## 2. Interaction with External Fields

- Let $A$ be the 4-potential $(\vec{A}, iA_0)$, where $\vec{A}$ and $A_0$ are the ordinary vector and scalar potentials. As in classical and non-relativistic mechanics, the modified Dirac equation can be obtained by the replacement

$$p \rightarrow p - eA$$

so that $$(i\hat{p} - ie\hat{A} + m)\psi = 0 \qquad (20)$$

where $\hat{A} = \gamma_\mu A_\mu$.

- If $A$ is independent of time, then stationary solutions of the form

$$\psi(\vec{r}, t) = \psi_0(\vec{r}) e^{-iEt}$$

exist. Substituting into (20) yields

$$(\vec{\alpha}\cdot\vec{p} + \beta m + eA_0 - e\vec{\alpha}\cdot\vec{A})\psi_0 = E\psi_0 \qquad (21)$$

### 2.1 Electron in a Central Potential

- Set $\vec{A} = 0$ and $A_0 = A_0(r)$, and define $V(r) = eA_0(r)$. For a central potential, $\vec{J}$ is still a constant of the motion, and all the results of Section 1.6 ~~still~~ apply. In particular,

$$\psi_{jLM} = \begin{pmatrix} \varphi_{jLM} \\ \chi_{jLM} \end{pmatrix}$$

with $$\left.\begin{aligned} \phi_{jLM} &= i\,g(r)\,\Omega_{jLM} \\ \chi_{jLM} &= -f(r)\,\Omega_{jL'M}\,. \end{aligned}\right\} \qquad (22)$$

The radial equations are the same as (19) except that $\varepsilon$ is replaced by $\varepsilon - V(r)$. Thus

$$\left.\begin{aligned} \frac{df}{dr} + (1-\kappa)\frac{f}{r} + (\varepsilon - m - V)\,g &= 0 \\ \frac{dg}{dr} + (1+\kappa)\frac{g}{r} - (\varepsilon + m - V)\,f &= 0\,. \end{aligned}\right\} \qquad (23)$$

With a spherically averaged potential and allowance for exchange, these equations become the Dirac-Hartree-Fock equations.

- For the hydrogen atom, $V(r) = -Ze^2/r$. The exact solutions can be written in terms of hypergeometric functions (see A. and B. pp. 122-125). Bethe and Salpeter (p. 69) give explicit solutions for $1s_{1/2}$, $2s_{1/2}$, $2p_{1/2}$, $2p_{3/2}$.

## 2.2 Non-Relativistic Approximations

- At low energies (ie $|\varepsilon - mc^2| \ll mc^2$), $\chi$ is much smaller than $\phi$, and an expansion of the solution in powers of $1/c$ may be useful. The equation to be solved is

$$i\frac{\partial\psi}{\partial t} = \left[ c\vec{\alpha}\cdot\left(\vec{p} - \frac{e}{c}\vec{A}\right) + \beta mc^2 + eA_0 \right]\psi \qquad (24)$$

- For convenience, define $\psi'$ by

$$\psi = \psi' e^{-imc^2 t}$$

to remove the high-frequency rest mass part of the energy. Then

$$i\frac{\partial\psi'}{\partial t} = \left[c\vec{\alpha}\cdot\left(\vec{p}-\frac{e}{c}\vec{A}\right)+(\beta-1)mc^2+eA_0\right]\psi' . \quad (25)$$

Making the usual decomposition

$$\psi' = \begin{pmatrix}\phi' \\ \chi'\end{pmatrix}$$

results in the pair of equations

$$i\frac{\partial\phi'}{\partial t} = c\vec{\sigma}\cdot\left(\vec{p}-\frac{e}{c}\vec{A}\right)\chi' + eA_0\phi' \quad (26)$$

$$i\frac{\partial\chi'}{\partial t} = c\vec{\sigma}\cdot\left(\vec{p}-\frac{e}{c}\vec{A}\right)\phi' + eA_0\chi' - 2mc^2\chi' \quad (27)$$

- Assume that $\chi'$ is $O(\phi/c)$. Then to a first approximation, the second equation gives

$$\chi' = \frac{1}{2mc}\,\vec{\sigma}\cdot\left(\vec{p}-\frac{e}{c}\vec{A}\right)\phi'$$

which justifies the assumption. Substituting this approximation into the first equation yields

$$i\frac{\partial\phi'}{\partial t} = \left\{\frac{1}{2m}\left[\vec{\sigma}\cdot\left(\vec{p}-\frac{e}{c}\vec{A}\right)\right]^2 + eA_0\right\}\phi' \quad (28)$$

- Using $(\vec{\sigma}\cdot\vec{A})(\vec{\sigma}\cdot\vec{B}) = \vec{A}\cdot\vec{B} + i\vec{\sigma}\cdot\vec{A}\times\vec{B}$, it follows that

$$\left[\vec{\sigma}\cdot\left(\vec{p}-\frac{e}{c}\vec{A}\right)\right]^2 = \left(\vec{p}-\frac{e}{c}\vec{A}\right)^2 - \frac{ie}{c}\vec{\sigma}\cdot\left(\vec{p}\times\vec{A}+\vec{A}\times\vec{p}\right)$$

$$= \left(\vec{p}-\frac{e}{c}\vec{A}\right)^2 - \frac{e}{c}\vec{\sigma}\cdot\nabla\times\vec{A}$$

Writing $\vec{H} = \nabla \times \vec{A}$, (26) becomes

$$i\frac{\partial \Phi'}{\partial t} = \left[ \frac{1}{2m}\left(\vec{p} - \frac{e}{c}\vec{A}\right)^2 + eA_0 - \frac{e}{2mc}\vec{\sigma}\cdot\vec{H} \right] \Phi' \quad (29)$$

This is the same as the non-relativistic Schrodinger equation except for the extra term $-\frac{e}{2mc}\vec{\sigma}\cdot\vec{H}$. This term represents the interaction of a particle with magnetic moment

$$\vec{\mu} = \frac{e\hbar}{2mc}\vec{\sigma} \quad (30)$$

with a magnetic field.

2.3 The Second Approximation

- Simplify the notation by defining

$$\vec{\pi} = \vec{p} - \frac{e}{c}\vec{A}.$$

To obtain the next term in the expansion, substitute $\chi' = \frac{1}{2mc}\vec{\sigma}\cdot\vec{\pi}\,\Phi'$ for $\chi'$ in all but the last term of (27) with the result

$$\chi = \frac{1}{2mc}\left[ \vec{\sigma}\cdot\vec{\pi} + \frac{eA_0}{2mc^2}\vec{\sigma}\cdot\vec{\pi} - \frac{i}{2mc^2}\frac{\partial}{\partial t}\vec{\sigma}\cdot\vec{\pi} \right]\Phi$$

Inserting this into (26) yields

$$i\left( \frac{\partial}{\partial t} + \frac{(\vec{\sigma}\cdot\pi)}{4m^2c^2}\frac{\partial}{\partial t}(\vec{\sigma}\cdot\vec{\pi}) \right)\Phi = \left\{ \frac{(\vec{\sigma}\cdot\pi)^2}{2m} + eA_0 + \frac{e}{4m^2c^2}(\vec{\sigma}\cdot\pi)A_0(\vec{\sigma}\cdot\vec{\pi}) \right\}\Phi \quad (31)$$

· The term $i(\vec{\sigma}\cdot\vec{\pi})\frac{\partial}{\partial t}(\vec{\sigma}\cdot\vec{\pi})\Phi$ is

$$i(\vec{\sigma}\cdot\vec{\pi})^2\frac{\partial\Phi}{\partial t} + i(\vec{\sigma}\cdot\vec{\pi})\left(-\frac{e}{c}\vec{\sigma}\cdot\frac{\partial\vec{A}}{\partial t}\right)\Phi$$

for time-dependent potentials. Include the second term above in the right-hand-side of (31) to obtain

$$i\left[1+\frac{(\vec{\sigma}\cdot\vec{\pi})^2}{4m^2c^2}\right]\frac{\partial\Phi}{\partial t} = \left\{\frac{(\vec{\sigma}\cdot\vec{\pi})^2}{2m} + \frac{ie}{4mc^3}(\vec{\sigma}\cdot\vec{p})(\vec{\sigma}\cdot\frac{\partial\vec{A}}{\partial t}) + eA_0 + \frac{e}{4m^2c^2}(\vec{\sigma}\cdot\vec{\pi})A_0(\vec{\sigma}\cdot\vec{\pi})\right\}\Phi \quad (32)$$

where $\vec{\pi}$ has been replaced by $\vec{p}$ in terms of $O(c^{-2})$ or smaller.

- To put (32) in the form $i\frac{\partial\Phi}{\partial t} = H'\Phi$, multiply through by $\left(1-\frac{(\vec{\sigma}\cdot\vec{\pi})^2}{4m^2c^2}\right)$ and retain terms up to $O(c^{-3})$.

$$i\frac{\partial\Phi}{\partial t} = \left\{\left(1-\frac{(\vec{\sigma}\cdot\vec{\pi})^2}{4m^2c^2}\right)\left(\frac{(\vec{\sigma}\cdot\vec{\pi})^2}{2m} + eA_0\right) + \frac{ie}{4mc^3}(\vec{\sigma}\cdot\vec{p})(\vec{\sigma}\cdot\frac{\partial\vec{A}}{\partial t}) + \frac{e}{4m^2c^2}(\vec{\sigma}\cdot\vec{\pi})A_0(\vec{\sigma}\cdot\vec{\pi})\right\}\Phi$$

$$= H'\Phi \quad (33)$$

- At first sight, this looks like a valid Schrödinger-like equation, but there are two difficulties.

1. $H'$ is not a Hermitian operator since it contains the term $\frac{p^2}{4mc^2}eA_0$ and $\frac{ie}{4mc^3}(\vec{\sigma}\cdot\vec{p})(\vec{\sigma}\cdot\frac{\partial\vec{A}}{\partial t})$.

2. The quantity $\int \varphi^* \varphi \, d\vec{r}$ is not conserved in time. Recall from the equation of continuity that the quantity which is conserved is

$$s_0 = \int [\varphi^* \varphi + \chi^* \chi] \, d\vec{r}$$

- Both ills are cured by the same medicine. Define an operator $Q$ and a wave function $\Phi = Q \varphi$ such that $\Phi$ can be normalized up to terms of $O(c^{-3})$

$$\text{ie} \int (\varphi^* \varphi + \chi^* \chi) \, d\vec{r} = \int \Phi^* \Phi \, d\vec{r} \qquad (34)$$

Using $\varphi = Q^{-1} \Phi$, it follows from (33) that $\Phi$ satisfies

$$i \frac{\partial}{\partial t} Q^{-1} \Phi = H' Q^{-1} \Phi$$

Multiply through by $Q$

$$i \frac{\partial}{\partial t} \Phi = \left[ Q H' Q^{-1} - i Q \left( \frac{\partial}{\partial t} Q^{-1} \right) \right] \Phi$$

$$= H \Phi . \qquad (35)$$

To determine $Q$, substitute $\chi = \dfrac{(\vec{\sigma} \cdot \vec{\pi})}{2mc} \varphi$ into (34). Then

$$\int \varphi^* \left[ 1 + \frac{(\vec{\sigma} \cdot \vec{\pi})^2}{4m^2c^2} \right] \varphi \, d\vec{r} = \int \Phi^* \Phi \, d\vec{r}$$

$$= \int \varphi^* Q^\dagger Q \varphi \, d\vec{r}$$

$$= \int \varphi^* Q^2 \varphi \, d\vec{r}$$

provided that $Q = Q^\dagger$.

$$\therefore\ Q \simeq \left[ 1 + \frac{(\vec{\sigma}\cdot\vec{\pi})^2}{8m^2c^2} \right]$$

and $Q^{-1} \simeq \left[ 1 - \frac{(\vec{\sigma}\cdot\vec{\pi})^2}{8m^2c^2} \right]$.

$$\therefore\ QH'Q^{-1} \simeq \frac{(\vec{\sigma}\cdot\vec{\pi})^2}{2m} - \frac{1}{8m^3c^2}(\vec{\sigma}\cdot\vec{\pi})^4 + eA_0$$

$$+ \frac{e}{8m^2c^2}\left[(\vec{\sigma}\cdot\vec{\pi})^2 A_0 - A_0(\vec{\sigma}\cdot\vec{\pi})^2\right] - \frac{e}{4m^2c^2}(\vec{\sigma}\cdot\vec{\pi})^2 A_0$$

$$+ \frac{ie}{4mc^3}(\vec{\sigma}\cdot\vec{p})\left(\vec{\sigma}\cdot\frac{\partial\vec{A}}{\partial t}\right) + \frac{e}{4m^2c^2}(\vec{\sigma}\cdot\vec{\pi})A_0(\vec{\sigma}\cdot\vec{\pi})$$

and
$$-iQ\left(\frac{\partial}{\partial t}Q^{-1}\right) \simeq -i\left(\frac{+e}{8mc^3}\right)\left[(\vec{\sigma}\cdot\vec{p})\left(\vec{\sigma}\cdot\frac{\partial A}{\partial t}\right) + \left(\vec{\sigma}\cdot\frac{\partial A}{\partial t}\right)(\vec{\sigma}\cdot\vec{p})\right]$$

The sum is thus

$$H = QH'Q^{-1} - iQ\left(\frac{\partial}{\partial t}Q^{-1}\right)$$

$$\simeq \frac{(\vec{\sigma}\cdot\vec{\pi})^2}{2m} - \frac{(\vec{\sigma}\cdot\vec{\pi})^4}{8m^3c^2} + eA_0$$

$$+ \frac{e}{8m^2c^2}\left[(\vec{\sigma}\cdot\vec{\pi})^2, A_0\right]_- + \frac{ie}{8mc^3}\left[(\vec{\sigma}\cdot\vec{p}), \left(\vec{\sigma}\cdot\frac{\partial\vec{A}}{\partial t}\right)\right]_-$$

$$- \frac{e}{4m^2c^2}(\vec{\sigma}\cdot\vec{\pi})^2 A_0 + \frac{e}{4m^2c^2}(\vec{\sigma}\cdot\vec{\pi})A_0(\vec{\sigma}\cdot\vec{\pi})$$

Everything is now self-conjugate except for the last two terms. However the non-Hermitian parts of these operators cancel as follows:

$$(\vec{\sigma}\cdot\vec{\pi})A_0(\vec{\sigma}\cdot\vec{\pi}) = A_0(\vec{\sigma}\cdot\vec{\pi})^2 - [A_0(\vec{\sigma}\cdot\vec{\pi})-(\vec{\sigma}\cdot\vec{\pi})A_0](\vec{\sigma}\cdot\vec{\pi})$$

$$= A_0(\vec{\sigma}\cdot\vec{\pi})^2 - \vec{\sigma}\cdot[A_0, \vec{p}]_-(\vec{\sigma}\cdot\vec{\pi})$$

$$= A_0(\vec{\sigma}\cdot\vec{\pi})^2 - i(\vec{\sigma}\cdot\nabla A_0)(\vec{\sigma}\cdot\vec{\pi})$$

$$= A_0(\vec{\sigma}\cdot\vec{\pi})^2 - i\nabla A_0\cdot\vec{\pi} + \vec{\sigma}\cdot\nabla A_0\times\vec{\pi}$$

$$\therefore\ -\frac{e}{4m^2c^2}(\vec{\sigma}\cdot\vec{\pi})^2A_0 + \frac{e}{4m^2c^2}(\vec{\sigma}\cdot\vec{\pi})A_0(\vec{\sigma}\cdot\vec{\pi})$$

$$= +\frac{e}{4m^2c^2}\left\{-[(\vec{\sigma}\cdot\pi)^2, A_0]_- - i\nabla A_0\cdot\vec{\pi} + \vec{\sigma}\cdot\nabla A_0\times\vec{\pi}\right\}$$

and
$$H = \frac{(\vec{\sigma}\cdot\vec{\pi})^2}{2m} - \frac{(\vec{\sigma}\cdot\vec{\pi})^4}{8m^3c^2} + eA_0$$

$$-\frac{e}{8m^2c^2}[(\vec{\sigma}\cdot\vec{\pi})^2, A_0]_- + \frac{ie}{8mc^3}\left[(\vec{\sigma}\cdot\vec{p}), (\vec{\sigma}\cdot\frac{\partial A}{\partial t})\right]_-$$

$$+\frac{e}{4m^2c^2}\left\{-i\nabla A_0\cdot\vec{\pi} + \vec{\sigma}\cdot\nabla A_0\times\vec{\pi}\right\}$$

Let us now make a definite choice of gauge so that $\nabla\cdot\vec{A} = 0$ and

$$\vec{E} = -\nabla A_0 + \frac{1}{c}\frac{\partial\vec{A}}{\partial t} \qquad \text{(coulomb gauge)}$$

Then $[(\vec{\sigma}\cdot\vec{p}), (\vec{\sigma}\cdot\frac{\partial\vec{A}}{\partial t})]_- = \vec{\sigma}\cdot\nabla\times\frac{\partial\vec{A}}{\partial t} + 2i\vec{\sigma}\cdot\frac{\partial\vec{A}}{\partial t}\times\vec{p}$

and $[(\vec{\sigma}\cdot\vec{\pi})^2, A_0]_- = -\nabla^2A_0 - 2i(\nabla A_0)\cdot\vec{\pi}$

The terms involving $\nabla A_0\cdot\vec{\pi}$ cancel and we are left with

$$H = \frac{(\vec{\sigma}\cdot\vec{\pi})^2}{2m} + eA_0 - \frac{(\vec{\sigma}\cdot\vec{\pi})^4}{8m^3c^2} - \frac{e}{4m^2c^2}\,\vec{\sigma}\cdot\vec{E}\times\vec{\pi}$$

$$+ \frac{e}{8m^2c^2}\nabla^2 A_0 + \frac{ie}{8m^2c^3}\,\vec{\sigma}\cdot\frac{\partial\vec{H}}{\partial t} \qquad (36)$$

where $\vec{\pi} = \vec{p} - \frac{e}{c}\vec{A}$

$$\vec{E} = -\nabla A_0 + \frac{1}{c}\frac{\partial\vec{A}}{\partial t}.$$

and only terms up to $O(c^{-3})$ should be retained.

Physical Interpretation

- The first two terms are the same as before.
- The third term represents the relativistic increase of mass with velocity. Recall that

$$E = (p^2c^2 + m^2c^4)^{1/2} + A_0$$

$$= mc^2\left(1 + \frac{p^2}{m^2c^2}\right)^{1/2} + A_0$$

$$\therefore\ E - mc^2 = \frac{p^2}{2m} - \frac{p^4}{8m^3c^2} + \cdots + A_0.$$

- The fourth term is the interaction energy between a moving magnetic dipole and an electric field. (spin-orbit interaction)
- Since $\nabla^2 A_0 = -4\pi\rho$, the fifth term vanishes except where charges are located.