

Form of the Spin-Orbit Hamiltonian

The spin free Schrodinger Hamiltonian for a one-electron atom is

$$\hat{H}^0 = -\frac{\hbar^2}{2m} \nabla^2 - \frac{e^2 Z}{4\pi\epsilon_0 r}$$

We know its eigenfunctions and eigenvalues and we are interested in the effect of spin. Usually we think of the electron as revolving about the nucleus but another view is to sit on the electron and watch the nucleus move relative to the electron. The nucleus carries a positive charge and generates a magnetic field at the location of the electron given by

$$\vec{B}(\vec{R}) = \frac{1}{c^2} \vec{V}_N \times \vec{F}_N(\vec{R})$$

Where \vec{V}_N is the velocity of the nucleus and $\vec{F}_N(\vec{R})$ is the force exerted on the electron by the nucleus. We note that the velocity of the nucleus is equal and opposite to the electrons' so we have

$$\vec{B}(\vec{r}) = \frac{1}{c^2} \vec{V} \times \frac{Ze\vec{r}}{4\pi\epsilon_0 r^3}$$

where \vec{r} is directed from the nucleus to the electron. Since the orbital angular momentum of the electron is $\vec{L} = \vec{r} \times m\vec{V}$, (m is the mass of the electron) we may write $\vec{B}(\vec{r}) = \frac{1}{c^2} \frac{Ze\hbar\vec{L}}{4\pi\epsilon_0 m r^3}$ where we measure \vec{L} in multiples of \hbar . This magnetic field interacts with the magnetic dipole moment of the electron $\vec{\mu} = -g\mu_B\vec{S}$ resulting in the spin-orbit interaction energy operator

$$\hat{H}_{so} = -\vec{\mu} \cdot \vec{B}(\vec{r}) = \frac{Ze^2\hbar^2 \hat{L} \cdot \hat{S}}{8\pi\epsilon_0 c^2 m^2 r^3} = W(r) \hat{L} \cdot \hat{S}$$

where $W(r) = \frac{Ze^2\hbar^2}{8\pi\epsilon_0 c^2 m^2 r^3}$.

A more detailed treatment by Thomas shows that we must multiply this expression for $\vec{B}(r)$ by $\frac{1}{2}$ and this correction has been included in the above equation. We will also derive this correct expression when we discuss the Pauli approximation to the Dirac equation. The perturbed Schrodinger Hamiltonian becomes

$$\hat{H} = \hat{H}^0 + W(r) \hat{L} \cdot \hat{S}.$$