Foldy-Wouthuysen Transformation

A unitary transformation U_F removes operators which couple the large to the small components.

Odd operators (off-diagonal in Pauli-Dirac basis): α^i, γ^i, $\gamma_5, \cdots$

Even operators (diagonal in Pauli-Dirac basis): $\mathbf{1}$, β, $\Sigma, \cdots$

$$\psi' = U_F \psi = e^{iS}\psi, \quad S = \text{hermitian} \tag{1}$$

First consider the case of a free particle, $H = \boldsymbol{\alpha} \cdot \boldsymbol{p} + \beta m$ not time-dependent.

$$i\frac{\partial \psi'}{\partial t} = e^{iS} H \psi = e^{iS} H e^{-iS} \psi' = H' \psi' \tag{2}$$

We want to find S such that H' contains no odd operators. We can try

$$e^{iS} = e^{\beta \boldsymbol{\alpha} \cdot \hat{\boldsymbol{p}} \theta} = \cos\theta + \beta \boldsymbol{\alpha} \cdot \hat{\boldsymbol{p}} \sin\theta, \quad \text{where } \hat{\boldsymbol{p}} = \boldsymbol{p}/|\boldsymbol{p}|. \tag{3}$$

$$\begin{aligned} H' &= (\cos\theta + \beta \boldsymbol{\alpha} \cdot \hat{\boldsymbol{p}} \sin\theta)(\boldsymbol{\alpha} \cdot \boldsymbol{p} + \beta m)(\cos\theta - \beta \boldsymbol{\alpha} \cdot \hat{\boldsymbol{p}} \sin\theta) \\ &= (\boldsymbol{\alpha} \cdot \boldsymbol{p} + \beta m)(\cos\theta - \beta \boldsymbol{\alpha} \cdot \hat{\boldsymbol{p}} \sin\theta)^2 \\ &= (\boldsymbol{\alpha} \cdot \boldsymbol{p} + \beta m) \exp(-2\beta \boldsymbol{\alpha} \cdot \hat{\boldsymbol{p}} \theta) \\ &= (\boldsymbol{\alpha} \cdot \boldsymbol{p}) \left(\cos 2\theta - \frac{m}{|\boldsymbol{p}|} \sin 2\theta \right) + \beta (m \cos 2\theta + |\boldsymbol{p}| \sin 2\theta). \end{aligned} \tag{4}$$

To eliminate $(\boldsymbol{\alpha} \cdot \boldsymbol{p})$ term we choose $\tan 2\theta = |\boldsymbol{p}|/m$, then

$$H' = \beta\sqrt{m^2 + |\boldsymbol{p}|^2}. \tag{5}$$

This is the same as the first hamilton we tried except for the β factor which also gives rise to negative energy solutions. In practice, we need to expand the hamilton for $|\boldsymbol{p}| \ll m$.

General case:

$$\begin{aligned} H &= \boldsymbol{\alpha} \cdot (\boldsymbol{p} - e\boldsymbol{A}) + \beta m + e\Phi \\ &= \beta m + \mathcal{O} + \mathcal{E}, \end{aligned} \tag{6}$$

$$\mathcal{O} = \boldsymbol{\alpha} \cdot (\boldsymbol{p} - e\boldsymbol{A}), \quad \mathcal{E} = e\Phi, \quad \beta\mathcal{O} = -\mathcal{O}\beta, \ \beta\mathcal{E} = \mathcal{E}\beta \tag{7}$$

H time-dependent $\Rightarrow$ S time-dependent

We can only construct S with a non-relativistic expansion of the transformed hamilton H' in a power series in $1/m$.

We'll expand to $\frac{p^4}{m^3}$ and $\frac{p\times(E,B)}{m^2}$.

$$H\psi = i\frac{\partial}{\partial t}\left(e^{-iS}\psi'\right) = e^{-iS}i\frac{\partial\psi'}{\partial t} + \left(i\frac{\partial}{\partial t}e^{-iS}\right)\psi'$$
$$\Rightarrow i\frac{\partial\psi'}{\partial t} = \left[e^{iS}\left(H - i\frac{\partial}{\partial t}\right)e^{-iS}\right]\psi' = H'\psi' \tag{8}$$

S is expanded in powers of $1/m$ and is "small" in the non-relativistic limit.

$$e^{iS}He^{-iS} = H + i[S,H] + \frac{i^2}{2!}[S,[S,H]] + \cdots + \frac{i^n}{n!}[S,[S,\cdots[S,H]]]. \tag{9}$$

$S = O(\frac{1}{m})$ to the desired order of accuracy

$$\begin{aligned} H' &= H + i[S,H] - \frac{1}{2}[S,[S,H]] - \frac{i}{6}[S,[S,[S,H]]] + \frac{1}{24}[S,[S,[S,[S,\beta m]]]] \\ &\quad -\dot{S} - \frac{i}{2}[S,\dot{S}] + \frac{1}{6}[S,[S,\dot{S}]] \end{aligned} \tag{10}$$

We will eliminate the odd operators order by order in $1/m$ and repeat until the desired order is reached.

First order $[O(1)]$:

$$H' = \beta m + \mathcal{E} + \mathcal{O} + i[S,\beta]m. \tag{11}$$

To cancel $\mathcal{O}$, we choose $S = -\frac{i\beta\mathcal{O}}{2m}$,

$$i[S,H] = -\mathcal{O} + \frac{\beta}{2m}[\mathcal{O},\mathcal{E}] = \frac{1}{m}\beta\mathcal{O}^2 \tag{12}$$
$$\frac{i^2}{2}[S,[S,H]] = -\frac{\beta\mathcal{O}^2}{2m} - \frac{1}{8m^2}[\mathcal{O},[\mathcal{O},\mathcal{E}]] - \frac{1}{2m^2}\mathcal{O}^3 \tag{13}$$
$$\frac{i^3}{3!}[S,[S,[S,H]]] = \frac{\mathcal{O}^3}{6m^2} - \frac{1}{6m^3}\beta\mathcal{O}^4 \tag{14}$$
$$\frac{i^4}{4!}[S,[S,[S,[S,H]]]] = \frac{\beta\mathcal{O}^4}{24m^3} \tag{15}$$
$$-\dot{S} = \frac{i\beta\dot{\mathcal{O}}}{2m} \tag{16}$$
$$-\frac{i}{2}[S,\dot{S}] = -\frac{i}{8m^2}[\mathcal{O},\dot{\mathcal{O}}] \tag{17}$$

Collecting everything,

$$H' = \beta\left(m + \frac{\mathcal{O}^2}{2m} - \frac{\mathcal{O}^4}{8m^3}\right) + \mathcal{E} - \frac{1}{8m^2}[\mathcal{O},[\mathcal{O},\mathcal{E}]] - \frac{i}{8m^2}[\mathcal{O},\dot{\mathcal{O}}] \tag{18}$$
$$+\frac{\beta}{2m}[\mathcal{O},\mathcal{E}] - \frac{\mathcal{O}^3}{3m^2} + \frac{i\beta\dot{\mathcal{O}}}{2m}$$
$$= \beta m + \mathcal{E}' + \mathcal{O}' \tag{19}$$

Now $\mathcal{O}'$ is $O(\frac{1}{m})$, we can transform H' by S' to cancel $\mathcal{O}'$,

$$S' = \frac{-i\beta}{2m}\mathcal{O}' = \frac{-i\beta}{2m}\left(\frac{\beta}{2m}[\mathcal{O},\mathcal{E}] - \frac{\mathcal{O}^3}{3m^2} + \frac{i\beta\dot{\mathcal{O}}}{2m}\right) \tag{20}$$

After transformation with S',

$$\begin{aligned} H'' = e^{iS'}\left(H' - i\frac{\partial}{\partial t}\right)e^{-iS'} &= \beta m + \mathcal{E}' + \frac{\beta}{2m}[\mathcal{O}',\mathcal{E}'] + \frac{i\beta\dot{\mathcal{O}}'}{2m} && (21)\\ &= \beta m + \mathcal{E}' + \mathcal{O}'', && (22)\end{aligned}$$

where $\mathcal{O}''$ is $O(\frac{1}{m^2})$, which can be cancelled by a third transformation, $S'' = \frac{-i\beta\mathcal{O}''}{2m}$

$$\begin{aligned} H''' &= e^{iS''}\left(H'' - i\frac{\partial}{\partial t}\right)e^{-iS''} = \beta m + \mathcal{E}' && (23)\\ &= \beta\left(m + \frac{\mathcal{O}^2}{2m} - \frac{\mathcal{O}^4}{8m^3}\right) + \mathcal{E} - \frac{1}{8m^2}[\mathcal{O},[\mathcal{O},\mathcal{E}]] - \frac{i}{8m^2}[\mathcal{O},\dot{\mathcal{O}}] && (24)\end{aligned}$$

Evaluating the operator products to the desired order of accuracy,

$$\begin{aligned} \frac{\mathcal{O}^2}{2m} &= \frac{(\boldsymbol{\alpha}\cdot(\boldsymbol{p}-e\boldsymbol{A}))^2}{2m} = \frac{(\boldsymbol{p}-e\boldsymbol{A})^2}{2m} - \frac{e}{2m}\boldsymbol{\Sigma}\cdot\boldsymbol{B} && (25)\\ \frac{1}{8m^2}\left([\mathcal{O},\mathcal{E}] + i\dot{\mathcal{O}}\right) &= \frac{e}{8m^2}(-i\boldsymbol{\alpha}\cdot\nabla\Phi - i\boldsymbol{\alpha}\cdot\dot{\boldsymbol{A}}) = \frac{ie}{8m^2}\boldsymbol{\alpha}\cdot\boldsymbol{E} && (26)\\ \left[\mathcal{O}, \frac{ie}{8m^2}\boldsymbol{\alpha}\cdot\boldsymbol{E}\right] &= \frac{ie}{8m^2}[\boldsymbol{\alpha}\cdot\boldsymbol{p}, \boldsymbol{\alpha}\cdot\boldsymbol{E}] \\ &= \frac{ie}{8m^2}\sum_{i,j}\alpha^i\alpha^j\left(-i\frac{\partial E^j}{\partial x^i}\right) + \frac{e}{4m^2}\boldsymbol{\Sigma}\cdot\boldsymbol{E}\times\boldsymbol{p} && (27)\\ &= \frac{e}{8m^2}(\nabla\cdot\boldsymbol{E}) + \frac{ie}{8m^2}\boldsymbol{\Sigma}\cdot(\nabla\times\boldsymbol{E}) + \frac{e}{4m^2}\boldsymbol{\Sigma}\cdot\boldsymbol{E}\times\boldsymbol{p}\end{aligned}$$

So, the effective hamiltonial to the desired order is

$$\begin{aligned} H''' &= \beta\left(m + \frac{(\boldsymbol{p}-e\boldsymbol{A})^2}{2m} - \frac{\boldsymbol{p}^4}{8m^3}\right) + e\Phi - \frac{e}{2m}\beta\boldsymbol{\Sigma}\cdot\boldsymbol{B} \\ &\quad - \frac{ie}{8m^2}\boldsymbol{\Sigma}\cdot(\nabla\times\boldsymbol{E}) - \frac{e}{4m^2}\boldsymbol{\Sigma}\cdot\boldsymbol{E}\times\boldsymbol{p} - \frac{e}{8m^2}(\nabla\cdot\boldsymbol{E}) && (28)\end{aligned}$$

The individual terms have a direct physical interpretation.

The first term in the parentheses is the expansion of

$$\sqrt{(\boldsymbol{p}-e\boldsymbol{A})^2 + m^2} \tag{29}$$

and $-\boldsymbol{p}^4/(8m^3)$ is the leading relativistic corrections to the kinetic energy.

The two terms

$$-\frac{ie}{8m^2}\boldsymbol{\Sigma}\cdot(\nabla\times\boldsymbol{E})-\frac{e}{4m^2}\boldsymbol{\Sigma}\cdot\boldsymbol{E}\times\boldsymbol{p} \tag{30}$$

together are the spin-orbit energy. In a spherically symmetric static potential, they take a very familar form. In this case $\nabla\times\boldsymbol{E}=0$,

$$\boldsymbol{\Sigma}\cdot\boldsymbol{E}\times\boldsymbol{p}=-\frac{1}{r}\frac{\partial\Phi}{\partial r}\boldsymbol{\Sigma}\cdot\boldsymbol{r}\times\boldsymbol{p}=-\frac{1}{r}\frac{\partial\Phi}{\partial r}\boldsymbol{\Sigma}\cdot\boldsymbol{L}, \tag{31}$$

and this term reduces to

$$H_{\mathrm{spin-orbit}}=\frac{e}{4m^2}\frac{1}{r}\frac{\partial\Phi}{\partial r}\boldsymbol{\Sigma}\cdot\boldsymbol{L}. \tag{32}$$

The last term is known as the Darwin term. In a coulomb potential of a nucleus with charge $Z|e|$, it takes the form

$$-\frac{e}{8m^2}(\nabla\cdot\boldsymbol{E})=-\frac{e}{8m^2}Z|e|\delta^3(r)=\frac{Ze^2}{8m^2}\delta^3(r)=\frac{Z\alpha\pi}{2m^2}\delta^3(r), \tag{33}$$

so it can only affect the S ($l=0$) states whose wavefunctions are nonzero at the origin.

For a Hydrogen-like (single electron) atom,

$$e\Phi=-\frac{Ze^2}{4\pi r},\quad \boldsymbol{A}=0. \tag{34}$$

The shifts in energies of various states due to these correction terms can be computed by taking the expectation values of these terms with the corresponding wavefunctions.

Darwin term (only for S ($l=0$) states):

$$\left\langle\psi_{ns}\left|\frac{Z\alpha\pi}{2m^2}\delta^3(r)\right|\psi_{ns}\right\rangle=\frac{Z\alpha\pi}{2m^2}|\psi_{ns}(0)|^2=\frac{Z^4\alpha^4 m}{2n^3}. \tag{35}$$

Spin-orbit term (nonzero only for $l\neq 0$):

$$\left\langle\frac{Z\alpha}{4m^2}\frac{1}{r^3}\boldsymbol{\sigma}\cdot\boldsymbol{r}\times\boldsymbol{p}\right\rangle=\frac{Z^4\alpha^4 m}{4n^3}\frac{[j(j+1)-l(l+1)-s(s+1)]}{l(l+1)(l+\frac{1}{2})}. \tag{36}$$

Relativistic corrections:

$$\left\langle-\frac{\boldsymbol{p}^4}{8m^3}\right\rangle=\frac{Z^4\alpha^4 m}{2n^4}\left(\frac{3}{4}-\frac{n}{l+\frac{1}{2}}\right). \tag{37}$$

We find

$$\Delta E(l=0) = \frac{Z^4\alpha^4 m}{2n^4}\left(\frac{3}{4}-n\right) \tag{38}$$

$$= \Delta E(l=1,j=\frac{1}{2}), \tag{39}$$

so $2S_{1/2}$ and $2P_{1/2}$ remain degenerate at this level. They are split by Lamb shift ($2S_{1/2} > 2P_{1/2}$) which can be calculated after you learn radiative corrections in QED. The $2P_{1/2}$ and $2P_{3/2}$ are split by the spin-orbit interaction (fine structure) which you should have seen before.

$$\Delta E(l=1, j=\frac{3}{2}) - \Delta E(l=1, j=\frac{1}{2}) = \frac{Z^4\alpha^4 m}{4n^3} \tag{40}$$