Last lecture:

- Heuristic derivation of Dirac equation: relativistic quantum mechanical wave equation which linear in space-time derivatives
- Dirac equation describes spin 1/2 - particles with Landé factor $g_s = 2$

13.4 Foldy-Wouthuysen Transformation:

Systematic approach to go for higher orders in the non-relativistic limit of Dirac equation: fine structure of hydrogen

$$i\hbar \frac{\partial \underbrace{\Psi}}{\partial t} = \hat{H}_D \underbrace{\Psi}_{\text{4-component Dirac spinor}}, \quad \hat{H}_D = c\vec{\alpha}\cdot(\vec{p} - q\vec{A}) + mc^2\beta + q\varphi, \quad \beta = \begin{pmatrix} \underbrace{I}_{=\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}} & 0 \\ \underbrace{0}_{\begin{pmatrix}0 & 0\\ 0 & 0\end{pmatrix}=} & -I \end{pmatrix}, \quad \vec{\alpha} = \begin{pmatrix} 0 & \vec{\sigma} \\ \vec{\sigma} & 0 \end{pmatrix}$$

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

$$\Rightarrow \hat{H}_D = mc^2 \beta$$

two sets of eigenvectors:

$\underline{E > 0}$ (particles): $\Psi = \begin{pmatrix} u \\ 0 \end{pmatrix}$, $\underline{E < 0}$ (antiparticles): $\Psi = \begin{pmatrix} 0 \\ v \end{pmatrix}$

two-component Weyl spinor

Either finite momenta or non-vanishing vector potential couples both Weyl spinors u, v

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

Implement this idea as a "Schrieffer – Wolff transformation" (see super-conductivity)

$$\underbrace{\Psi'}_{u,v \text{ decoupled}} = \underbrace{e^{\hat S}}_{\text{unitary}} \underbrace{\Psi}_{u,v \text{ coupled}} , \qquad e^{\hat S} \text{ unitary: } e^{\hat S^+} = e^{-\hat S} \Rightarrow \hat S^+ = -\hat S \text{ anti-hermitian}$$

$$i\hbar \frac{\partial}{\partial t}\left\{ e^{-\hat S}\Psi' \right\} = -i\hbar \frac{\partial \hat S}{\partial t} e^{-\hat S}\Psi + i\hbar\, e^{-\hat S}\frac{\partial \Psi'}{\partial t} = \hat H \Psi = \hat H e^{-\hat S}\Psi' \quad \Big| \cdot e^{\hat S}$$

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

After 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 non-relativistic limit

Definition: An operator $\hat{\mathcal{E}}$ or $\hat{\mathcal{O}}$ is called even or odd if it is diagonal or off-diagonal in Weyl spinors

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

examples: $\beta = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}$, $\vec\alpha = \begin{pmatrix} 0 & \vec\sigma \\ \vec\sigma & 0 \end{pmatrix}$

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

$$\hat H = \underbrace{mc^2\beta + q\varphi}_{=\hat{\mathcal{E}}} + c\,\vec\alpha\left(\hat{\vec p} - q\vec A\right)$$

to be considered as a perturbation

small momenta   weak vector potential

assume: $e^{\hat{S}}$, $\hat{S}$ is supposed to be small, $\frac{\partial \hat{S}}{\partial t} = 0$ (stationary $\varphi, \vec{A}$)

Side consideration: λ as a smallness parameter

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

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

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

$\vdots$ $\vdots$

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

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

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

Lowest order:

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

negligible in lowest order

aim: eliminate odd terms in lowest order

condition: $\hat{O} + mc^2 [\underbrace{\hat{S}}_{\text{has to be determined}}, \beta]_- = 0$ $(*)$ $\Rightarrow$ $\hat{O}(1 - 2kmc^2) = 0$

$\Rightarrow k = \frac{1}{2mc^2}$

Ansatz: $\hat{S} = \underbrace{k}_{\text{prefactor}} \beta \hat{O}$ $\Rightarrow$ determine k such that $(*)$ is fulfilled

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

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

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

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

Result: $\hat{S} = \frac{1}{2mc^2}\beta\hat{O}$

↑ This is small as we divide by rest energy mc^2

$$\hat{O} = c\vec{\alpha}\cdot(\vec{p} - q\vec{A})$$

Transformed Hamiltonian turns ~~out~~ to have the following form after a long but straight-forward calculation:

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

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

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

↑ They would have be eliminated by a higher order Schrieffer-Wolff transformation

Term of order $\frac{1}{mc^2}$: nonrelativistic limit of last lecture

$$\frac{1}{2mc^2} c^2 \beta \underbrace{\left[(\vec{\hat{p}} - q\vec{A}) \cdot \vec{\sigma} \right] \left[(\vec{\hat{p}} - q\vec{A}) \cdot \vec{\alpha} \right]}$$

analyzed last time

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

Term of order $\frac{1}{(mc^2)^3}$: special relativistic correction of kin. energy

$$-\frac{1}{8m^3c^6} \beta c^4 \left[(\vec{\hat{p}} - q\vec{A}) \cdot \vec{\sigma} \right]^4 \underset{\vec{A}=\vec{0}}{=} -\frac{1}{8m^3c^2} \beta \vec{\hat{p}}^4$$

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

Term of order $\frac{1}{(mc^2)^2}$: Darwin term + spin orbit coupling $\quad \vec{A} = \vec{0}$

$$[\hat{O}, \hat{\varepsilon}]_- = [c\vec{\alpha} \cdot \vec{\hat{p}}, q\varphi]_- = cq \frac{\hbar}{i} \vec{\nabla}\varphi \underset{\vec{E} = -\vec{\nabla}\varphi}{=} -i\hbar cq \vec{\alpha} \cdot \vec{E}$$

$$[\hat{O}, [\hat{O}, \hat{\varepsilon}]_-]_- = [c\vec{\alpha} \cdot \vec{\hat{p}}, -i\hbar cq \vec{\alpha} \vec{E}]_- = -i\hbar c^2 q [\vec{\alpha} \cdot \underset{=\vec{A}}{\vec{\hat{p}}}, \vec{\alpha} \underset{\vec{B}}{\vec{E}}]_-$$

$$(\vec{\sigma} \cdot \vec{A})(\vec{\sigma} \cdot \vec{B}) \overset{\text{last}}{\underset{\text{time}}{=}} \vec{A} \cdot \vec{B} + i \vec{\sigma} \cdot (\vec{A} \times \vec{B})$$

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

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

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

$$\vec{E} = -\vec{\nabla} \varphi$$

$$\varphi = \frac{q}{4\pi\varepsilon_0 r}, \quad q = -e$$

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

$$- \frac{1}{8 m^2 c^4} 4 c^2 q \vec{S} (\vec{E} \times \vec{p}) \overset{q=-e}{=} \ldots = \frac{e^2}{8 \pi \varepsilon_0 m^2 c^2 r^3} \vec{L} \cdot \vec{S}$$

spin-orbit coupling

Dirac theory describes properly the measured fine structure of hydrogen

13.5 Central Potential:

basic notion: " get rid off angles, focus on radius"

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

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

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

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

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

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

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

$$[\hat{H}, \vec{S}]_- = c[\vec{\alpha}\hat{\vec{p}}, \vec{S}]_- = \frac{c\hbar}{i}\hat{p}_l[\alpha_l, \vec{\Sigma}]_- = +ic\hbar\,\varepsilon_{ijk}\alpha_j \hat{p}_k \neq 0$$

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

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

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

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

We expect to find eigenfunctions of $\hat{H}$, $\vec{J}^2$ and $\hat{J}_z$!