbf{x})$.
  - I'll do it the modern way and build off all our work in quantum field theory. We had a Dirac Lagrangian. The Euler-Lagrange

equation is also called the Dirac equation (it looks similar to the above) **but it operates on an operator** $\psi(t, \mathbf{x})$.

  - We know how to solve DE's for complex functions like χ but not for operators. So the first thing I do is to convert the operator equation into a wavefunction equation. The trick is to use an inner product.

- The Dirac wavefunction equation is hard to solve in closed form. Usually it is expanded in powers of v/c. We will see that the Schrodinger Hamiltonian is modified so that $H \rightarrow H + \Delta V$ where $\Delta V = \frac{e^2}{2|\mathbf{x}|^3 \mathrm{m}^2} \mathbf{S} \cdot \mathbf{L} + \ldots$

- Since ΔV is small, the term makes a small perturbation on the original Schrodinger energy levels. Because there are two values of spin, the energy splits into two close values, known as the *fine structure*.



Hydrogen fine structure

- Spectral lines of H found to be composed of closely spaced *doublets*. Splitting is due to interactions between electron spin S and the orbital angular momentum L => *spin-orbit coupling*.
- Hα line is single line according to the Bohr or Schrödinger theory. Occurs at 656.47 nm for H and 656.29 nm for D (isotope shift, $\Delta\lambda$~0.2 nm).
- Spin-orbit coupling produces fine-structure splitting of ~0.016 nm. Corresponds to an internal magnetic field on the electron of about 0.4 Tesla.

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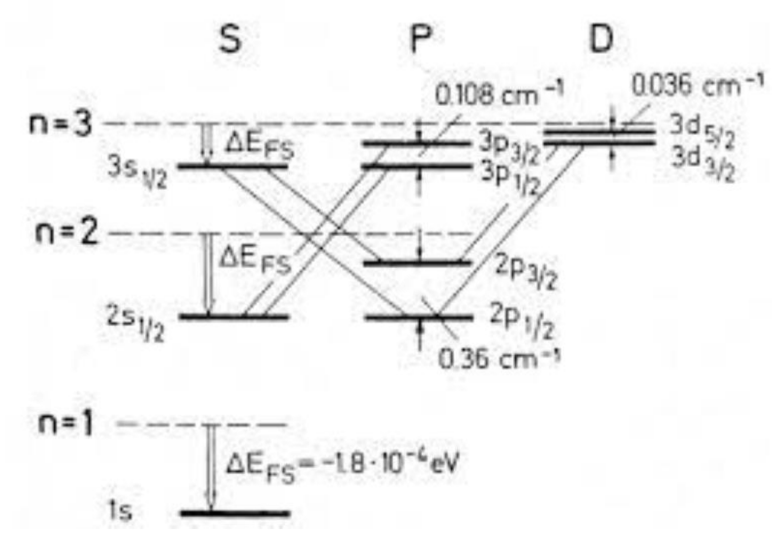

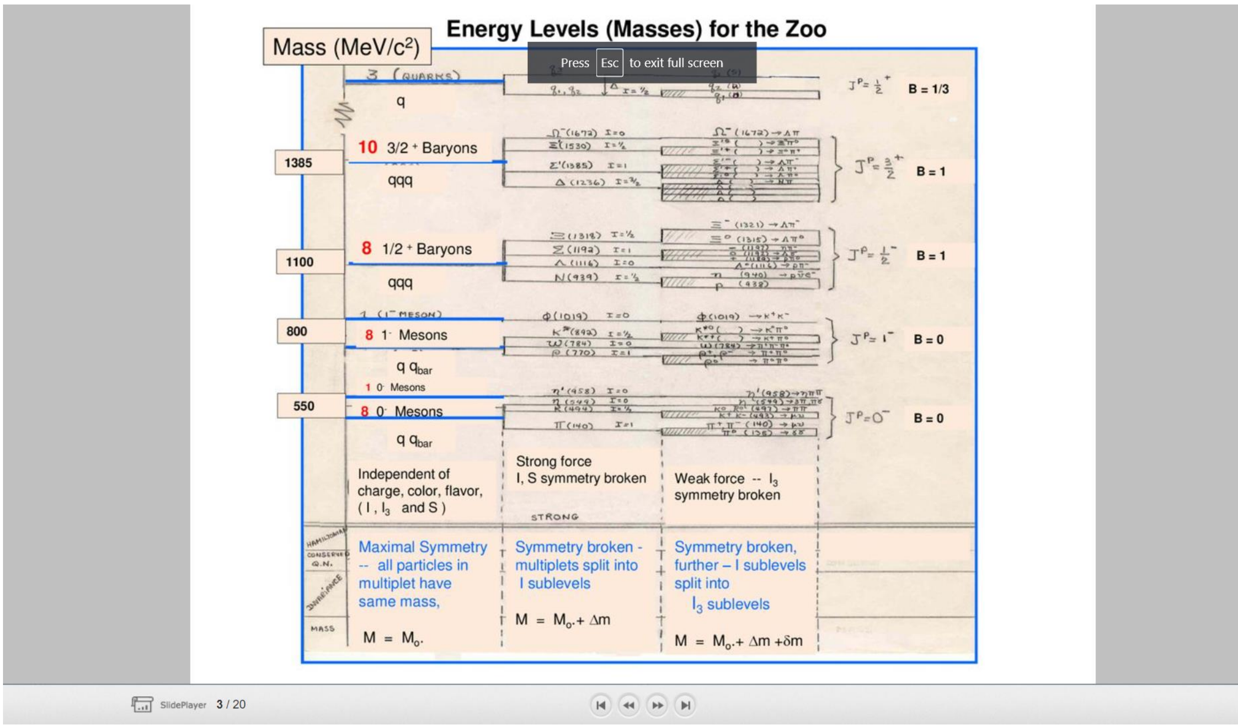

Energy Levels (Masses) for the Zoo

Mass (MeV/c^2)

q

10 3/2$^+$ Baryons

qqq

8 1/2$^+$ Baryons

qqq

8 1$^-$ Mesons

q q_{bar}

1 0$^-$ Mesons

8 0$^-$ Mesons

q q_{bar}

Independent of charge, color, flavor, (I , I_3 and S)

Strong force
I, S symmetry broken

Weak force -- I_3 symmetry broken

Maximal Symmetry -- all particles in multiplet have same mass,

M = M_o.

Symmetry broken - multiplets split into I sublevels

M = M_o.+ Δm

Symmetry broken, further – I sublevels split into I_3 sublevels

M = M_o.+ Δm +δm

- Going forward ...

We'll review why energy levels appear in angular momentum multiplets, and how to use the angular-momentum algebra and perturbation theory to compute energy-splitting. Then we'll begin using similar techniques to understand the particle zoo. Instead of the angular-momentum algebra, we'll look at the SU(3) algebra and instead of energy levels we'll look at mass levels.

2 From field theory to the Schrodinger equation

2.1 General quantum field theory in a nutshell

- The program of quantum physics starts with the action, which is the integral of a Lagrangian $S = \int \mathcal{L}$.
- In quantum field theory (QFT), the Lagrangian is dependent on canonical fields $\phi^i(x)$ and canonical field-momenta
$$\pi^i(x) = \frac{\partial \mathcal{L}}{\partial \dot{\phi}^i}(x)$$
where the indices are simply used to distinguish field components.
$$S = \int d^4x \mathcal{L}(\phi^i, \pi^i).$$
- One of the axioms of field theory is that the action must be Lorentz-invariant. This axiom imposes constraints on the permissible Lagrangians.
- Another axiom of field theory is that the fields in our universe, obey the Euler-Lagrange equations – that is, those fields are extrema of the action.
- Yet another axiom of field theory, is that the fields are actually operators on a Hilbert space, and that their commutation relations are given by Dirac's conditions relating canonical variables (fields) to canonical momenta.

2.2 A particular case – free Dirac fields

- The Dirac action for a <u>free</u> spin-$\frac{1}{2}$ particle:
$$\mathcal{S} = \int d^4x \mathcal{L} = \int d^4x \psi^\dagger(x)\gamma_0 \left(i\partial\!\!\!/ - m\right) \psi(x) \tag{1}$$

  - ψ is a 4-spinor – a vector with 4 complex components.
  - $\gamma^0, \gamma^1, \gamma^2, \gamma^3$ are 4x4 matrices.
  - $\not{\partial} \equiv \sum_\mu \gamma^\mu \partial_\mu$

- Equation of motion:

  $$\frac{\delta \mathcal{S}}{\delta \psi^\dagger} = 0$$

  implies the Dirac equation

  $$\boldsymbol{\left(i\not{\partial} - m\right) \psi(x) = 0}$$

  where $\boldsymbol{\psi}$ is a 4-tuplet of operators.[1]

2.3 A more interesting case – free Dirac fields interacting with an external electromagnetic field

This will be the way we model an electron in the presence of the electromagnetic field of a proton. The proton is heavy, so the electron doesn't have much effect on the proton's electromagnetic field. We can treat that EM field as *external.*

- The Lagrangian for a Dirac particle in the presence of an external electromagnetic field is

  $$\mathcal{L} = \bar{\psi}\left(i\gamma^\mu \partial_\mu - m\right)\psi - e\bar{\psi}\gamma^\mu A_\mu \psi \tag{2}$$

  where A_μ is an external field (the electromagnetic 4-potential)– by which I mean that it is a real-valued (**NOT** an operator[2] 4-vector whose values are 'given', rather than derived.

- The equation of motion for the Dirac operator field in an external electromagnetic field is

  $$\left(i\boldsymbol{\not{\partial}} - m - e\boldsymbol{\gamma}^\mu A_\mu\right)\boldsymbol{\psi}(x) = 0. \tag{3}$$

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[1] Notice that in the Lagrangian, we were dealing with complex numbers, but when we write the Euler-Lagrange equation and perform other manipulations, we re-interpret the fields as operators. This sort of makes sense if you think about path integrals. In the path integral, there is an exponential of the action, and the action is an integral over complex functions. All manipulations of interest, including Euler-Lagrange equations, are done as functional integrals weighted by the exponential of the action – corresponding to the operator interpretation.

[2] Although as Zwiebach points out, A is a function of $\mathbf{x}$ which in turn is an operator on the space of functions.

2.4 From operator equation to wavefunction equation

In previous sessions, we saw that the Dirac field is an operator on a Hilbert space of particle and antiparticle states. Ultimately, we are interested in the energies of bound states of an electron state in the presence of a proton's EM field. From those energies we can obtain the hydrogen spectrum.

- In the very early days of QM, Schrodinger had come up with a prescription for finding the energy states.
  - Find the classical Hamiltonian H as a function of coordinates $\mathbf{x}$ and momenta $\mathbf{p}$.
  - Rewrite $\mathbf{p}$ as a differential operator $-i\boldsymbol{\nabla}$.
  - Then apply the rewritten Hamiltonian to a function ψ and solve the eigenvalue equation

    $$H\psi = E\psi$$

    . Here, the ψ are wavefunctions and **not field operators. The energies E are the bound state energies.**
  - **There is also an identification between the Hamiltonian and the time derivative operator:**

    $$i\partial_t\psi(t,\mathbf{x}) = \mathbf{H}\psi(\mathbf{t},\mathbf{x}).$$

- **At first, no-one knew what the function ψ represented. It took years for people to eventually interpret it as "state" with a probability amplitude.**

- Dirac didn't start with a field theory. He started with a Schrodinger-style equation that was Lorentz invariant. This did a good job of predicting bound state energies. **However, Dirac and others were unable to interpret Dirac's wavefunction the same way that they had interpreted Schrodinger's wavefunction. There were serious problems that required a new concept, *holes*, which was an unsatisfactory ad hoc construction to fix the interpretation issues. THAT EVENTUALLY LED TO THE CONCLUSION THAT A PROPER THEORY OF THE ELECTRON REQUIRED A FIELD THEORY, AND AN INTERPRETATION OF ψ AS A FIELD AND NOT A DIRAC WAVEFUNCTION.**

- Rather than directly imitating Zwiebach's lecture which follows Dirac's approach of looking for a relativistic wave function equation, I'll arrive at the same endpoint by starting from our field theory results. Later I'll return to Zwiebach's approach.

- Use Dirac's bra-ket notation to represent states (vectors in a Hilbert space) – $|\xi\rangle$.

- A special state is denoted $|\Omega\rangle$ and is the lowest-energy eigenstate of the Hamiltonian. It is generally called *the vacuum state.*

- Define a complex 4-tuplet called a **Dirac wavefunction** by

  $$\xi_i(x) \equiv \langle\Omega|\boldsymbol{\psi}_i(x)|\xi\rangle.$$

  Here we've return very temporarily to $\boldsymbol{\psi}_i$ as referring to the Dirac **field operator.**

- **We'll work with this to get energy eigenvalues, but the Dirac wavefunction isn't to be interpreted as a Schrodinger wavefunction. The analysis of 100 years assures us that the eigenvalue procedure is valid.**

- **Then we can use eq. (3) to get**

  $$\left(i\boldsymbol{\partial\!\!\!/} - m - e\boldsymbol{\gamma}^\mu A_\mu\right)\boldsymbol{\xi}(x) = 0. \tag{4}$$

  The difference between this equation and the previous Dirac equation, is that ξ is a set of complex numbers, whereas ψ is a set of operators!

2.5 From state equation to Schrodinger equation

The above Dirac equation is what we had in previous notes. Now I want to connect this to Zwiebach lecture 4.4. **He uses slightly different notation – surprise, surprise!** I'll convert mine to his.

- Following convention, Zwiebach calls his complex wavefunction ψ instead of ξ. This is often confusing because we previously had used ψ as a field operator. From now on, when discussing the Dirac equation, we'll use ψ to denote the Dirac wavefunction, rather than the Dirac field operator!

- Zwiebach also writes the 4 components of the wavefunction as

$$\psi = \begin{pmatrix} \chi \\ \eta \end{pmatrix}$$

  where χ and η are both 2-spinors (i.e. complex doublets). He usually refers to χ as the Pauli spinor.

- Now rewrite the Dirac equation, eq. (4) by explicitly isolating the time derivative (and don't forget we are replacing ξ by ψ).

$$i\partial_t \psi(t, \mathbf{x}) = \gamma^0 \gamma^j \left(-i\partial_j\right) \psi(t, \mathbf{x}) + \left(m\gamma^0 + e\gamma^0\gamma^\mu A_\mu(t, \mathbf{x})\right) \psi(t, \mathbf{x}) \tag{5}$$

- Zwiebach follows conventions of the Dirac wavefunction approach and uses the Dirac representation of γ matrices.

$$\gamma^0 = \begin{pmatrix} \mathbf{I}_2 & 0 \\ 0 & -\mathbf{I}_2 \end{pmatrix}, \gamma^i = \begin{pmatrix} 0 & -\sigma_i \\ \sigma_i & 0 \end{pmatrix} \tag{6}$$

- Take eq. (5), write $\psi = \begin{pmatrix} \chi \\ \eta \end{pmatrix}$, and expand the γ matrices in the Dirac representation, and get

$$\left(i\partial_t - eA_0\right) \begin{pmatrix} \chi \\ \eta \end{pmatrix} = \begin{pmatrix} m\mathbf{I}_{2\text{x}2} & \left(-i\partial_j + eA_j\right)\sigma_j \\ \left(-i\partial_j + eA_j\right)\sigma_j & -m\mathbf{I}_{2\text{x}2} \end{pmatrix} \begin{pmatrix} \chi \\ \eta \end{pmatrix} \tag{7}$$

  EXERCISE: Derive this equation.

- For the case of the Hydrogen atom, the vector potential A_i is 0 (no magnetic field) and we write $A_0 = -\phi$, so the equation becomes

$$\left(i\partial_t + e\phi\right) \begin{pmatrix} \chi \\ \eta \end{pmatrix} = \begin{pmatrix} m\mathbf{I}_{2\text{x}2} & \left(-i\partial_j\right)\sigma_j \\ \left(-i\partial_j\right)\sigma_j & -m\mathbf{I}_{2\text{x}2} \end{pmatrix} \begin{pmatrix} \chi \\ \eta \end{pmatrix} \tag{8}$$

- Now for a magic trick! We saw that Schrodinger identified the operator $i\partial_t$ with the Hamiltonian, and that the eigenvalue equation is $H\psi = E\psi$. **So, from now on, whenever we see $\imath\partial_t\psi$, we'll replace it by $E\psi$.**

- Let's make that substitution and rewrite eq. (8) in components as

$$\begin{aligned} \left(E' + e\phi\right)\mathbf{I}_{2\text{x}2}\chi &= \left(-i\partial_j\right)\sigma_j\eta \\ \left(E' + 2m + e\phi\right)\mathbf{I}_{2\text{x}2}\eta &= \left(-i\partial_j\right)\sigma_j\chi \end{aligned} \tag{9}$$

  where $E' = E - m$.

- Now rewrite the second equation as

  $$\eta = \frac{(-i\partial_j)\,\sigma_j\chi}{(E' + 2m + e\phi)} \tag{10}$$

  and substitute η into the first equation.

  $$(E' + e\phi)\,\mathbf{I}_{2\text{x}2}\chi = (-i\partial_j)\,\sigma_j\frac{(-i\partial_j)\,\sigma_j\chi}{(E' + 2m + e\phi)} \tag{11}$$

- We can re-organize terms a bit so that this equation becomes

  $$\begin{aligned} E'\chi &= \left(-e\phi - \frac{1}{2m}\boldsymbol{\nabla}\boldsymbol{\cdot}\boldsymbol{\sigma}\left(1 + \frac{E' + e\phi}{2m}\right)^{-1}\boldsymbol{\nabla}\boldsymbol{\cdot}\boldsymbol{\sigma}\right)\chi \\ &\approx \left(-e\phi - \frac{1}{2m}\boldsymbol{\nabla}\boldsymbol{\cdot}\boldsymbol{\sigma}\left(1 - \frac{E' + e\phi}{2m}\right)\boldsymbol{\nabla}\boldsymbol{\cdot}\boldsymbol{\sigma}\right)\chi \end{aligned} \tag{12}$$

  where we've used the nonrelativistic approximation that $E' + e\phi << 2m$.

- Recall that

  $$\partial_i(\phi\chi) = (\partial_i\phi)\chi + \phi(\partial_i\chi).$$

  Therefore

  $$\boldsymbol{\nabla}\boldsymbol{\cdot}\boldsymbol{\sigma}\,(\phi\boldsymbol{\nabla}\boldsymbol{\cdot}\boldsymbol{\sigma}\chi) = (\boldsymbol{\nabla\phi}\boldsymbol{\cdot}\boldsymbol{\sigma})\,(\boldsymbol{\nabla\chi}\boldsymbol{\cdot}\boldsymbol{\sigma}) + \phi\boldsymbol{\nabla}\boldsymbol{\cdot}\boldsymbol{\sigma}\boldsymbol{\nabla}\boldsymbol{\cdot}\boldsymbol{\sigma}\chi \tag{13}$$

  Recall from the notes to Zwiebach lecture 4.3 that

  $$(\boldsymbol{\sigma}\cdot a)(\boldsymbol{\sigma}\cdot b) = (\mathbf{a}\cdot\mathbf{b})\mathbf{I}_{2\text{x}2} + \mathbf{i}\boldsymbol{\sigma}\cdot(\mathbf{a}\times\mathbf{b}). \tag{14}$$

  Applying this to the above, we get

  $$\boldsymbol{\nabla}\boldsymbol{\cdot}\boldsymbol{\sigma}\,(\phi\boldsymbol{\nabla}\boldsymbol{\cdot}\boldsymbol{\sigma}\chi) = (\boldsymbol{\nabla}\phi\cdot\boldsymbol{\nabla}\chi)\,\mathbf{I}_{2\text{x}2} + i\boldsymbol{\sigma}\cdot(\boldsymbol{\nabla}\phi\times\boldsymbol{\nabla}\chi) + \phi\boldsymbol{\nabla}^2\chi \tag{15}$$

  so that we can rewrite eq. (12) as

  $$\begin{aligned} (E' + e\phi)\chi &\approx -\frac{1}{2m}\boldsymbol{\nabla}\boldsymbol{\cdot}\boldsymbol{\sigma}\left(1 - \frac{E' + e\phi}{2m}\right)\boldsymbol{\nabla}\boldsymbol{\cdot}\boldsymbol{\sigma}\chi \\ &= i\frac{e}{4m^2}\boldsymbol{\sigma}\cdot(\boldsymbol{\nabla}\phi\times\boldsymbol{\nabla}\chi) \\ &\quad + \left(-\frac{1}{2m}\left(1 - \frac{E + e\phi}{2m}\right)\boldsymbol{\nabla}^2 + \frac{e}{4m^2}\,(\boldsymbol{\nabla}\phi\cdot\boldsymbol{\nabla})\right)\chi \end{aligned} \tag{16}$$

- The non-relativistic expansion is in terms of order $1/m$. We have

$$E' + e\phi = \mathcal{O}(\frac{1}{m}).$$

  The term $E' + e\phi$ also appears on the RHS, multiplied by $\frac{1}{m^2}$, so altogether that term is $\mathcal{O}(\frac{1}{m^3})$ and can therefore be suppressed relative to other terms of order $\frac{1}{m^2}$.

- The relativistic term of particular interest to us is the spin-orbit term (the only term involving spin). For the hydrogen atom,

$$\phi(t, \mathbf{x}) = \frac{\mathrm{e}}{|\mathbf{x}|}$$

  and therefore

$$\boldsymbol{\nabla}\phi(t, \mathbf{x}) = -\mathrm{e}\frac{\mathbf{x}}{|\mathbf{x}|^{\mathbf{3}}}.$$

  So we can rewrite eq.(16) as

$$E'\chi = \left(-\frac{1}{2m}\boldsymbol{\nabla}^2 - \frac{e^2}{|\mathbf{x}|} + \frac{e^2}{4|\mathbf{x}|^{\mathbf{3}}\mathrm{m}^{\mathbf{2}}}\sigma \cdot (\mathbf{x} \times (-\mathbf{i}\boldsymbol{\nabla})) + ...\right)\chi \qquad (17)$$

  Noting that $-i\boldsymbol{\nabla} = \mathbf{p}$, we can replace the term $(\mathbf{x} \times (-\mathbf{i}\boldsymbol{\nabla}))$ on the RHS, with $(\mathbf{x} \times \mathbf{p})$, which – recognizing the definition of orbital angular momentum – becomes $\mathbf{L}$.

- Finally we have

$$\begin{aligned} E'\chi &= \left(-\frac{1}{2m}\boldsymbol{\nabla}^2 - \frac{e^2}{|\mathbf{x}|} + \frac{e^2}{4|\mathbf{x}|^3\mathrm{m}^2}\boldsymbol{\sigma} \cdot \mathbf{L} + ...\right)\chi \\ &= \left(-\frac{1}{2m}\boldsymbol{\nabla}^2 - \frac{e^2}{|\mathbf{x}|} + \frac{e^2}{2|\mathbf{x}|^3\mathrm{m}^2}\mathbf{S} \cdot \mathbf{L} + ...\right)\chi \end{aligned} \qquad (18)$$

  where we used $\mathbf{S} = \boldsymbol{\sigma}/\mathbf{2}$.

- This should be familiar-looking. It is an eigenvalue equation where the eigenvalue is $E' = E - m$, and the RHS is of the form $H\chi$ with

$$H = \frac{\mathbf{p^2}}{2m} + V(\mathbf{x}) + \frac{e^2}{2|\mathbf{x}|^3\mathrm{m}^2}\mathbf{S} \cdot \mathbf{L} + ...$$

  The potential is just $-e^2/|\mathbf{x}|$.[3]

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[3] Zwiebach includes other terms such as the Darwin term proportional to $\boldsymbol{\nabla}\phi \cdot \boldsymbol{\nabla}$ but for now, our focus is only on the spin-orbit contribution.