# 250(1): Systematic Development of the Dirac Hamiltonian

This note considers the spin orbit Hamiltonian from the fermion equation or chiral representation of the Dirac equation:

$$\hat{H} = \frac{e}{4m^2c^2}\left(\underline{\sigma}\cdot\left(-i\hbar\underline{\nabla} - e\underline{A}\right)\phi\,\underline{\sigma}\cdot\left(\underline{p} - e\underline{A}\right)\right)\psi \quad -(1)$$

in which the $\underline{p}$ in the second bracket is a function on its

the original spin orbit Hamiltonian:

$$\hat{H}_{SO} = \frac{e}{4m^2c^2}\left(\underline{\sigma}\cdot\left(-i\hbar\underline{\nabla}\right)\phi\,\underline{\sigma}\cdot\underline{p}\right)\psi \quad -(2)$$

It will be shown that the inclusion of the vector potential $\underline{A}$ produces new observable effects. These will have their counterparts in particle collision theory and low energy nuclear reactors.

The Hamiltonian (1) can be expanded as:

$$\begin{aligned}
\hat{H} = & -\frac{ie\hbar}{4m^2c^2}\left(\underline{\sigma}\cdot\underline{\nabla}\left(\phi\,\underline{\sigma}\cdot\underline{p}\,\psi\right)\right) \\
& - \frac{e^2}{4m^2c^2}\,\underline{\sigma}\cdot\underline{A}\,\phi\,\underline{\sigma}\cdot\underline{p}\,\psi \qquad -(3) \\
& + \frac{ie^2\hbar}{4m^2c^2}\left(\underline{\sigma}\cdot\underline{\nabla}\left(\phi\,\underline{\sigma}\cdot\underline{A}\,\psi\right)\right) \\
& + \frac{e^3\phi}{4m^2c^2}\,\underline{\sigma}\cdot\underline{A}\,\underline{\sigma}\cdot\underline{A}\,\psi
\end{aligned}$$

2) There are three new hamiltonians, each giving new effects. This note will start the development of these hamiltonians.

Hamiltonian 1

This is:

$$\hat{H}_1 = \frac{e^3 \phi}{4m^2c^2} \underline{\sigma} \cdot \underline{A} \, \underline{\sigma} \cdot \underline{A} \quad -(4)$$

If $\underline{A}$ is real valued:

$$\hat{H}_1 = \frac{e^3 \phi A^2}{4m^2c^2} \quad -(5)$$

If it is assumed that $\phi$ is Coulombic then:

$$\phi = -\frac{e}{4\pi\epsilon_0 r} \quad -(6)$$

so

$$\hat{H}_1 = -\frac{e^4}{16\pi\epsilon_0 m^2c^2} \frac{A^2}{r} \quad -(7)$$

It has a similar $e^4$ dependence to the well known energy levels of the hydrogen atom:

$$E_n = \frac{-\mu e^4}{32\pi^2\epsilon_0^2\hbar^2} \frac{1}{n^2} \quad -(8)$$

If there exists a vector potential $\underline{A}$ in an atom or molecule then eq. (7) produces observable effects.

3) There are several ways of interpreting and developing eq. (7). The simplest is to use the general result:

$$\underline{A} = \frac{1}{2} \underline{B} \times \underline{r} \quad -(9)$$

so

$$\underline{\sigma} \cdot \underline{A} \, \underline{\sigma} \cdot \underline{A} = \frac{1}{4} \underline{B} \times \underline{r} \cdot \underline{B} \times \underline{r} \quad -(10)$$

$$= \frac{1}{4} B^2 r^2 - (\underline{B} \cdot \underline{r})(\underline{B} \cdot \underline{r})$$

If

$$\underline{B} \perp \underline{r} \quad -(11)$$

then

$$A^2 = \frac{1}{4} B^2 r^2 \quad -(12)$$

Taking the ensemble average:

$$\langle A^2 \rangle = \frac{1}{4} \langle r^2 \rangle B^2 \quad -(13)$$

and eq. (7) becomes:

$$\hat{H}_1 = - \frac{e^4}{64 \pi \epsilon_0 m^2 c^2 r} \langle r^2 \rangle B^2 \quad -(14)$$

for a Coulomb potential, or in general:

$$\boxed{\hat{H}_1 = \frac{e^3 \phi}{4 m^2 c^2} \langle r^2 \rangle B^2} \quad -(15)$$

Quantum mechanical perturbation theory can be applied to the result (15) as usual. As usual with this type of theory, eq. (15) is a precise result, and should be looked for experimentally.

†) Eq. (15) is a type of field induced spin orbit coupling.

As in note 248(6), eq. (1), there also exists the hamiltonian:

$$\hat{H}_2 = \frac{e^2}{2m} \underline{\sigma} \cdot \underline{A} \, \underline{\sigma} \cdot \underline{A} \quad -(16)$$

The Pauli algebra in eqs. (4) and (16) can be developed using the identity given by E. Merzbacher, "Quantum Mechanics" (Wiley, 1970), p. 605, eq. (24.63):

$$\underline{\sigma} \cdot \underline{p} = \frac{1}{r^2} (\underline{\sigma} \cdot \underline{r})(\underline{\sigma} \cdot \underline{r})(\underline{\sigma} \cdot \underline{p})$$

$$= \underline{\sigma} \cdot \hat{\underline{r}} \left( \hat{\underline{r}} \cdot \underline{p} + \frac{i}{r} \underline{\sigma} \cdot (\underline{r} \times \underline{p}) \right) \quad -(17)$$

where

$$\hat{\underline{r}} = \frac{\underline{r}}{r}, \quad -(18)$$

and

$$\underline{L} = \underline{r} \times \underline{p} \quad -(19)$$

Therefore:

$$\underline{\sigma} \cdot \underline{A} = \underline{\sigma} \cdot \hat{\underline{r}} \left( \hat{\underline{r}} \cdot \underline{A} + \frac{i}{r} \underline{\sigma} \cdot (\underline{r} \times \underline{A}) \right) \quad -(20)$$

It follows that:

$$\underline{\sigma} \cdot \underline{A} \, \underline{\sigma} \cdot \underline{A} = \underline{\sigma} \cdot \hat{\underline{r}} \, \underline{\sigma} \cdot \hat{\underline{r}} \left( \hat{\underline{r}} \cdot \underline{A} + \frac{i}{r} \underline{\sigma} \cdot (\underline{r} \times \underline{A}) \right)^2$$

$$= \left(\underline{\hat{r}}\cdot\underline{A} + \frac{i}{r}\,\underline{\sigma}\cdot(\underline{r}\times\underline{A})\right)^2$$

because:

$$\underline{\sigma}\cdot\underline{\hat{r}}\,\underline{\sigma}\cdot\underline{\hat{r}} = 1 \quad -(22)$$

Therefore the hamiltonian (16) for example can be written as:

$$\hat{H}_2 = \frac{e^2}{2m}\left(\underline{\hat{r}}\cdot\underline{A} + \frac{i}{r}\,\underline{\sigma}\cdot(\underline{r}\times\underline{A})\right)^2 \quad -(23)$$

$$= \frac{e^2}{2m}\left(\underline{\hat{r}}\cdot\underline{A}\,\underline{\hat{r}}\cdot\underline{A} + \frac{2i}{r}\,\underline{\sigma}\cdot(\underline{r}\times\underline{A})(\underline{\hat{r}}\cdot\underline{A}) - \frac{1}{r^2}\,\underline{\sigma}\cdot(\underline{r}\times\underline{A})\,\underline{\sigma}\cdot(\underline{r}\times\underline{A})\right)$$

Now consider the hamiltonian:

$$\boxed{\hat{H}_{22} = \frac{e^2}{mr}\, i\,\underline{\sigma}\cdot(\underline{r}\times\underline{A})(\underline{\hat{r}}\cdot\underline{A})} \quad -(24)$$

- This hamiltonian leads to a new type of ESR and NMR as follows.

Consider the ~~rotating~~ electromagnetic potential:

$$\underline{A} = \frac{A^{(0)}}{\sqrt{2}}\,(\underline{i} - i\underline{j})\,e^{i(\Omega t - kZ)} \quad -(25)$$

where $\Omega$ is the rotating angular frequency.

Using standard physics initially for the sake of argument, eq. (25) gives the

6) results:

$$\underset{\sim}{r} \cdot \underline{A} = \frac{A^{(0)}}{\sqrt{2}}(X - iY)e^{i\phi} \quad -(26)$$

$$\underline{r} \times \underline{A} = \begin{vmatrix} \underline{i} & \underline{j} & \underline{k} \\ X & Y & Z \\ 1 & -i & 0 \end{vmatrix} \frac{1}{\sqrt{2}} A^{(0)} e^{i\Omega t}$$

$$= \frac{A^{(0)}}{\sqrt{2}} e^{i\phi}(-iX - Y)\underline{k} + \dots,$$

So

$$\underline{r} \times \underline{A}\ \underline{r} \cdot \underline{A} = -\frac{A^{(0)2}}{2} e^{2i\phi}(iX + Y)(X - iY)\underline{k} + \dots$$

$$= -\frac{A^{(0)2}}{2}(\cos 2\phi + i\sin 2\phi)(2YX + i(X^2 - Y^2))\underline{k} + \dots$$

$$-(27)$$

The imaginary part of this result is:

$$\mathrm{Im}(\underline{r} \times \underline{A}\ \underline{r} \cdot \underline{A})$$

$$= -\frac{A^{(0)2}}{2} i\left(2YX \sin 2\phi + (X^2 - Y^2)\cos 2\phi\right)\underline{k} + \dots \quad -(28)$$

Therefore the Hamiltonian (24) has the real and physical component:

$$\hat{H}_{22} = \frac{e^2 A^{(0)2}}{2mr^2}\left(2XY \sin 2\phi + (X^2 - Y^2)\cos 2\phi\right)\sigma_Z \quad -(29)$$

and resonance occurs between the states of $\sigma_Z$.

Finally, if we consider

Finally consider the average of the Hamiltonian (24):

$$\langle \hat{H}_{22} \rangle = \frac{e^2}{mr^2} i \underline{\sigma} \cdot (\underline{r} \times \underline{A})(\underline{r} \cdot \underline{A}^*) \quad -(30)$$

where $A^*$ is the complex conjugate of $\underline{A}$:

$$\underline{A}^* = \frac{1}{\sqrt{2}} (\underline{i} + i\underline{j}) \exp(-i\phi) \quad -(31)$$

and

$$\phi = \Omega t - kZ. \quad -(32).$$

Then

$$\underline{r} \cdot \underline{A}^* = X + iY \quad -(33)$$

and

$$\underline{r} \times \underline{A} \; \underline{r} \cdot \underline{A}^* = -\frac{A^{(0)2}}{2} (iX + Y)(X + iY) \quad -(34)$$

$$= -\frac{A^{(0)2}}{2} i (X^2 + Y^2)$$

Therefore:

$$\boxed{\langle \hat{H}_{22} \rangle = \frac{e^2 A^{(0)2}}{2mr^2} (X^2 + Y^2) \sigma_Z} \quad -(35)$$

and resonance can be induced between the states of $\underline{\sigma_Z}$. If the following definition is made:

$$B^{(0)} := \frac{A^{(0)}}{\sqrt{2}\, r} \quad -(36)$$

the Hamiltonian (35) becomes:

$$\langle \hat{H}_{22} \rangle = \frac{e^2 B^{(0)}}{m} \langle X^2 + Y^2 \rangle \sigma_Z \quad -(37)$$

which is very similar to the second order hamiltonian obtained in a static magnetic field:

$$H_2 = \frac{e^2}{8m} B^2 \langle X^2 + Y^2 \rangle \quad -(38)$$

the difference is that eqn. (37) premultiplies $\sigma_Z$, so eq. (37) leads to electron spin resonance induced by an electromagnetic field, i.e. another type of RFR.