8 Foldy-Wouthuysen Transformation

We now have the Dirac equation with interactions. For a given problem we can solve for the spectrum and wavefunctions (ignoring the negative energy solutions for a moment), for instance, the hydrogen atom, We can compare the solutions to those of the schrödinger equation and find out the relativistic corrections to the spectrum and the wavefunctions. In fact, the problem of hydrogen atom can be solved exactly. However, the exact solutions are problem-specific and involve unfamiliar special functions, hence they not very illuminating. You can find the exact solutions in many textbooks and also in Shulten's notes. Instead, in this section we will develop a systematic approximation method to solve a system in the non-relativistic regime ($E-m \ll m$). It corresponds to take the approximation we discussed in the previous section to higher orders in a systematic way. This allows a physical interpretation for each term in the approximation and tells us the relative importance of various effects. Such a method has more general applications for different problems.

In Foldy-Wouthuysen transformation, we look for 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, $\Sigma, \cdots$

$$\psi' = U_F \psi = e^{iS}\psi, \quad S = \text{hermitian} \tag{171}$$

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

$$i\frac{\partial \psi'}{\partial t} = e^{iS} H\psi = e^{iS} H e^{-iS}\psi' = H'\psi' \tag{172}$$

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

$$e^{iS} = e^{\beta\boldsymbol{\alpha}\cdot\hat{\boldsymbol{p}}\theta} = \cos\theta + \beta\boldsymbol{\alpha}\cdot\hat{\boldsymbol{p}}\sin\theta, \quad \text{where } \hat{\boldsymbol{p}} = \boldsymbol{p}/|\boldsymbol{p}|. \tag{173}$$

$$\begin{aligned} H' &= (\cos\theta + \beta\boldsymbol{\alpha}\cdot\hat{\boldsymbol{p}}\sin\theta)(\boldsymbol{\alpha}\cdot\boldsymbol{p} + \beta m)(\cos\theta - \beta\boldsymbol{\alpha}\cdot\hat{\boldsymbol{p}}\sin\theta) \\ &= (\boldsymbol{\alpha}\cdot\boldsymbol{p} + \beta m)(\cos\theta - \beta\boldsymbol{\alpha}\cdot\hat{\boldsymbol{p}}\sin\theta)^2 \\ &= (\boldsymbol{\alpha}\cdot\boldsymbol{p} + \beta m)\exp(-2\beta\boldsymbol{\alpha}\cdot\hat{\boldsymbol{p}}\theta) \\ &= (\boldsymbol{\alpha}\cdot\boldsymbol{p})\left(\cos 2\theta - \frac{m}{|\boldsymbol{p}|}\sin 2\theta\right) + \beta\left(m\cos 2\theta + |\boldsymbol{p}|\sin 2\theta\right). \end{aligned} \tag{174}$$

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

$$H' = \beta\sqrt{m^2 + |\boldsymbol{p}|^2}. \tag{175}$$

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:

$$\begin{aligned} H &= \boldsymbol{\alpha}\cdot(\boldsymbol{p}-e\boldsymbol{A})+\beta m+e\Phi \\ &= \beta m+\mathcal{O}+\mathcal{E}, \end{aligned} \tag{176}$$

$$\mathcal{O}=\boldsymbol{\alpha}\cdot(\boldsymbol{p}-e\boldsymbol{A}), \quad \mathcal{E}=e\Phi, \quad \beta\mathcal{O}=-\mathcal{O}\beta,\ \beta\mathcal{E}=\mathcal{E}\beta \tag{177}$$

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 $\frac{p\times(E,B)}{m^2}$.

$$\begin{aligned} H\psi = i\frac{\partial}{\partial t}\left(e^{-iS}\psi'\right) &= e^{-iS}i\frac{\partial\psi'}{\partial t}+\left(i\frac{\partial}{\partial t}e^{-iS}\right)\psi' \\ \Rightarrow i\frac{\partial\psi'}{\partial t} &= \left[e^{iS}\left(H-i\frac{\partial}{\partial t}\right)e^{-iS}\right]\psi' = H'\psi' \end{aligned} \tag{178}$$

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

$$e^{iS}He^{-iS}=H+i[S,H]+\frac{i^2}{2!}[S,[S,H]]+\cdots+\frac{i^n}{n!}[S,[S,\cdots[S,H]]]. \tag{179}$$

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

$$\begin{aligned} H' &= H+i[S,H]-\frac{1}{2}[S,[S,H]]-\frac{i}{6}[S,[S,[S,H]]]+\frac{1}{24}[S,[S,[S,[S,\beta m]]]] \\ &\quad -\dot{S}-\frac{i}{2}[S,\dot{S}]+\frac{1}{6}[S,[S,\dot{S}]] \end{aligned} \tag{180}$$

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

First order $[O(1)]$:

$$H'=\beta m+\mathcal{E}+\mathcal{O}+i[S,\beta]m. \tag{181}$$

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

$$i[S,H] = -\mathcal{O}+\frac{\beta}{2m}[\mathcal{O},\mathcal{E}]=\frac{1}{m}\beta\mathcal{O}^2 \tag{182}$$

$$\frac{i^2}{2}[S,[S,H]] = -\frac{\beta\mathcal{O}^2}{2m}-\frac{1}{8m^2}[\mathcal{O},[\mathcal{O},\mathcal{E}]]-\frac{1}{2m^2}\mathcal{O}^3 \tag{183}$$

$$\frac{i^3}{3!}[S,[S,[S,H]]] = \frac{\mathcal{O}^3}{6m^2}-\frac{1}{6m^3}\beta\mathcal{O}^4 \tag{184}$$

$$\frac{i^4}{4!}[S,[S,[S,[S,H]]]] = \frac{\beta\mathcal{O}^4}{24m^3} \tag{185}$$

$$-\dot{S} = \frac{i\beta\dot{\mathcal{O}}}{2m} \tag{186}$$

$$-\frac{i}{2}[S,\dot{S}] = -\frac{i}{8m^2}[\mathcal{O},\dot{\mathcal{O}}] \tag{187}$$

Collecting everything,

$$
\begin{aligned}
H' &= \beta\left(m+\frac{\mathcal{O}^2}{2m}-\frac{\mathcal{O}^4}{8m^3}\right)+\mathcal{E}-\frac{1}{8m^2}[\mathcal{O},[\mathcal{O},\mathcal{E}]]-\frac{i}{8m^2}[\mathcal{O},\dot{\mathcal{O}}] \qquad (188)\\
&\quad +\frac{\beta}{2m}[\mathcal{O},\mathcal{E}]-\frac{\mathcal{O}^3}{3m^2}+\frac{i\beta\dot{\mathcal{O}}}{2m}\\
&= \beta m+\mathcal{E}'+\mathcal{O}' \qquad (189)
\end{aligned}
$$

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

$$
S'=\frac{-i\beta}{2m}\mathcal{O}'=\frac{-i\beta}{2m}\left(\frac{\beta}{2m}[\mathcal{O},\mathcal{E}]-\frac{\mathcal{O}^3}{3m^2}+\frac{i\beta\dot{\mathcal{O}}}{2m}\right) \qquad (190)
$$

After transformation with S',

$$
\begin{aligned}
H''=e^{iS'}\left(H'-i\frac{\partial}{\partial t}\right)e^{-iS'} &= \beta m+\mathcal{E}'+\frac{\beta}{2m}[\mathcal{O}',\mathcal{E}']+\frac{i\beta\dot{\mathcal{O}}'}{2m} \qquad (191)\\
&= \beta m+\mathcal{E}'+\mathcal{O}'', \qquad (192)
\end{aligned}
$$

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

$$
\begin{aligned}
H''' &= e^{iS''}\left(H''-i\frac{\partial}{\partial t}\right)e^{-iS''}=\beta m+\mathcal{E}' \qquad (193)\\
&= \beta\left(m+\frac{\mathcal{O}^2}{2m}-\frac{\mathcal{O}^4}{8m^3}\right)+\mathcal{E}-\frac{1}{8m^2}[\mathcal{O},[\mathcal{O},\mathcal{E}]]-\frac{i}{8m^2}[\mathcal{O},\dot{\mathcal{O}}] \qquad (194)
\end{aligned}
$$

Evaluating the operator products to the desired order of accuracy,

$$
\begin{aligned}
\frac{\mathcal{O}^2}{2m} &= \frac{(\boldsymbol{\alpha}\cdot(\boldsymbol{p}-e\boldsymbol{A}))^2}{2m}=\frac{(\boldsymbol{p}-e\boldsymbol{A})^2}{2m}-\frac{e}{2m}\boldsymbol{\Sigma}\cdot\boldsymbol{B} \qquad (195)\\
\frac{1}{8m^2}\left([\mathcal{O},\mathcal{E}]+i\dot{\mathcal{O}}\right) &= \frac{e}{8m^2}(-i\boldsymbol{\alpha}\cdot\nabla\Phi-i\boldsymbol{\alpha}\cdot\dot{\boldsymbol{A}})=\frac{ie}{8m^2}\boldsymbol{\alpha}\cdot\boldsymbol{E} \qquad (196)\\
\left[\mathcal{O},\frac{ie}{8m^2}\boldsymbol{\alpha}\cdot\boldsymbol{E}\right] &= \frac{ie}{8m^2}[\boldsymbol{\alpha}\cdot\boldsymbol{p},\boldsymbol{\alpha}\cdot\boldsymbol{E}]\\
&= \frac{ie}{8m^2}\sum_{i,j}\alpha^i\alpha^j\left(-i\frac{\partial E^j}{\partial x^i}\right)+\frac{e}{4m^2}\boldsymbol{\Sigma}\cdot\boldsymbol{E}\times\boldsymbol{p} \qquad (197)\\
&= \frac{e}{8m^2}(\nabla\cdot\boldsymbol{E})+\frac{ie}{8m^2}\boldsymbol{\Sigma}\cdot(\nabla\times\boldsymbol{E})+\frac{e}{4m^2}\boldsymbol{\Sigma}\cdot\boldsymbol{E}\times\boldsymbol{p}
\end{aligned}
$$

So, the effective hamiltonial to the desired order is

$$
\begin{aligned}
H''' &= \beta\left(m+\frac{(\boldsymbol{p}-e\boldsymbol{A})^2}{2m}-\frac{\boldsymbol{p}^4}{8m^3}\right)+e\Phi-\frac{e}{2m}\beta\boldsymbol{\Sigma}\cdot\boldsymbol{B}\\
&\quad -\frac{ie}{8m^2}\boldsymbol{\Sigma}\cdot(\nabla\times\boldsymbol{E})-\frac{e}{4m^2}\boldsymbol{\Sigma}\cdot\boldsymbol{E}\times\boldsymbol{p}-\frac{e}{8m^2}(\nabla\cdot\boldsymbol{E}) \qquad (198)
\end{aligned}
$$

The individual terms have a direct physical interpretation.

The first term in the parentheses is the expansion of

$$\sqrt{(\boldsymbol{p} - e\boldsymbol{A})^2 + m^2} \tag{199}$$

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

The two terms

$$-\frac{ie}{8m^2}\boldsymbol{\Sigma} \cdot (\nabla \times \boldsymbol{E}) - \frac{e}{4m^2}\boldsymbol{\Sigma} \cdot \boldsymbol{E} \times \boldsymbol{p} \tag{200}$$

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

$$\boldsymbol{\Sigma} \cdot \boldsymbol{E} \times \boldsymbol{p} = -\frac{1}{r}\frac{\partial \Phi}{\partial r}\boldsymbol{\Sigma} \cdot \boldsymbol{r} \times \boldsymbol{p} = -\frac{1}{r}\frac{\partial \Phi}{\partial r}\boldsymbol{\Sigma} \cdot \boldsymbol{L}, \tag{201}$$

and this term reduces to

$$H_{\text{spin-orbit}} = \frac{e}{4m^2}\frac{1}{r}\frac{\partial \Phi}{\partial r}\boldsymbol{\Sigma} \cdot \boldsymbol{L}. \tag{202}$$

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

$$-\frac{e}{8m^2}(\nabla \cdot \boldsymbol{E}) = -\frac{e}{8m^2}Z|e|\delta^3(r) = \frac{Ze^2}{8m^2}\delta^3(r) = \frac{Z\alpha\pi}{2m^2}\delta^3(r), \tag{203}$$

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

For a Hydrogen-like (single electron) atom,

$$e\Phi = -\frac{Ze^2}{4\pi r}, \quad \boldsymbol{A} = 0. \tag{204}$$

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):

$$\left\langle \psi_{ns} \left| \frac{Z\alpha\pi}{2m^2}\delta^3(r) \right| \psi_{ns} \right\rangle = \frac{Z\alpha\pi}{2m^2}|\psi_{ns}(0)|^2 = \frac{Z^4\alpha^4 m}{2n^3}. \tag{205}$$

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

$$\left\langle \frac{Z\alpha}{4m^2}\frac{1}{r^3}\boldsymbol{\sigma} \cdot \boldsymbol{r} \times \boldsymbol{p} \right\rangle = \frac{Z^4\alpha^4 m}{4n^3}\frac{[j(j+1) - l(l+1) - s(s+1)]}{l(l+1)(l+\frac{1}{2})}. \tag{206}$$

Relativistic corrections:

$$\left\langle -\frac{\boldsymbol{p}^4}{8m^3} \right\rangle = \frac{Z^4\alpha^4 m}{2n^4}\left(\frac{3}{4} - \frac{n}{l+\frac{1}{2}}\right). \tag{207}$$

We find

$$\Delta E(l=0) = \frac{Z^4\alpha^4 m}{2n^4}\left(\frac{3}{4} - n\right) \tag{208}$$

$$= \Delta E(l=1, j=\frac{1}{2}), \tag{209}$$

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.

$$\Delta E(l=1, j=\frac{3}{2}) - \Delta E(l=1, j=\frac{1}{2}) = \frac{Z^4\alpha^4 m}{4n^3} \tag{210}$$

9 Klein Paradox and the Hole Theory

So far we have ignored the negative solutions. However, the negative energy solutions are required together with the positive energy solutions to form a complete set. If we try to localize an electron by forming a wave packet, the wavefunction will be composed of some negative energy components. There will be more negative energy components if the electron is more localized by the uncertainty relation $\Delta x \Delta p \sim \hbar$. The negative energy components can not be ignored if the electron is localized to distances comparable to its compton wavelength $\hbar/mc$, and we will encounter many paradoxes and dilemmas. An example is the Klein paradox described below.

In order to localize electrons, we must introduce strong external forces confining them to the desired region. Let's consider a simplified situation that we want to confine a free electron of energy E to the region $z < 0$ by a one-dimensional step-function potential of height V as shown in Fig. 1. Now in the $z < 0$ half space there is an incident positive energy plan wave of momentum $k > 0$ along the z axis,

$$\psi_{\text{inc}}(z) = e^{ikz}\begin{pmatrix} 1 \\ 0 \\ \frac{k}{E+m} \\ 0 \end{pmatrix}, \quad \text{(spin-up)}. \tag{211}$$

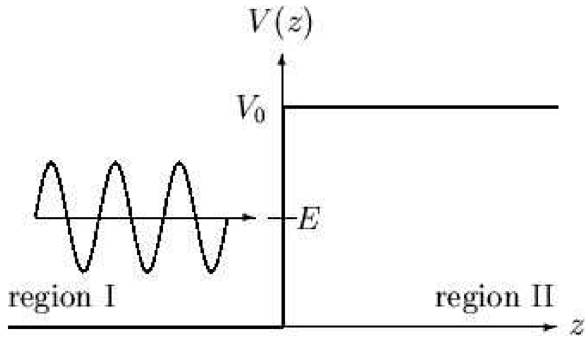

Figure 1: Electrostatic potential idealized with a sharp boundary, with an incident free electron wave moving to the right in resion I.

The reflected wave in $z < 0$ region has the form

$$\psi_{\text{ref}}(z) = a\, e^{-ikz} \begin{pmatrix} 1 \\ 0 \\ \frac{-k}{E+m} \\ 0 \end{pmatrix} + b\, e^{-ikz} \begin{pmatrix} 0 \\ 1 \\ 0 \\ \frac{k}{E+m} \end{pmatrix}, \tag{212}$$

and the transmitted wave in the $z > 0$ region (in the presence of the constant potential V) has a similar form

$$\psi_{\text{trans}}(z) = c\, e^{iqz} \begin{pmatrix} 1 \\ 0 \\ \frac{q}{E-V+m} \\ 0 \end{pmatrix} + d\, e^{-iqz} \begin{pmatrix} 0 \\ 1 \\ 0 \\ \frac{-q}{E-V+m} \end{pmatrix}, \tag{213}$$

with an effetive momentum q of

$$q = \sqrt{(E-V)^2 - m^2}. \tag{214}$$

The total wavefunction is

$$\psi(z) = \theta(-z)[\psi_{\text{inc}}(z) + \psi_{\text{ref}}(z)] + \theta(z)\psi_{\text{trans}}(z). \tag{215}$$

Requiring the continuity of $\psi(z)$ at $z = 0$, $\psi_{\text{inc}}(0) + \psi_{\text{ref}}(0) = \psi_{\text{trans}}(0)$, we obtain

$$1 + a = c \tag{216}$$

$$b = d \tag{217}$$

$$(1-a)\frac{k}{E+m} = c\,\frac{q}{E-V+m} \tag{218}$$

$$b\,\frac{k}{E+m} = d\,\frac{-q}{E-V+m} \tag{219}$$

From these equations we can see

$$
\begin{aligned}
& b = d = 0 \quad \text{(no spin-flip)} && (220)\\
& 1 + a = c && (221)\\
& 1 - a = rc \quad \text{where } r = \frac{q}{k}\frac{E+m}{E-V+m} && (222)\\
\Rightarrow\ & c = \frac{2}{1+r}, \quad a = \frac{1-r}{1+r}. && (223)
\end{aligned}
$$

As long as $|E-V| < m$, q is imaginary and the transmitted wave decays exponentially. However, when $V \geq E+m$ the transmitted wave becomes oscillatory again. The probablity currents $\boldsymbol{j} = \psi^\dagger \boldsymbol{\alpha} \psi = \psi^\dagger \alpha^3 \psi \hat{\boldsymbol{z}}$, for the incident, transmitted, and reflected waves are

$$
\begin{aligned}
j_{\text{inc}} &= 2\frac{k}{E+M}, \\
j_{\text{trans}} &= 2c^2 \frac{q}{E-V+m}, \\
j_{\text{ref}} &= 2a^2 \frac{k}{E+m}. \qquad (224)
\end{aligned}
$$

we find

$$
\begin{aligned}
\frac{j_{\text{trans}}}{j_{\text{inc}}} &= c^2 r = \frac{4r}{(1+r)^2} \quad (< 0 \text{ for } V \geq E+m), \\
\frac{j_{\text{ref}}}{j_{\text{inc}}} &= a^2 = \left(\frac{1-r}{1+r}\right)^2 \quad (> 1 \text{ for } V \geq E+m). \qquad (225)
\end{aligned}
$$

Although the conservation of the probabilities looks satified: $j_{\text{inc}} = j_{\text{trans}} + j_{\text{ref}}$, but we get the paradox that the reflected flux is larger than the incident one!

There is also a problem of causality violation of the single particle theory which you can read in Prof. Gunion's notes, p.14–p.15.

Hole Theory

In spite of the success of the Dirac equation, we must face the difficulties from the negative energy solutions. By their very existence they require a massive reinterpretation of the Dirac theory in order to prevent atomic electrons from making radiative transitions into negative-energy states. The transition rate for an electron in the ground state of a hydrogen atom to fall into a negative-energy state may be calculated by applying semiclassical radiation theory. The rate for the electron to make a transition into the energy interval $-mc^2$ to $-2mc^2$ is

$$\sim \frac{2\alpha^6}{\pi}\frac{mc^2}{\hbar} \simeq 10^8 \text{sec}^{-1} \qquad (226)$$

and it blows up if all the negative-energy states are included, which clearly makes no sense.

A solution was proposed by Dirac as early as 1930 in terms of a many-particle theory. (This shall not be the final standpoint as it does not apply to scalar particle, for instance.) He assumed that all negative energy levels are filled up in the vacuum state. According to the Pauli exclusion principle, this prevents any electron from falling into these negative energy states, and thereby insures the stability of positive energy physical states. In turn, an electron of the negative energy sea may be excited to a positive energy state. It then leaves a hole in the sea. This hole in the negative energy, negatively charged states appears as a positive energy positively charged particle—the positron. Besides the properties of the positron, its charge $|e| = -e > 0$ and its rest mass m_e, this theory also predicts new observable phenomena:

—The annihilation of an electron-positron pair. A positive energy electron falls into a hole in the negative energy sea with the emission of radiation. From energy momentum conservarion at least two photons are emitted, unless a nucleus is present to absorb energy and momentum.

—Conversely, an electron-positron pair may be created from the vacuum by an incident photon beam in the presence of a target to balance energy and momentum. This is the process mentioned above: a hole is created while the excited electron acquires a positive energy.

Thus the theory predicts the exisstence of positrons which were in fact observed in 1932. Since positrons and electrons may annihilate, we must abandon the interpretation of the Dirac equation as a wave equation. Also, the reason for discarding the Klein-Gordon equation no longer hold and it actually describes spin-0 particles, such as pions. However, the hole interpretation is not satisfactory for bosons, since there is no Pauli exclusion principle for bosons.

Even for fermions, the concept of an infinitely chaged unobservable sea looks rather queer. We have instead to construct a true many-body theory to accommodate particles and antiparticles in a consistent way. This is achieved in the quantume theory of fields which will be the subject of the rest of this course.