249(2): 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 as in 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 ϕ 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.

) 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.

4) 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:

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

(21)

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

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 potential:

$$\underline{A} = A^{(0)}\left(\underline{i} + i\underline{j}\right)e^{-i\Omega t} \quad -(25)$$

where Ω is the rotation angular frequency.

Using standard physics initially for a rather d[illegible] argument, eq. (25) gives the rotating magnetic flux density:

$$\underline{B} = \underline{\nabla} \times \underline{A} \quad -(26)$$

In order for this $\underline{B}$ to be non-zero $\underline{A}$ is defined as:

$$\underline{A} = B^{(0)} \left(Y \underline{i} + i X \underline{j} \right) e^{-i\Omega t} \quad -(27)$$

so

$$\underline{B} = \underline{\nabla} \times \underline{A} = B^{(0)} e^{-i\Omega t} \begin{vmatrix} \underline{i} & \underline{j} & \underline{k} \\ \partial/\partial X & \partial/\partial Y & \partial/\partial Z \\ Y & iX & 0 \end{vmatrix}$$

$$= B^{(0)} e^{-i\Omega t} (i - 1) \underline{k} \quad -(28)$$

$$= B^{(0)} (i-1)(\cos \Omega t - i \sin \Omega t) \underline{k}$$

The real and physical part of this magnetic flux density is:

$$\boxed{\text{Real } \underline{B} = B^{(0)} \underline{k} (\sin \Omega t - \cos \Omega t)} \quad -(29)$$

and oscillates with time along the Z axis.

In order to illustrate the existence of the new type of ESR or NMR consider:

$$\underline{r} = X \underline{i} + Y \underline{j} + Z \underline{k} \quad -(30)$$

inside an atom or molecule. It follows that:

$$\underline{r} \cdot \underline{A} = B^{(0)} XY(1+i) \exp(-i\Omega t) \quad -(31)$$

and

$$\underline{r} \times \underline{A} = B^{(0)} e^{-i\Omega t} \begin{vmatrix} \underline{i} & \underline{j} & \underline{k} \\ X & Y & Z \\ Y & iX & 0 \end{vmatrix} \quad -(32)$$

$$= B^{(0)} e^{-i\Omega t} \left((Y^2 + iX^2) \underline{k} + XZ(\underline{j} - i\underline{i}) \right)$$

For simplicity of development consider the Z component:

$$(\underline{r} \times \underline{A})_Z = B^{(0)} e^{-i\Omega t} (Y^2 + iX^2) \underline{k} \quad -(33)$$

then the hamiltonian:

$$\hat{H}_{22} = \frac{e^2}{mr} i\underline{\sigma} \cdot (\underline{r} \times \underline{A})(\hat{\underline{r}} \cdot \underline{A}) \quad -(34)$$

can be calculated from eqs. (31) and (33) and contains real and imaginary parts. The real part is the physical part. So:

$$\hat{H}_{22} = \frac{i e^2 B^{(0)2}}{mr^2} \sigma_Z e^{-2i\Omega t} (Y^2 + iX^2) XY(1+i)$$

$$= \frac{e^2 B^{(0)2} XY}{mr^2} (Y^2 + iX^2)(i-1) \sigma_Z e^{-2i\Omega t}$$

$$= \frac{e^2 B^{(0)2} XY}{mr^2} \left(i(Y^2 - X^2) - (X^2 + Y^2) \right) e^{-2i\Omega t} \sigma_Z$$

$$= \frac{e^2 B^{(0)2} XY \sigma_Z}{mr^2} \left(\cos 2\Omega t - i \sin 2\Omega t \right) \left(i(Y^2 - X^2) - (X^2 + Y^2) \right) \quad -(35)$$

The real and physical part of the hamiltonian is:

$$\text{Real } \hat{H}_{22} = \frac{e^2 B^{(0)2} XY}{mr^2} \left((Y^2 - X^2) \sin 2\Omega t - (X^2 + Y^2) \cos 2\Omega t \right) \sigma_Z \quad -(36)$$

where

$$r^2 = X^2 + Y^2 + Z^2. \quad -(37)$$

For a homogeneous sample on averaging:

$$\langle X^2 - Y^2 \rangle = 0 \quad -(38)$$

So:

$$\boxed{\langle \hat{H}_{22} \rangle = -\frac{e^2}{m} B^{(0)2} \sigma_Z \left\langle \frac{XY(X^2 + Y^2)}{X^2 + Y^2 + Z^2} \right\rangle \cos 2\Omega t} \quad -(39)$$

<u>Summary</u>

There exist the hamiltonians:

$$\hat{H}_{22} = \frac{ie^2}{mr^2} \underline{\sigma} \cdot \underline{r} \times \underline{A} \; \underline{r} \cdot \underline{A} \quad -(40)$$

and

$$\hat{H}_{12} = \frac{ie^3 \phi}{4m^2 c^2 r^2} \underline{\sigma} \cdot \underline{r} \times \underline{A} \; \underline{r} \cdot \underline{A} \quad -(41)$$

T & A is chosen to be <u>complex valued</u>

i) Such these Hamiltonians give rise to new types of ESR and NMR of great potential utility.

The vector potential $\underline{A}$ can be an externally applied vector potential or an internal atomic or molecular vector potential. In such examples the real parts of $\hat{H}_{22}$ and $\hat{H}_{12}$ are the physically meaningful parts.

In order to re-express the Hamiltonians (40) and (41) in more familiar format it is possible to relate $\underline{r}$ to the magnetic dipole moment and to replace $\underline{A}$ by $\underline{B}$ using:

$$\underline{A} = \frac{1}{2}\underline{B} \times \underline{r} \quad - (42)$$

In order to prove eq. (42) note that:

$$\underline{B} = \underline{\nabla} \times \underline{A} \quad - (43)$$

so

$$\underline{A} = \frac{1}{2}\left(\underline{\nabla} \times \underline{A}\right) \times \underline{r} \quad - (44)$$

and

$$\underline{B} = \frac{1}{2}\,\underline{\nabla} \times \left(\underline{B} \times \underline{r}\right)$$

$$= \frac{1}{2}\left(\underline{B}\left(\underline{\nabla}\cdot\underline{r}\right) - \left(\underline{\nabla}\cdot\underline{B}\right)\underline{r} + \left(\underline{r}\cdot\underline{\nabla}\right)\underline{B} - \left(\underline{B}\cdot\underline{\nabla}\right)\underline{r}\right)$$

$$= \frac{1}{2}\left(\underline{B}\left(\underline{\nabla}\cdot\underline{r}\right) + \left(\underline{r}\cdot\underline{\nabla}\right)\underline{B}\right) = \underline{B} \quad - (45)$$

QED

Eq. (42) can now be used in eqs. (40) and (41) to express them in terms of $\underline{B}$ in general:

$$\hat{H}_{22} = \frac{ie^2}{4mr^2}\,\underline{\sigma}\cdot(\underline{r}\times(\underline{B}\times\underline{r}))(\underline{r}\cdot\underline{B}\times\underline{r}) \quad -(46)$$

$$\hat{H}_{12} = \frac{ie^3\phi}{4m^2c^2r^2}\,\underline{\sigma}\cdot(\underline{r}\times(\underline{B}\times\underline{r}))(\underline{r}\cdot\underline{B}\times\underline{r}) \quad -(47)$$

and resonance occurs between states of $\underline{\sigma}$.

In general the rotating magnetic field is:

$$\underline{B} = B^{(0)}(\underline{i} - i\underline{j})\,e^{i\Omega t} \quad -(48)$$

The electromagnetic field is:

$$\underline{B} = \frac{B^{(0)}}{\sqrt{2}}(\underline{i} - i\underline{j})\,e^{i(\omega t - \kappa Z)} \quad -(49)$$

The field in eq. (48) is rotating and the field in eq. (49) is rotating and translating. They are both circularly polarized, but cause elliptically polarized.

Computer Algebra

This code used to work out the real parts of H_{22} and H_{12} from eqs. (46) to (49).