Relativistic effects on light matter interactions

We continue to describe light semi-classically but improve our description of matter by considering relativistic effects. We will discover spin as an essentially relativistic attribute of elementary particles which resembles an intrinsic magnetic moment in the non relativistic limit.

This chapter is devoted to understanding of how this intrinsic magnetic moment interacts with other magnetic moments due to relative motion of the ion and the electrons. We will learn how these interactions modify energy levels described by n, l, m and the associated selection rules.

First we will briefly review relativistic Q. Mech of free particle.

Relativistic relation of E, momentum p and rest mass m:

$$E^2 = m^2c^4 + p^2c^2 \Rightarrow -\hbar^2\frac{\partial^2\psi}{\partial t^2} = m^2c^4\psi - \hbar^2c^2\nabla^2\psi$$

$E \leftarrow i\hbar\frac{\partial}{\partial t}$, $p \leftarrow -i\hbar\nabla$ → Klein Gordon eqn

Note that the KG equation is satisfied by $e^{i(kx \pm Et/\hbar)}$

Try $\psi = A e^{i(kx \pm Et/\hbar)}$

KG eqn $\Rightarrow$ $E^2 = m^2c^4 + c^2k^2\hbar^2 \Rightarrow E \to \pm\infty$ as $|k| \to \infty$

Note $e^{i(kx + Et/\hbar)}$ not allowed by S.Eq. since TDSE and TISE would give the energies differing by sign.

However KG Eqn must be correct. So we need a different description for relativistic particles which will not lead to the apparently catastrophic scenario of E of particles going to $-\infty$ → Global sink!

Dirac's proposal: $\hat{H} = c\vec{\alpha}\cdot\hat{\vec{p}} + \beta mc^2$ | Retain $E = i\hbar\frac{\partial}{\partial t}$

Motivation was to avoid double derivative of time but treat the spatial coordinates in the same footing as t (or ct more precisely) to be consistent with Sp. Relativity.

The hope was that with suitable choice of $\vec{\alpha}$ and $\beta$ the Eq will merge into KG Eqn yet the description of particles will still be consistent with $E = i\hbar\frac{\partial}{\partial t}$

$\therefore (E - c\vec{\alpha}\cdot\hat{\vec{p}} - \beta mc^2)\psi = 0$ → Dirac Wave Eq$^n$.

with $i\hbar\frac{\partial\psi}{\partial t} = E\psi = H\psi$

Let us consider $\psi$ not as a scalar field in configuration space but are column matrices $\underline{\Psi} = \begin{bmatrix}\psi_1\\ \psi_2\\ \vdots\\ \psi_N\end{bmatrix}$ for each point in coordinate sp.

(This actually become apparent a bit later.)

$\therefore \underline{\underline{H}}, \underline{\underline{\alpha}}$ and $\underline{\underline{\beta}}$ are $N\times N$ matrix and owing to the Hermiticity of $\underline{\underline{H}}$, $\vec{\underline{\underline{\alpha}}} = \vec{\underline{\underline{\alpha}}}^\dagger$ and $\underline{\beta} = \underline{\beta}^\dagger$; Note $\vec{\underline{\underline{\alpha}}} = \hat{i}\underline{\underline{\alpha}}^1 + \hat{j}\underline{\underline{\alpha}}^2 + \hat{k}\underline{\underline{\alpha}}^3$

To find $\vec{\underline{\underline{\alpha}}}$ and $\underline{\beta}$ Dirac equated:

$$(E + \vec{\underline{\underline{\alpha}}}\cdot\hat{\vec{p}} + \underline{\underline{\beta}}mc^2)(\underline{E} - c\vec{\underline{\underline{\alpha}}}\cdot\hat{\vec{p}} - \underline{\underline{\beta}}mc^2)\underline{\Psi} = 0$$

to

$$[\hat{E}^2 - \hat{p}^2c^2 - m^2c^4]\underline{\Psi} = 0 \text{ the KG eq}^n$$

$$\left[E^2 - c^2\left[\sum_{k=1}^{3}(\alpha^k)^2\hat{p}_k^2 + \sum_{(k<l)}^{3}\sum^{3}(\alpha^k\alpha^l + \alpha^l\alpha^k)\hat{p}_k\hat{p}_l\right] - mc^3\left[\sum_{k=1}^{3}(\alpha^k\beta + \beta\alpha^k)\hat{p}_k\right] - m^2c^4\underline{\beta}^2\right]\underline{\Psi} = 0$$

Comparing above with the KG eq$^n$:

$$(\alpha^1)^2 = (\alpha^2)^2 = (\alpha^3)^2 = \beta^2 = 1 \quad \text{— (A)}$$

$$\left[\begin{aligned}&[\alpha^1, \alpha^2]_+ = [\alpha^2, \alpha^3]_+ = [\alpha^3, \alpha^1]_+ = 0\\ &[\alpha^1, \beta]_+ = [\alpha^2, \beta]_+ = [\alpha^3, \beta]_+ = 0\end{aligned}\right] \text{(B)}$$

Note that $\{\alpha^k\}$ and $\beta$ are scalar then the set of (A) equation would have been enough but then they would not satisfy (B). So $\{\alpha^k\}$ and $\beta$ must have more components in them and that leads to the matrix form.

Now if we consider a 2×2 matrix for $\{\alpha^k\}$ and $\beta$, or more simply for $A^2 = B^2 = 1$ and $AB + BA = 0$ then we can show easily that if we start with $x$

A possible (non unique) choice of $\underline{\underline{\alpha}}^1, \underline{\underline{\alpha}}^2, \underline{\underline{\alpha}}^3, \underline{\underline{\beta}}$ was readily available from the idea of quaternions

$$\underset{\substack{\downarrow \\ 4\times 4}}{\vec{\underline{\underline{\alpha}}}} = \begin{pmatrix} 0 & \vec{\underline{\underline{\sigma}}} \\ \vec{\underline{\underline{\sigma}}} & 0 \end{pmatrix} \qquad \underset{\substack{\downarrow \\ 2\times 2}}{\vec{\underline{\underline{\sigma}}}} = \hat{i}\,\underset{\substack{\downarrow \\ \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}}}{\underline{\underline{\sigma}}^1} + \hat{j}\,\underset{\substack{\downarrow \\ \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}}}{\underline{\underline{\sigma}}^2} + \hat{k}\,\underset{\substack{\downarrow \\ \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}}}{\underline{\underline{\sigma}}^3}$$

and $\underline{\underline{\beta}} = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}$ ; $I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$

Similarly $\Psi = \begin{bmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{bmatrix}$, $\Psi^\dagger = (\psi_1^* \ \psi_2^* \ \psi_3^* \ \psi_4^*)$ $(\vec{r}, t)$

$$\rho(\vec{r}, t) = \Psi^\dagger \Psi = \sum_{i=1}^{4} |\psi_i(\vec{r}, t)|^2$$

$$\Rightarrow \frac{\partial \rho}{\partial t} + \nabla \cdot (\Psi^\dagger c \underline{\underline{\vec{\alpha}}} \Psi) \quad \text{(Show HW)}$$

Charged particle in EM field:

$$\left[(E - q\Phi) - c\,\underline{\underline{\vec{\alpha}}} \cdot (\hat{\vec{p}} - q\vec{A}) - \beta mc^2\right]\Psi = 0$$

For time independent A and $\Phi$, as is the case for quasi static environment, due to a slowly moving ion, we can write

$$\Psi = \begin{bmatrix} \psi(r) \\ \eta(r) \end{bmatrix} e^{-iEt/\hbar} \quad \text{where } \underline{\psi}(r) = \begin{bmatrix} \psi_1 \\ \psi_2 \end{bmatrix}, \ \underline{\eta}(r) = \begin{bmatrix} \psi_3 \\ \psi_4 \end{bmatrix} \ \text{(A)}$$

$$E\,\underline{\psi}(r) = c(-i\hbar\nabla - q\vec{A}) \cdot \underline{\underline{\vec{\sigma}}}\,\underline{\eta}(r) + (q\Phi + mc^2)\underline{\psi}(r)$$

$$E\,\underline{\eta}(r) = c(-i\hbar\nabla - q\vec{A}) \cdot \underline{\underline{\vec{\sigma}}}\,\underline{\psi}(r) + (q\Phi - mc^2)\underline{\eta}(r) \quad \text{(B)}$$

Let $E = E' + mc^2$ and $|E'|$ as well as $|q\Phi|$ both $\ll mc^2$

$$E'\underline{\psi}(r) = c(-i\hbar\nabla - q\vec{A}) \cdot \underline{\underline{\vec{\sigma}}}\,\underline{\eta}(r) + q\Phi\,\underline{\psi}(r) \quad \text{(A1)}$$

$$(E' + 2mc^2)\underline{\eta}(r) = c(-i\hbar\nabla - q\vec{A}) \cdot \underline{\underline{\vec{\sigma}}}\,\underline{\psi}(r) + q\Phi\,\underline{\eta}(r) \quad \text{(B1)}$$

considering only the dominant terms,

Now (B1) $\longrightarrow \underline{\eta}(r) = \frac{1}{2mc}(-i\hbar\nabla - q\vec{A})\cdot\underline{\sigma}\,\underline{\Psi}(r)$ — (B2)

since the term with $c$ or $c^2$ are far too greater than the other term.

$$\Rightarrow \frac{\eta(r)}{\Psi(r)} \approx \frac{p}{mc} \approx \frac{v}{c} \Rightarrow \underset{\text{weak}}{|\eta(r)|} \ll \underset{\text{strong}}{|\Psi(r)|}$$

Substituting $\eta(r)$ from (B2) in (A1)

$$E'\underline{\Psi} = \frac{1}{2m}\left[(-i\hbar\nabla - q\vec{A})\cdot\sigma\right]^2\underline{\Psi} + q\phi\underline{\Psi}$$

Use $(\vec{\underline{\sigma}}\cdot\vec{\underline{D}})(\vec{\underline{\sigma}}\cdot\vec{\underline{B}}) = \vec{\underline{D}}\cdot\vec{\underline{B}} + i\vec{\underline{\sigma}}\cdot(\vec{\underline{D}}\times\vec{\underline{B}})$

put $\vec{\underline{D}} = (-i\nabla - q\vec{A})I$; $\vec{B} = (-\nabla - q\vec{A})\underline{\Psi}$ $(-i\hbar\nabla - q\vec{A})\underline{\Psi}$

$$\therefore \left[(-i\hbar\nabla - q\vec{A})\cdot\sigma\right]^2\underline{\Psi} = (-i\hbar\nabla - q\vec{A})\cdot(-i\hbar\nabla - q\vec{A})$$
$$+ i\vec{\underline{\sigma}}\cdot\left[(-i\hbar\nabla - q\vec{A})\times(-i\hbar\nabla - q\vec{A})\right]\underline{\Psi}$$

$\hookrightarrow (-\hbar^2\nabla\times\nabla\underline{\Psi} + i\hbar q A\times\nabla\underline{\Psi} + iq\nabla\times(A\underline{\Psi}) + q^2 A\times A\underline{\Psi}$

$\hookrightarrow = iq\hbar[A\times\nabla\Psi + \Psi(\nabla\times A) + \nabla\Psi\times A]\underline{\Psi}$

$= i\hbar q(\nabla\times A)\underline{\Psi}$

$$\therefore E'\underline{\Psi} = \frac{1}{2m}(-i\hbar\nabla - q\vec{A})\cdot(-i\hbar\nabla - q\vec{A}) - \frac{\hbar q}{2m}\vec{\sigma}\cdot\underset{\vec{B}}{(\nabla\times A)} - e\phi\Big]\underline{\Psi}$$

$q = -e$

$$E'\underline{\Psi} = \left[\frac{1}{2m}(-i\hbar\nabla + e\vec{A})\cdot(-i\hbar\nabla + e\vec{A}) + \frac{e\hbar}{2m}(\vec{\underline{\sigma}}\cdot\vec{B}) - e\phi\right]\underline{\Psi}$$ — (A2)

$\hookrightarrow$ Pauli Eq$^n$

Intrinsic magnetic moment: $\frac{e\hbar}{2m}\vec{\sigma} = \mu_B\vec{\sigma} \longrightarrow$ SPIN

Conventionally: $(-\mu_B\vec{\sigma})$

. The above equation is actually the Heuristically argued Pauli theory to explain Stern Gerlach type experiments. which showed the existence of SPIN. Non relativistic limit of 4 component Dirac theory is then two component. Recall that the Pauli theory. Which is we are only talking about the "strong" component.