

252(1) : Expression of Free Particle Kinetic Energy in Terms of Angular Momentum

Angular momentum being is fundamental to quantum mechanics so, it is important to incorporate it into the Hamiltonian of Dirac's equation:

$$H\psi = \left(mc^2 + e\phi + \frac{1}{2m} \underline{\sigma} \cdot (\underline{p} - e\underline{A}) \left(1 + \frac{e\phi}{2mc^2} \right) \underline{\sigma} \cdot (\underline{p} - e\underline{A}) \right) \psi$$

$$\left(mc^2 + e\phi + \frac{1}{2m} \underline{\sigma} \cdot \underline{p} \underline{\sigma} \cdot \underline{p} - \frac{e}{2m} (\underline{\sigma} \cdot \underline{A} \underline{\sigma} \cdot \underline{p} + \underline{\sigma} \cdot \underline{p} \underline{\sigma} \cdot \underline{A}) \right)$$

$$+ \frac{e^2}{2m} \underline{\sigma} \cdot \underline{A} \underline{\sigma} \cdot \underline{A} + \frac{e}{4m^2 c^2} \underline{\sigma} \cdot (\underline{p} - e\underline{A}) \phi \underline{\sigma} \cdot (\underline{p} - e\underline{A}) \right) \psi \quad \text{--- (1)}$$

This same Hamiltonian can be developed with particle physics and QED theory, and with ECE theory. Angular momentum is incorporated at a fundamental level by considering:

$$H_1 \psi = \frac{1}{2m} \underline{\sigma} \cdot \underline{p} \underline{\sigma} \cdot \underline{p} \psi \quad \text{--- (2)}$$

where:

$$\underline{\sigma} \cdot \underline{p} = \frac{\underline{\sigma} \cdot \underline{r}}{r^2} (\underline{r} \cdot \underline{p} + i \underline{\sigma} \cdot \underline{L}) \quad \text{--- (3)}$$

and

$$\underline{L} = \underline{r} \times \underline{p} \quad \text{--- (4)}$$

$$\underline{S} = \frac{1}{2} \hbar \underline{\sigma} \quad \text{--- (5)}$$

Therefore two types of angular momentum are

2) included at the outset, the orbital \underline{L} and spin \underline{S} .
 The total angular momentum operator is:

$$\underline{J} \psi = (\underline{L} + 2\underline{S}) \psi \quad - (6)$$

and the total angular momentum is conserved.

From eq. (3):

$$\begin{aligned} \underline{\sigma} \cdot \underline{p} \underline{\sigma} \cdot \underline{p} &= \frac{\underline{\sigma} \cdot \underline{r} \underline{\sigma} \cdot \underline{r}}{r^4} (\underline{r} \cdot \underline{p} + i \underline{\sigma} \cdot \underline{L}) (\underline{r} \cdot \underline{p} + i \underline{\sigma} \cdot \underline{L}) \\ &= \frac{1}{r^2} (\underline{r} \cdot \underline{p} \underline{r} \cdot \underline{p} + i \underline{r} \cdot \underline{p} \underline{\sigma} \cdot \underline{L} + i \underline{\sigma} \cdot \underline{L} \underline{r} \cdot \underline{p} - \underline{\sigma} \cdot \underline{L} \underline{\sigma} \cdot \underline{L}) \\ &= \frac{1}{r^2} (\underline{r} \cdot \underline{p} \underline{r} \cdot \underline{p} + i \underline{r} \cdot \underline{p} \underline{\sigma} \cdot \underline{L} + i \underline{\sigma} \cdot \underline{L} \underline{r} \cdot \underline{p} - L^2 - i \underline{\sigma} \cdot \underline{L} \times \underline{L}) \end{aligned} \quad - (7)$$

This classical equation is quantized with:

$$\underline{r} \cdot \underline{p} \psi = \frac{\hbar}{i} r \frac{d\psi}{dr} \quad - (8)$$

$$L^2 \psi = \hbar^2 l(l+1) \psi \quad - (9)$$

$$\underline{L} \times \underline{L} \psi = i \hbar \underline{L} \psi \quad - (10)$$

$$\underline{S} \cdot \underline{L} \psi = \frac{\hbar^2}{2} (j(j+1) - l(l+1) - s(s+1)) \psi \quad - (11)$$

Therefore:

$$\underline{r} \cdot \underline{p} (\underline{r} \cdot \underline{p} \psi) = \frac{\hbar}{i} r \left(\frac{d}{dr} \left(\frac{\hbar}{i} r \frac{d}{dr} \right) \psi \right) \quad - (12)$$

using the Leibnitz theorem:

$$\begin{aligned}
 3) \quad \underline{r} \cdot \underline{p} (\underline{r} \cdot \underline{p} \psi) &= -\hbar^2 r \left(\left(\frac{d}{dr} \left(r \frac{d}{dr} \right) \right) \psi + \frac{dr}{dr} \frac{d\psi}{dr} \right) \\
 &= -\hbar^2 r \left(\frac{dr}{dr} \frac{d\psi}{dr} + r \frac{d^2\psi}{dr^2} + \frac{dr}{dr} \frac{d\psi}{dr} \right) \\
 &= -\hbar^2 \left(2r \frac{d\psi}{dr} + r^2 \frac{d^2\psi}{dr^2} \right) \\
 &= -\hbar^2 \frac{d}{dr} \left(r^2 \frac{d\psi}{dr} \right) \quad - (13)
 \end{aligned}$$

Now we: $\underline{p} = -i\hbar \underline{\nabla}$ - (14)

to find that eq. (7) is:

$$\begin{aligned}
 -\frac{\hbar^2}{2m} \nabla^2 \psi &= \frac{1}{2m} \left(-\frac{\hbar^2}{r^2} \frac{d}{dr} \left(r^2 \frac{d\psi}{dr} \right) - \frac{l(l+1)\hbar^2}{r^2} \psi \right) \\
 &+ \frac{\hbar}{r} \left(\frac{d}{dr} (\underline{\sigma} \cdot \underline{L} \psi) + \underline{\sigma} \cdot \underline{L} \frac{d\psi}{dr} \right) + \frac{\hbar}{r^2} \underline{\sigma} \cdot \underline{L} \psi \\
 &\quad - (15)
 \end{aligned}$$

Now we: $\frac{d}{dr} (\underline{\sigma} \cdot \underline{L} \psi) = \underline{\sigma} \cdot \underline{L} \frac{d\psi}{dr}$ - (16)

using eqs. (5) and (11).

Therefore the Hamiltonian H_1 can be expressed as follows:

4):

$$\begin{aligned}
 H_1 \psi &= -\frac{\hbar^2}{2m} \nabla^2 \psi = -\frac{\hbar^2}{2m} \left(\frac{1}{r^2} \frac{d}{dr} \left(r^2 \frac{d\psi}{dr} \right) + \frac{l(l+1)}{r^2} \psi \right) \\
 &\quad + \frac{1}{2m} \left(\frac{2}{r} \left(2 \underline{S} \cdot \underline{L} \frac{d\psi}{dr} + \frac{\underline{S} \cdot \underline{L}}{r} \psi \right) \right) \\
 &= -\frac{\hbar^2}{2m} \left(\frac{1}{r^2} \frac{d}{dr} \left(r^2 \frac{d\psi}{dr} \right) + l(l+1) \psi \right) \\
 &\quad + \frac{1}{2m} \left(\frac{2}{r} \underline{S} \cdot \underline{L} \left(2 \frac{d\psi}{dr} + \frac{1}{r} \psi \right) \right) \quad - (17)
 \end{aligned}$$

The Laplacian in spherical polar coordinates is:

$$\begin{aligned}
 \nabla^2 \psi &= \frac{1}{r^2} \frac{d}{dr} \left(r^2 \frac{d\psi}{dr} \right) + \frac{1}{r^2 \sin \theta} \frac{d}{d\theta} \left(\sin \theta \frac{d\psi}{d\theta} \right) \\
 &\quad + \frac{1}{r^2 \sin^2 \theta} \frac{d^2 \psi}{d\phi^2} \quad - (18)
 \end{aligned}$$

and the spherical harmonics are defined by:

$$L^2 Y_l^m = l(l+1) \hbar^2 Y_l^m \quad - (19)$$

$$\text{Therefore if: } \psi = Y_l^m \quad - (20)$$

The first contribution of terms in eq. (17) is the Laplacian term.

5) The overall result is therefore:

$$\boxed{-\frac{\hbar^2}{2m} \underline{\sigma} \cdot \underline{\nabla} \underline{\sigma} \cdot \underline{\nabla} \psi = -\frac{\hbar^2}{2m} \nabla^2 \psi + \frac{1}{m} \left(\frac{s \cdot L}{r} \left(2 \frac{d\psi}{dr} + \frac{1}{r} \psi \right) \right)} \quad - (21)$$

where $\psi = Y_l^m e^{-r/a_0} \quad - (22)$

The spherical harmonics are part of the hydrogenic wave functions and eq. (21) is expressed in the spherical polar coordinates. It is seen that spin orbit coupling occurs at a fundamental level

Eq. (21) can be written as:

$$-\frac{\hbar^2}{2m} \underline{\sigma} \cdot \underline{\nabla} \underline{\sigma} \cdot \underline{\nabla} \psi = -\frac{\hbar^2}{2m} \nabla^2 \psi + \frac{\hbar^2}{2mr} (j(j+1) - l(l+1) - s(s+1)) \left(2 \frac{d\psi}{dr} + \frac{1}{r} \psi \right) \quad - (23)$$

giving two new types of energy expectation value

$$E_1 = \frac{\hbar^2}{m} (j(j+1) - l(l+1) - s(s+1)) \int \psi^* \frac{1}{r} \frac{d\psi}{dr} d\tau \quad - (24)$$

and:

$$b) E_2 = \frac{\hbar^2}{2m} (j(j+1) - l(l+1) - s(s+1)) \int \psi^* \frac{1}{r^3} \psi d\tau \quad - (25)$$

This analysis for a free electron can be extended to the H atom by considering:

$$H_2 \psi = \left(e\psi + \frac{1}{2m} \underline{\sigma} \cdot \underline{p} \underline{\sigma} \cdot \underline{p} \right) \psi \quad - (26)$$

is a non-relativistic approximation. The usual Hamiltonian of the H atom for example is:

$$H_1 = -\frac{\hbar^2}{2m} \nabla^2 - \frac{e^2}{4\pi\epsilon_0 r} \quad - (27)$$

giving the well known hydrogenic wave functions instead of the spherical harmonics. Eq. (21) is therefore extended to:

$$H_3 \psi = -\frac{\hbar^2}{2m} \underline{\sigma} \cdot \underline{\nabla} \underline{\sigma} \cdot \underline{\nabla} \psi - \frac{e^2}{4\pi\epsilon_0 r} \psi$$

$$= -\frac{\hbar^2}{2m} \nabla^2 \psi - \frac{e^2}{4\pi\epsilon_0 r} \psi + \frac{1}{m} \left(\frac{\underline{s} \cdot \underline{L}}{r} \left(2 \frac{d\psi}{dr} + \frac{1}{r} \psi \right) \right) \quad - (28)$$

which has to be solved numerically.