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Physics 115 - Seminar 5

Spin-Orbit Interaction through the Dirac Equation

Since the Dirac equation is useful for describing electrons, let us insert the potential for the electron in the hydrogen atom, $\hat{V} = -\frac{e^2}{r}$. (Note that we are still approximating the proton as infinitely massive.) The Dirac equation is then

$$\left(c\hat{\boldsymbol{\alpha}} \cdot \hat{\boldsymbol{P}} + \hat{\beta}mc^2 + \hat{V}\right)|\psi\rangle = E\,|\psi\rangle\,. \tag{1}$$

If we again write $|\psi\rangle$ as

$$|\psi\rangle = \begin{bmatrix} \chi \\ \Phi \end{bmatrix}, \tag{2}$$

the Dirac equation becomes

$$\begin{bmatrix} E - \hat{V} - mc^2 & -c\hat{\boldsymbol{\sigma}} \cdot \hat{\boldsymbol{P}} \\ -c\hat{\boldsymbol{\sigma}} \cdot \hat{\boldsymbol{P}} & E - \hat{V} + mc^2 \end{bmatrix} \begin{bmatrix} \chi \\ \Phi \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}, \tag{3}$$

which leads to two coupled differential equations:

$$\left(E - \hat{V} - mc^2\right)\chi - c\hat{\boldsymbol{\sigma}} \cdot \hat{\boldsymbol{P}}\Phi = 0, \tag{4}$$

$$\left(E - \hat{V} + mc^2\right)\Phi - c\hat{\boldsymbol{\sigma}} \cdot \hat{\boldsymbol{P}}\chi = 0. \tag{5}$$

Combining these equations by eliminating Φ, we get

$$\left(E - \hat{V} - mc^2\right)\chi = c\hat{\boldsymbol{\sigma}} \cdot \hat{\boldsymbol{P}}\left[\frac{1}{E - \hat{V} + mc^2}\right] c\hat{\boldsymbol{\sigma}} \cdot \hat{\boldsymbol{P}}\chi. \tag{6}$$

On the LHS, we make the substitution $E_S = E - mc^2$, where E_S is the energy from Schrödinger's equation, and on the RHS we approximate

$$\begin{aligned} \frac{1}{E - \hat{V} + mc^2} &= \frac{1}{2mc^2 + E_S - \hat{V}} = \frac{1}{2mc^2}\left(1 + \frac{E_S - \hat{V}}{2mc^2}\right)^{-1} \\ &\approx \frac{1}{2mc^2}\left(1 - \frac{E_S - \hat{V}}{2mc^2}\right) = \frac{1}{2mc^2} - \frac{E_S - \hat{V}}{4m^2c^4}. \end{aligned} \tag{7}$$

If we only kept the lowest term in this expansion, $1/2mc^2$, we would get the familiar nonrelativistic Schrödinger equation. Keeping the higher order term allows us to see the fine structure. Now we make our substitutions into Eq. (6) to get

$$E_S\chi = \left[\frac{\hat{P}^2}{2m} + V - \frac{\hat{\boldsymbol{\sigma}} \cdot \hat{\boldsymbol{P}}\left(E_S - \hat{V}\right)\hat{\boldsymbol{\sigma}} \cdot \hat{\boldsymbol{P}}}{4m^2c^2}\right]\chi. \tag{8}$$

In order to get rid of the E_S on the RHS, we use the fact that $\hat{V}$ and $\hat{\boldsymbol{\sigma}}$ commute and that we only need $E_S - V$ to lower (v^2/c^2) order to write

$$\begin{aligned}\left(E_S - \hat{V}\right)\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{P}}\chi &= \hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{P}}\left(E_S - \hat{V}\right)\chi + \hat{\boldsymbol{\sigma}}\cdot\left[E_S - \hat{V}, \hat{\boldsymbol{P}}\right]\chi \\ &= \left(\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{P}}\right)\frac{\hat{P}^2}{2m}\chi + \hat{\boldsymbol{\sigma}}\cdot\left[\hat{\boldsymbol{P}}, \hat{V}\right]\chi.\end{aligned} \tag{9}$$

Now, Eq. (8) becomes

$$\begin{aligned}E_S\chi &= \left[\frac{\hat{P}^2}{2m} + \hat{V} - \frac{\hat{P}^4}{8m^3c^2} - \frac{\left(\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{P}}\right)\cdot\left(\hat{\boldsymbol{\sigma}}\cdot\left[\hat{\boldsymbol{P}}, \hat{V}\right]\right)}{4m^2c^2}\right]\chi \\ &= \left[\frac{\hat{P}^2}{2m} + \hat{V} - \frac{\hat{P}^4}{8m^3c^2} - \frac{i\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{P}}\times\left[\hat{\boldsymbol{P}}, \hat{V}\right]}{4m^2c^2} - \frac{\hat{\boldsymbol{P}}\cdot\left[\hat{\boldsymbol{P}}, \hat{V}\right]}{4m^2c^2}\right]\chi.\end{aligned} \tag{10}$$

The first two terms are just the Hamiltonian for the nonrelativistic Schrödinger equation. The third term is the relativistic correction to the kinetic energy. We are concerned with the fourth term, the spin- orbit interaction $H_{S.O.}$. To analyze this term, note first that

$$\begin{aligned}\left[\hat{\boldsymbol{P}}, \hat{V}\right]|\psi\rangle &= \left(\hat{\boldsymbol{P}}\hat{V} - \hat{V}\hat{\boldsymbol{P}}\right)|\psi\rangle = \left(i\hbar\nabla\frac{e^2}{r} - \frac{e^2}{r}i\hbar\nabla\right)|\psi\rangle \\ &= i\hbar e^2\left(\left(\nabla\frac{1}{r}\right)|\psi\rangle + \frac{1}{r}\nabla|\psi\rangle - \frac{1}{r}\nabla|\psi\rangle\right) = -i\hbar e^2\frac{\hat{\boldsymbol{r}}}{r^3}|\psi\rangle\ .\end{aligned} \tag{11}$$

This gives

$$\begin{aligned}H_{S.O.} &= \frac{-i\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{P}}\times\left[\hat{\boldsymbol{P}}, \hat{V}\right]}{4m^2c^2} = \frac{-i\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{P}}\times\left[-i\hbar e^2\frac{\hat{\boldsymbol{r}}}{r^3}\right]}{4m^2c^2} \\ &= \frac{-\hbar e^2\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{P}}\times\hat{\boldsymbol{r}}}{4m^2c^2r^3} = \frac{e^2}{2m^2c^2r^3}\left(\frac{\hbar}{2}\hat{\boldsymbol{\sigma}}\right)\cdot\left(\hat{\boldsymbol{r}}\times\hat{\boldsymbol{P}}\right) \\ &= \frac{e^2}{2m^2c^2r^3}\hat{\boldsymbol{S}}\cdot\hat{\boldsymbol{L}}.\end{aligned} \tag{12}$$

As you can recall (or go look up in your notes), this is the same as the $H_{S.O.}$ found by making corrections to the Schrödinger equation. However, the $H_{S.O.}$ found earlier had a factor of 1/2 (known as the Thomas factor) randomly tacked on. Using the Dirac equation, the Thomas factor drops out automatically.