13.4 Foldy - Wouthuysen Transformation:

Systematic approach to go for higher orders in the nonrelativistic limit for the Dirac equation $\longrightarrow$ finestructure of hydrogen atom

$$i\hbar \frac{\partial \Psi}{\partial t} = \hat{H}\Psi, \quad \hat{H} = c\vec{\alpha}(\hat{\vec{p}} - q\vec{A}) + mc^2\beta + q\varphi, \quad \vec{\alpha} = \begin{pmatrix} 0 & \vec{\sigma} \\ \vec{\sigma} & 0 \end{pmatrix}$$

starting point: $\vec{p} = \vec{0}, \vec{A} = \vec{0}, \varphi = 0 \hat{=}$ restframe + vanishing ~~electromagnetic~~ field

$$\Rightarrow \hat{H} = mc^2\beta, \quad \beta = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}$$

two sets of eigenvectors:

$E > 0$ (particle): $\Psi = \begin{pmatrix} u \\ 0 \end{pmatrix}$, $E < 0$ (antiparticle): $\Psi = \begin{pmatrix} 0 \\ v \end{pmatrix}$

Either finite momentum or non-vanishing electromagnetic field couple both Weyl spinors u, v

Foldy-Wouthuysen transformation: decoupling of Weyl spinors in the non-relativistic limit

$$\Psi' = e^{\hat{S}}\Psi, \quad e^{\hat{S}} \text{ unitary} \hat{=} e^{-\hat{S}} = e^{\hat{S}^+} \Rightarrow \hat{S}^+ = -\hat{S}$$

Schrieffer-Wolff transformation: superconductivity

$$i\hbar \frac{\partial}{\partial t}(e^{-\hat{S}}\Psi') = -i\hbar \frac{\partial \hat{S}}{\partial t} e^{-\hat{S}}\Psi' + i\hbar \underline{e^{-\hat{S}}} \frac{\partial \Psi'}{\partial t} = \hat{H} e^{-\hat{S}}\Psi' \quad \Big| \; e^{+\hat{S}}\cdot$$

$$i\hbar \frac{\partial}{\partial t}\Psi' = \hat{H}'\Psi', \quad \hat{H}' = e^{+\hat{S}}\left(\hat{H} + i\hbar \frac{\partial \hat{S}}{\partial t}\right)e^{-\hat{S}} = \boxed{e^{\hat{S}}\left(\hat{H} - \underline{i\hbar \frac{\partial}{\partial t}}\right)e^{-\hat{S}}} \quad (*)$$

After the Schrieffer – Wolff transformation: decoupling

$$\hat{H}' = \begin{pmatrix} \hat{H}'_+ & 0 \\ 0 & \hat{H}'_- \end{pmatrix}$$

If not exactly then at least perturbatively; i.e. in nonrelativistic limit

Definition: An operator $\hat{\mathcal{E}}$ or $\hat{O}$ is called even or odd if it is diagonal in upper/lower Weyl spinors or couples upper/lower Weyl spinors

$$\hat{\mathcal{E}} = \begin{pmatrix} * & 0 \\ 0 & * \end{pmatrix}, \qquad \hat{O} = \begin{pmatrix} 0 & * \\ * & 0 \end{pmatrix}$$

examples: $\underbrace{\beta = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}}_{\text{even}}$, $\underbrace{\vec{\alpha} = \begin{pmatrix} 0 & \vec{\sigma} \\ \vec{\sigma} & 0 \end{pmatrix}}_{\text{odd}}$

In principle each operator can be decomposed into an even and an odd operator.

Example: $\hat{H} = \underbrace{mc^2\beta}_{\text{unperturbed, even}} + \underbrace{\hat{\mathcal{E}}}_{\text{even}} + \underbrace{\hat{O}}_{\underbrace{\text{odd}}_{\text{perturbation}}}$; $\hat{\mathcal{E}} = q\varphi$, $\hat{O} = c\vec{\alpha}\cdot(\underbrace{\vec{p}}_{\text{small momenta}} - q\underbrace{\vec{A}}_{\text{weak vector potential}})$

$\Rightarrow$ $\hat{S}$ is supposed to be small $\Rightarrow$ Investigate (*)

First Term:

$$\hat{F}(\lambda) = e^{\lambda\hat{S}}\,\hat{H}\,e^{-\hat{S}\lambda} \qquad \hat{F}(0) = \hat{H}$$

λ ← artificial smallness parameter

$$\hat{F}'(\lambda) = e^{\lambda\hat{S}}[\hat{S},\hat{H}]_-\,e^{-\hat{S}\lambda} \qquad \hat{F}'(0) = [\hat{S},\hat{H}]_-$$

$$\hat{F}''(\lambda) = e^{\lambda\hat{S}}[\hat{S},[\hat{S},\hat{H}]_-]_-\,e^{-\hat{S}\lambda} \qquad \hat{F}''(0) = [\hat{S},[\hat{S},\hat{H}]_-]_-$$

Taylor series in λ:

$$\hat{F}(\underbrace{1}_{=\lambda}) = e^{\hat{S}} \hat{H} e^{-\hat{S}} = \underbrace{\hat{H} + [\hat{S}, \hat{H}]_-}_{\text{lowest order}} + \frac{1}{2}[\hat{S},[\hat{S},\hat{H}]_-]_- + \ldots = \hat{H}'$$

Formal notation for nested commutators: $(\mathrm{ad}\,\hat{S})\hat{H} = [\hat{S}, \hat{H}]_-$

$$e^{\hat{S}} \hat{H} e^{-\hat{S}} = \sum_{k=0}^{\infty} \frac{1}{k!} (\mathrm{ad}\,\hat{S})^k \hat{H}$$

<u>Second Term:</u> neglect time dependences

$$-e^{-\hat{S}}\, i\hbar \frac{\partial}{\partial t} e^{\hat{S}} = i\hbar \left\{ \frac{\partial \hat{S}}{\partial t} + \frac{1}{2}\left[\hat{S}, \frac{\partial \hat{S}}{\partial t}\right]_- + \frac{1}{6}\left[\hat{S},\left[\hat{S}, \frac{\partial \hat{S}}{\partial t}\right]_-\right]_- + \ldots \right\}$$

Application to Dirac Hamiltonian: lowest order elimination of odd $\hat{O}$

$$\hat{H}' = \hat{H} + [\hat{S},\hat{H}]_- + \ldots = mc^2\beta + \underbrace{\hat{\varepsilon}}_{\text{small}} + \hat{O} + [\underbrace{\hat{S}}_{\text{small}}, mc^2\beta \cancel{+ \underbrace{\hat{\varepsilon} + \hat{O}}_{\text{small}}}]_- + \ldots$$

lowest order approx.

Eliminate odd terms in lowest order:

$$\text{Condition: } \underbrace{\hat{O}}_{\text{given}} + mc^2 [\underbrace{\hat{S}}_{=?}, \beta]_- = 0 \Rightarrow \hat{O} - 2\kappa mc^2 \hat{O} = 0 \rightarrow \kappa = \frac{1}{2mc^2}$$

Ansatz: $\hat{S} = \kappa\beta\hat{O}$, coefficient $\kappa = ?$

$$\beta\hat{O} = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}\begin{pmatrix} 0 & B \\ A & 0 \end{pmatrix} = \begin{pmatrix} 0 & B \\ -A & 0 \end{pmatrix}$$

$$\hat{O}\beta = \begin{pmatrix} 0 & B \\ A & 0 \end{pmatrix}\begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix} = \begin{pmatrix} 0 & -B \\ A & 0 \end{pmatrix}$$

$$\beta\hat{O} + \hat{O}\beta = [\beta, \hat{O}]_+ = 0 \quad (**)$$

$$\beta = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}$$

$$[\hat{S}, \beta]_- = \kappa[\beta\hat{O}, \hat{\beta}]_- = \kappa\{\beta\underbrace{\hat{O}\beta}_{\overset{(**)}{=} -\beta\beta\hat{O}} - \beta\beta\hat{O}\} = -2\kappa\underbrace{\beta^2}_{=1}\hat{O} = -2\kappa\hat{O}$$

Result: $\hat{S} = -\frac{1}{2mc^2}\beta\hat{O}$, $\hat{O} = c\vec{\alpha}(\vec{\hat{p}} - q\vec{\hat{A}})$

Transformed Hamiltonian after a long but straight-forward calculation:

$$\hat{H}' = mc^2\beta + \hat{\mathcal{E}}' + \hat{O}'$$

$$\hat{\mathcal{E}}' = \hat{\mathcal{E}} + \frac{1}{2mc^2}\beta\hat{O}^2 - \frac{1}{8m^2c^4}[\hat{O},[\hat{O},\hat{\mathcal{E}}]_-]_- - \frac{1}{8m^3c^6}\beta\hat{O}^4 + \dots$$

$$\hat{O}' = \frac{1}{2mc^2}\beta[\hat{O},\hat{\mathcal{E}}]_- - \frac{1}{3m^2c^4}\hat{O}^3 - \frac{1}{48m^3c^6}\beta[\hat{O},[\hat{O},[\hat{O},\hat{\mathcal{E}}]_-]_-]_- + \dots$$

one needs to perform subsequent unitary transformations to higher order in order to eliminate higher-order odd terms.

Physical interpretation:

- Term of order $1/mc^2$: nonrelativistic limit from last lecture

$$\frac{1}{2mc^2}c^2\beta\underbrace{[(\vec{\hat{p}} - q\vec{\hat{A}})\cdot\vec{\sigma}][(\vec{\hat{p}} - q\vec{\hat{A}})\cdot\vec{\sigma}]}_{\text{analyzed previously}}$$

$= \hat{O}/c$

$$= \underbrace{\frac{1}{2m}(\vec{\hat{p}} - q\vec{\hat{A}})^2}_{\text{Landé factor: } g_\ell = 1} + \underbrace{\frac{-q}{m}\vec{\hat{S}}\cdot\vec{\hat{B}}}_{\text{Landé factor } g_S = 2}$$

- Term of order $1/m^3c^6$:

$$-\frac{1}{8m^3c^6}\beta c^4(\vec{\hat{p}} - q\vec{\hat{A}})^4 \overset{\vec{A}=\vec{0}}{=} -\frac{1}{8m^3c^2}\beta\vec{\hat{p}}^4$$

special relativistic correction of energy momentum dispersion

$$E = \sqrt{\vec{p}^2c^2 + m^2c^4} = mc^2 + \frac{\vec{p}^2}{2m} - \frac{1}{8m^3c^2}\vec{p}^4 + \dots \checkmark$$

• Term of order $1/m^2c^4$: $\qquad \vec E = -\,\mathrm{grad}\,\varphi$

$$[\hat O, \hat{\mathcal E}]_- = [c\vec\alpha(\hat{\vec p} - \cancel{q\vec A}), q\varphi]_- = cq\,\vec\alpha\,[\hat{\vec p}, \varphi]_- = cq\frac{\hbar}{i}\vec\alpha\cdot\vec\nabla\varphi$$

$$= -i\hbar c q\,\vec\alpha\cdot\vec E$$

$$[\hat O, [\hat O, \hat{\mathcal E}]_-]_- = [c\vec\alpha\cdot(\hat{\vec p} - q\vec A),\ i\hbar c q\,\vec\alpha\cdot\vec E]_-$$

$(\vec\sigma\cdot\vec A)(\vec\sigma\cdot\vec B)$ last time $\vec A\cdot\vec B + i\,\vec\sigma(\vec A\times\vec B)$

$$(\vec\alpha\cdot\vec A)(\vec\alpha\cdot\vec B) = \begin{pmatrix}0 & \sigma_j\\ \sigma_j & 0\end{pmatrix}\begin{pmatrix}0 & \sigma_k\\ \sigma_k & 0\end{pmatrix}A_jB_k = \begin{pmatrix}\sigma_j\sigma_k & 0\\ 0 & \sigma_j\sigma_k\end{pmatrix}A_jB_k$$

$$= \vec A\cdot\vec B\ I_{4\times4} + i\underbrace{\begin{pmatrix}\vec\sigma & 0\\ 0 & \vec\sigma\end{pmatrix}}_{=\frac{2}{\hbar}\hat{\vec S}}\cdot(\vec A\times\vec B)$$

$$= \dots = \hbar^2c^2q\,\mathrm{div}\,\vec E + \cancel{2i\hbar c^2 q\,\hat{\vec S}\cdot\mathrm{rot}\,\vec E}$$
$$+ 4c^2q\,\hat{\vec S}\cdot(\vec E\times\hat{\vec p}) + \cancel{4c^2q^2\,\vec S\cdot(\vec A\times\vec E)}$$

$\vec A = \vec 0$, $\vec E = -\,\mathrm{grad}\,\varphi$, $\quad \varphi = \frac{q}{4\pi\varepsilon_0 r}$

1) $-\frac{1}{8m^2c^4}\hbar^2c^2q\,\mathrm{div}\,\vec E = \dots = \frac{\hbar^2e^2}{8m^2c^2\varepsilon_0}\,\delta(\vec r)$ Darwin term ✓

2) $\frac{-1}{8m^2c^4}\,4c^2q\,\hat{\vec S}\cdot(\vec E\times\hat{\vec p}) = \dots \overset{q=-e}{=} \frac{e^2}{8\pi\varepsilon_0 m^2c^2r^3}\,\hat{\vec L}\cdot\hat{\vec S}$ spin orbit coupling ✓

Dirac theory describes properly the measured fine structure of hydrogen atom.

13.5 Central Potential: "get rid of the angles, focus on radius"

$\vec{A} = \vec{0}$, $\varphi(\vec{x}) = \varphi(r)$, $r = |\vec{x}|$

$$i\hbar \frac{\partial}{\partial t} \Psi = \hat{H} \Psi, \quad \hat{H} = c\,\vec{\alpha}\cdot\hat{\vec{p}} + mc^2\beta + q\,\varphi(r)$$

1) orbital angular momentum: $\hat{\vec{L}} = \vec{x} \times \hat{\vec{p}}$

$$[\varphi(r), \hat{L}_i]_- = [\varphi(r), \varepsilon_{ijk} x_j \hat{p}_k]_- = i\hbar\, \varepsilon_{ijk} x_j \underbrace{\partial_k \varphi(r)}_{= \frac{\varphi'(r)}{r} x_k} \equiv 0$$

$$\boxed{[\hat{H}, \hat{L}_i]_-} = c\,[\vec{\alpha}\cdot\hat{\vec{p}}, \hat{L}_i]_- = \dots = \boxed{-i\hbar\, \varepsilon_{ijk}\, \alpha_j\, \hat{p}_k} \neq 0$$

2) spin angular momentum: $\hat{\vec{S}} = \frac{\hbar}{2}\vec{\Sigma}$, $\vec{\Sigma} = \begin{pmatrix} \vec{\sigma} & 0 \\ 0 & \vec{\sigma} \end{pmatrix}$

note: $[\beta, \vec{S}]_- = 0$

$$\boxed{[\hat{H}, \hat{\vec{S}}]_-} = c\,[\vec{\alpha}\cdot\hat{\vec{p}}, \hat{\vec{S}}]_- = \frac{c\hbar}{2}\, \hat{p}_l\, [\alpha_l, \vec{\Sigma}]_- = \boxed{+i\hbar c\, \vec{\alpha}\times\hat{\vec{p}}} \neq 0$$

$$\alpha_l \Sigma_i = \begin{pmatrix} 0 & \sigma_l \\ \sigma_l & 0 \end{pmatrix}\begin{pmatrix} \sigma_i & 0 \\ 0 & \sigma_i \end{pmatrix} = \begin{pmatrix} 0 & \sigma_l\sigma_i \\ \sigma_l\sigma_i & 0 \end{pmatrix} = \begin{pmatrix} 0 & \delta_{li} + i\varepsilon_{lij}\sigma_j \\ \delta_{li} + i\varepsilon_{lij}\sigma_j & 0 \end{pmatrix}$$

$$\Rightarrow [\alpha_l, \Sigma_i]_- = 2i\,\varepsilon_{lij}\,\alpha_j$$

Conclusion: $[\hat{H}, \underbrace{\hat{\vec{L}} + \hat{\vec{S}}}_{= \hat{\vec{J}}}]_- = 0$ total angular momentum operator

$$\Rightarrow [\hat{H}, \hat{\vec{J}}^2]_- = 0 = [\hat{H}, \hat{J}_z]_-$$

We expect that we can find eigenfunctions of $\hat{H}$, $\hat{\vec{J}}^2$ and $\hat{J}_z$.