Appendix D

Relativistic Quantum Mechanics of Fermions

Electron has a spin and its magnitude is 1/2. The relativistic equation of eq.(C.1.2) has only one component of the field ϕ, and therefore it cannot describe the spin one half particle such as electron. Therefore, one has to consider some other equations for electron, and this equation is discovered by Dirac as we describe below.

D.1 Derivation of Dirac Equation

The procedure of obtaining Dirac equation is rather simple. One starts from eq.(C.1.1) and tries to factorize it into a linear equation for E and $\boldsymbol{p}$. This can be realized as

$$E^2 - \boldsymbol{p}^2 - m^2 = (E - \boldsymbol{p}\cdot\boldsymbol{\alpha} - m\beta)(E + \boldsymbol{p}\cdot\boldsymbol{\alpha} + m\beta) = 0 \qquad (D.1.1)$$

where $\boldsymbol{\alpha}$ and β are four by four matrices, and they satisfy the following anti-commutation relations

$$\{\alpha_i, \alpha_j\} = 2\delta_{ij}, \qquad \{\alpha_i, \beta\} = 0, \qquad \beta^2 = 1$$

where i and j run $i, j = x, y, z$. Some of the representations are given in Appendix A.6. The relativistic quantum mechanical equation for a free electron discovered by Dirac is given as

$$\left(i\frac{\partial}{\partial t} + i\boldsymbol{\nabla}\cdot\boldsymbol{\alpha} - m\beta\right)\psi = 0 \qquad (D.1.2)$$

where ψ denotes the wave function and should have four components since $\boldsymbol{\alpha}$ and β are four by four matrices,

$$\psi = \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{pmatrix}. \qquad (D.1.3)$$

In the four components of the wave function, two of them correspond to the spin degrees of freedom and the other two components represent the positive and negative energy states. The static Dirac equation becomes

$$(-i\boldsymbol{\nabla}\cdot\boldsymbol{\alpha}+m\beta)\,\psi = E\psi. \qquad (D.1.4)$$

If the energy eigenvalue contains the negative energy states, which is indeed the case, then the negative energy states must be physical, in contrast to the boson case. For fermions, the negative energy states play a very important role in quantum field theory.

D.2 Negative Energy States

The negative energy states in the Dirac equation are essential for describing the vacuum of quantum field theory, and Dirac interpreted that the vacuum of quantum field theory must be occupied completely by the negative energy states. Because of the Pauli principle, the vacuum is stable as long as the states are full. If one creates a hole in the vacuum, then this corresponds to a new particle with the same mass of the particle which one considers. This can be easily seen since, from the vacuum energy

$$E_v = -\sum_n \sqrt{\boldsymbol{p}_n^2 + m^2}$$

one extracts the state n_0 which is one hole state

$$E_v^{1hole} = -\sum_{n\neq n_0} \sqrt{\boldsymbol{p}_n^2 + m^2}.$$

Therefore one obtains a hole state energy

$$E^h \equiv E_v^{1hole} - E_v = \sqrt{\boldsymbol{p}_{n_0}^2 + m^2} \qquad (D.2.1)$$

which means that the hole state has the same mass as the original fermion. Further, if the fermion has a charge e, then the hole state must have an opposite charge which can be seen in the same way as the energy case.

$$\text{hole charge}\quad e_h \equiv \left(\sum_{n\neq n_0} e - \sum_n e\right) = -e\ . \qquad (D.2.2)$$

D.3 Hydrogen Atom

The Dirac equation is most successful for describing the spectrum of hydrogen atom. One writes the Dirac equation for the hydrogen-like atoms as

$$\left(-i\boldsymbol{\nabla}\cdot\boldsymbol{\alpha}+m\beta-\frac{Ze^2}{r}\right)\psi=E\psi \qquad (D.3.1)$$

where Z denotes the charge of nucleus. Before presenting the solution of the above equation, we should make some comments on this equation. It is of course clear that there is no system which is composed of one electron, except a free electron state. Therefore, even though eq.(D.3.1) shows a simple one body problem for an electron with the potential which is measured from the coordinate center, the realistic problem must be at least two body problem, a system composed of electron and proton. In addition, there must be some contributions from photons and virtual pairs of electron and positron in the intermediate states. If one wishes to discuss the problem of hydrogen atom in the field theoretical treatment, it becomes extremely difficult. This is clear since, in this case, one has to evaluate the system as a many body problem. Even a reliable treatment of the center of mass effects is a non-trivial issue if one starts from the Dirac equation.

D.3.1 Conserved Quantities

The Dirac Hamiltonian for electron in hydrogen atom is written as

$$H=-i\boldsymbol{\nabla}\cdot\boldsymbol{\alpha}+m\beta-\frac{Ze^2}{r}. \qquad (D.3.2)$$

Now, one defines the total angular momentum $\boldsymbol{J}$ and an operator K by

$$\boldsymbol{J}=\boldsymbol{L}+\frac{1}{2}\boldsymbol{\Sigma} \qquad (D.3.3a)$$

$$K=\beta(\boldsymbol{\Sigma}\cdot\boldsymbol{L}+1) \qquad (D.3.3b)$$

where $\boldsymbol{\Sigma}$ is extended to 4×4 matrix of $\boldsymbol{\sigma}$ and is defined as

$$\boldsymbol{\Sigma}=\begin{pmatrix}\boldsymbol{\sigma} & \mathbf{0}\\ \mathbf{0} & \boldsymbol{\sigma}\end{pmatrix}.$$

In this case, it is easy to prove that $\boldsymbol{J}$ and K commute with the Hamiltonian H

$$[H,\boldsymbol{J}]=0, \quad [H,K]=0. \qquad (D.3.4)$$

Therefore, the energy eigenvalues can be specified by the eigenvalues of $\boldsymbol{J}^2$ and K

$$\boldsymbol{J}^2\psi^{\kappa}_{j,j_m}=j(j+1)\psi^{\kappa}_{j,j_m} \qquad (D.3.5a)$$

$$K\psi^{\kappa}_{j,j_m}=\kappa\psi^{\kappa}_{j,j_m} \qquad (D.3.5b)$$

where κ takes values according to

$$\kappa=\mp\left(j+\frac{1}{2}\right) \quad \text{for} \quad j=\ell\pm\frac{1}{2}. \qquad (D.3.6)$$

D.3.2 Energy Spectrum

In this case, the energy eigenvalue of the Dirac Hamiltonian in hydrogen atom is given as

$$E_{n,j} = m\left[1 - \frac{(Z\alpha)^2}{n^2 + 2\left(n - (j+\frac{1}{2})\right)\left[\sqrt{(j+\frac{1}{2})^2 - (Z\alpha)^2} - (j+\frac{1}{2})\right]}\right]^{\frac{1}{2}} \qquad (D.3.7)$$

where α denotes the fine structure constant and is given as

$$\alpha = \frac{1}{137}.$$

The quantum number n runs as $n = 1, 2\cdots$. The energy $E_{n,j}$ can be expanded to order α^4

$$E_{n,j} - m = -\frac{m(Z\alpha)^2}{2n^2} - \frac{m(Z\alpha)^4}{2n^4}\left(\frac{n}{j+\frac{1}{2}} - \frac{3}{4}\right) + \mathcal{O}\left((Z\alpha)^6\right). \qquad (D.3.8)$$

The first term in the energy eigenvalue is the familiar energy spectrum of the hydrogen atom in the non-relativistic quantum mechanics.

D.3.3 Ground State Wave Function ($1s_{\frac{1}{2}}$ – state)

It may be worth to write the Dirac wave function of the lowest state in a hydrogen-like atom. We denote the ground state wave function by

$$\psi^{(-1)}_{\frac{1}{2},m_s}(\boldsymbol{r}) \quad \text{for} \quad 1s_{\frac{1}{2}} - \text{state}$$

since $\kappa = -1$ and $s = \frac{1}{2}$. The energy eigenvalue $E_{1s_{\frac{1}{2}}}$ is simply written as

$$E_{1s_{\frac{1}{2}}} = m\sqrt{1 - (Z\alpha)^2}.$$

The ground state wave function is explicitly given as

$$\psi^{(-1)}_{\frac{1}{2},m_s}(\boldsymbol{r}) = \begin{pmatrix} f^{(-1)}(r) \\ -i\boldsymbol{\sigma}\cdot\hat{\boldsymbol{r}}\, g^{(-1)}(r) \end{pmatrix} \frac{\chi_{m_s}}{\sqrt{4\pi}} \qquad (D.3.9)$$

where χ_{m_s} denotes the two component spinor and is given as

$$\chi_{\frac{1}{2}} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \qquad \chi_{-\frac{1}{2}} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

$\hat{\boldsymbol{r}}$ is defined as

$$\hat{\boldsymbol{r}} = \frac{\boldsymbol{r}}{r}.$$

The radial wave functions $f^{(-1)}(r)$ and $g^{(-1)}(r)$ can be analytically written

$$f^{(-1)}(r) = N\rho^{\sqrt{1-(Z\alpha)^2}}\frac{e^{-\rho}}{\rho} \tag{D.3.10a}$$

$$g^{(-1)}(r) = N\rho^{\sqrt{1-(Z\alpha)^2}}\frac{e^{-\rho}}{\rho}\left[\frac{\epsilon\left(\sqrt{1-(Z\alpha)^2}-1\right)-Z\alpha}{\sqrt{1-(Z\alpha)^2}+1-Z\alpha\epsilon}\right] \tag{D.3.10b}$$

where ρ and ϵ are defined as

$$\rho = \sqrt{m^2 - E^2_{1s_{\frac{1}{2}}}}\, r = Z\alpha r$$

$$\epsilon = \sqrt{\frac{m - E_{1s_{\frac{1}{2}}}}{m + E_{1s_{\frac{1}{2}}}}} = \frac{1-\sqrt{1-(Z\alpha)^2}}{Z\alpha}.$$

N is a normalization constant and should be determined from

$$\int_0^\infty \left[\left(f^{(-1)}(r)\right)^2 + \left(g^{(-1)}(r)\right)^2\right] r^2 dr = 1.$$

D.4 Lamb Shifts

The important consequence of the Dirac equation in hydrogen atom is that the energy eigenvalues are specified by the total angular momentum j apart from the principal quantum number n, and indeed this is consistent with experimental observations.

There is one important deviation of the experiment from the Dirac prediction, that is, the degeneracy of $2p_{\frac{1}{2}}$−state and $2s_{\frac{1}{2}}$−state is resolved. The $2p_{\frac{1}{2}}$−state is lower than the $2s_{\frac{1}{2}}$−state in hydrogen atom. This splitting is originated from the second order effect of the vector field $\boldsymbol{A}$ which affects only on the $2s_{\frac{1}{2}}$−state. Intuitively, the second order effects must be always attractive. However, in the calculation of the Lamb shift, one has to consider the renormalization of the mass term, and due to this renormalization effect, the second order contribution of the vector field $\boldsymbol{A}$ becomes repulsive, and therefore the $2s_{\frac{1}{2}}$−state becomes higher than the $2p_{\frac{1}{2}}$−state.

D.4.1 Quantized Vector Field

Here, we briefly explain how to evaluate the Lamb shift in the non-relativistic kinematics. In this calculation, the quantized electromagnetic field $\boldsymbol{A}$ should be employed

$$\hat{\boldsymbol{A}}(x) = \sum_{\boldsymbol{k}} \sum_{\lambda=1}^{2} \frac{1}{\sqrt{2V\omega_{\boldsymbol{k}}}} \epsilon(\boldsymbol{k},\lambda) \left[c_{\boldsymbol{k},\lambda} e^{-ikx} + c^{\dagger}_{\boldsymbol{k},\lambda} e^{ikx} \right] \qquad (D.4.1)$$

where $c_{\boldsymbol{k},\lambda}$ and $c^{\dagger}_{\boldsymbol{k},\lambda}$ denote the creation and annihilation operators which satisfy the following commutation relations

$$[c_{\boldsymbol{k},\lambda},\ c^{\dagger}_{\boldsymbol{k}',\lambda'}] = \delta_{\boldsymbol{k},\boldsymbol{k}'}\delta_{\lambda,\lambda'}$$

and all other commutation relations vanish.

D.4.2 Non-relativistic Hamiltonian

We start from the Hamiltonian for electron in the hydrogen atom with the electromagnetic interaction

$$H = \frac{\hat{\boldsymbol{p}}^2}{2m_0} - \frac{Ze^2}{r} - \frac{e}{m_0}\hat{\boldsymbol{p}}\cdot\hat{\boldsymbol{A}} \qquad (D.4.2)$$

where the $\hat{\boldsymbol{A}}^2$ term is ignored in the Hamiltonian.

D.4.3 Second Order Perturbation Energy

Now, the second order perturbation energy due to the electromagnetic interaction for a free electron state can be written as

$$\delta E = -\sum_{\lambda}\sum_{\boldsymbol{k}}\sum_{\boldsymbol{p}'}\left(\frac{e}{m_0}\right)^2 \frac{1}{2V\omega_{\boldsymbol{k}}} \frac{|\langle \boldsymbol{p}'|\epsilon(\boldsymbol{k},\lambda)\cdot\hat{\boldsymbol{p}}|\boldsymbol{p}\rangle|^2}{E_{\boldsymbol{p}'}+k-E_{\boldsymbol{p}}} \qquad (D.4.3)$$

where $|\boldsymbol{p}\rangle$ and $|\boldsymbol{p}'\rangle$ denote the free electron state with its momentum. Since the photon energy ($\omega_{\boldsymbol{k}} = k$) is much larger than the energy difference of the electron states ($E_{\boldsymbol{p}'} - E_{\boldsymbol{p}}$)

$$|E_{\boldsymbol{p}'} - E_{\boldsymbol{p}}| << k \qquad (D.4.4)$$

one obtains

$$\delta E = -\frac{1}{6\pi^2}\Lambda\left(\frac{e}{m_0}\right)^2 \boldsymbol{p}^2 \qquad (D.4.5)$$

where Λ is the cutoff momentum of photon. This divergence is proportional to the cutoff Λ which is not the logarithmic divergence. However, this is essentially due to the non-relativistic treatment, and if one carries out the relativistic calculation of quantum field theory, then the divergence becomes logarithmic.

D.4.4 Mass Renormalization and New Hamiltonian

Defining the effective mass δm as

$$\delta m = \frac{1}{3\pi^2}\Lambda e^2 \qquad (D.4.6)$$

the free energy of electron can be written as

$$E_F = \frac{\boldsymbol{p}^2}{2m_0} - \frac{\boldsymbol{p}^2}{2m_0^2}\delta m \simeq \frac{\boldsymbol{p}^2}{2(m_0+\delta m)} \qquad (D.4.7)$$

where one should keep only the term up to order of e^2 because of the perturbative expansion. Now, one defines the renormalized (physical) electron mass m by

$$m = m_0 + \delta m \qquad (D.4.8)$$

and rewrites the Hamiltonian H in terms of the renormalized electron mass m

$$H = \frac{\hat{\boldsymbol{p}}^2}{2m} - \frac{Ze^2}{r} + \frac{\hat{\boldsymbol{p}}^2}{2m^2}\delta m - \frac{e}{m}\hat{\boldsymbol{p}}\cdot\hat{\boldsymbol{A}}. \qquad (D.4.9)$$

Here, the third term ($\frac{\hat{\boldsymbol{p}}^2}{2m^2}\delta m$) corresponds to the counter term which cancels out the second order perturbation energy [eq.(D.4.3)].

D.4.5 Lamb Shift Energy

Using eq.(D.4.3), one can calculate the second order perturbation energy due to the electromagnetic interaction for the $2s_{1/2}$ electron state in hydrogen atom

$$\Delta E_{2s_{1/2}} = \frac{1}{6\pi^2}\Lambda\left(\frac{e}{m}\right)^2\langle 2s_{1/2}|\hat{\boldsymbol{p}}^2|2s_{1/2}\rangle$$

$$-\sum_{\lambda}\sum_{\boldsymbol{k}}\sum_{n\ell}\left(\frac{e}{m}\right)^2\frac{1}{2V\omega_{\boldsymbol{k}}}\frac{|\langle n\ell|\epsilon(\boldsymbol{k},\lambda)\cdot\hat{\boldsymbol{p}}|2s_{1/2}\rangle|^2}{E_{n,\ell}+k-E_{2s_{1/2}}} \qquad (D.4.10)$$

where the first term comes from the counter term. This energy can be rewritten as

$$\Delta E_{2s_{1/2}} = \frac{1}{6\pi^2}\left(\frac{e}{m}\right)^2\sum_{n,\ell}|\langle n,\ell|\hat{\boldsymbol{p}}|2s_{1/2}\rangle|^2\int_0^{\Lambda}dk\frac{E_{n,\ell}-E_{2s_{1/2}}}{E_{n,\ell}+k-E_{2s_{1/2}}} \qquad (D.4.11)$$

where the following identity equation is employed

$$\sum_{n,\ell}|\langle n,\ell|\hat{\boldsymbol{p}}|2s_{1/2}\rangle|^2 = \langle 2s_{1/2}|\hat{\boldsymbol{p}}^2|2s_{1/2}\rangle. \qquad (D.4.12)$$

Further, neglecting the dependence of $E_{n,\ell}$ in the energy denominator because of eq.(D.4.4), one can carry out the summation of $\sum_{n,\ell}$ in eq.(D.4.11) as

$$\sum_{n,\ell}|\langle n,\ell|\hat{\boldsymbol{p}}|2s_{1/2}\rangle|^2(E_{n,\ell}-E_{2s_{1/2}}) = \frac{1}{2}\langle 2s_{1/2}|\left[[\hat{\boldsymbol{p}},\hat{H}_0],\hat{\boldsymbol{p}}\right]|2s_{1/2}\rangle$$

$$= 2\pi Ze^2\langle 2s_{1/2}|\delta(\boldsymbol{r})|2s_{1/2}\rangle \qquad (D.4.13)$$

where $\hat{H}_0$ is the unperturbed Hamiltonian of hydrogen atom

$$\hat{H}_0 = \frac{\hat{\boldsymbol{p}}^2}{2m} - \frac{Ze^2}{r}.$$

Choosing the value of the cutoff Λ as

$$\Lambda \sim m$$

one obtains the energy shift for the $2s_{1/2}$ electron state

$$\Delta E_{2s_{1/2}} \simeq 1040 \ \text{MHz}$$

which is close to a right Lamb shift for the $2s_{1/2}$ state

$$\Delta E^{exp}_{2s_{1/2}} = 1057.862 \ \pm 0.020 \ \text{MHz}.$$

It should be noted that there is no energy shift for the $2p_{1/2}$ state.