Lecture #20

Plane wave solutions of the Dirac equation

Spherical spinors

Hydrogen-like systems … again (Relativistic version)

Dirac energy levels

Chapter 2, pages 48-53, Lectures on Atomic Physics

Chapter 15, pages 696-716, Bransden & Joachain, Quantum Mechanics

Plane wave solutions of the Dirac equation

The Dirac equation for the free particle with spin ½ is

$$i\hbar\frac{\partial}{\partial t}\Psi = -i\hbar c\,\boldsymbol{\alpha}\cdot\nabla\Psi + \beta mc^{2}\Psi \quad \text{or} \quad \left[E - c\,\boldsymbol{\alpha}\cdot\mathbf{p} - \beta mc^{2}\right]\Psi = 0$$

We look for solutions in the form

$$\Psi(\mathbf{r},t) = A\,u\,e^{i(\mathbf{pr}-Et)/\hbar}$$

4-component spinor

constant

$$\left[c\,\boldsymbol{\alpha}\cdot\mathbf{p} + \beta mc^{2}\right]u = Eu$$

Plane wave solutions of the Dirac equation: p=0

First, we consider the case p=0. We label the solutions u(0).

$$\beta = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix} \quad \Longrightarrow \quad \begin{pmatrix} mc^2 & 0 & 0 & 0 \\ 0 & mc^2 & 0 & 0 \\ 0 & 0 & -mc^2 & 0 \\ 0 & 0 & 0 & -mc^2 \end{pmatrix} u(0) = Eu(0)$$

The eigenvalues are

$$E_+ = mc^2 \quad (twice)$$

$$E_- = -mc^2 (twice).$$

The eigenvectors are

$$u^{(1)}(0) = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} \quad u^{(2)}(0) = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} \quad u^{(3)}(0) = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} \quad u^{(4)}(0) = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$$

Plane wave solutions of the Dirac equation: general case

$$\left[c\,\boldsymbol{\alpha}\cdot\mathbf{p}+\beta mc^2\right]u = Eu \qquad \alpha_i = \begin{pmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{pmatrix} \qquad \beta = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}$$

We use the following designations: $u = \begin{pmatrix} u_A \\ u_B \end{pmatrix}, \quad u_A = \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} \quad u_B = \begin{pmatrix} u_3 \\ u_4 \end{pmatrix}.$

$$\begin{pmatrix} 0 & c\,\boldsymbol{\sigma}\cdot\boldsymbol{p} \\ c\,\boldsymbol{\sigma}\cdot\boldsymbol{p} & 0 \end{pmatrix}\begin{pmatrix} u_A \\ u_B \end{pmatrix} + \begin{pmatrix} mc^2 I & 0 \\ 0 & -mc^2 I \end{pmatrix}\begin{pmatrix} u_A \\ u_B \end{pmatrix} = E\begin{pmatrix} u_A \\ u_B \end{pmatrix}$$

$$\begin{pmatrix} mc^2 I & c\,\boldsymbol{\sigma}\cdot\boldsymbol{p} \\ c\,\boldsymbol{\sigma}\cdot\boldsymbol{p} & -mc^2 I \end{pmatrix}\begin{pmatrix} u_A \\ u_B \end{pmatrix} = E\begin{pmatrix} u_A \\ u_B \end{pmatrix}$$

$$mc^2 u_A + c\,\boldsymbol{\sigma}\cdot\boldsymbol{p}u_B = Eu_A \qquad \rightarrow \qquad u_A = \frac{c\,\boldsymbol{\sigma}\cdot\boldsymbol{p}}{E-mc^2}u_B$$

$$-c\,\boldsymbol{\sigma}\cdot\boldsymbol{p}u_A - mc^2 u_B = Eu_B \qquad \rightarrow \qquad u_B = \frac{c\,\boldsymbol{\sigma}\cdot\boldsymbol{p}}{E+mc^2}u_A$$

Plane wave solutions of the Dirac equation: general case

Combining $u_A = \frac{c\,\boldsymbol{\sigma}\cdot\boldsymbol{p}}{E - mc^2} u_B$ and $u_B = \frac{c\,\boldsymbol{\sigma}\cdot\boldsymbol{p}}{E + mc^2} u_A$

we obtain $\left(E - mc^2\right)\left(E + mc^2\right) u_A = c^2 \boldsymbol{\sigma}\cdot\boldsymbol{p}\;\boldsymbol{\sigma}\cdot\boldsymbol{p}\; u_A = c^2 \boldsymbol{p}^2 u_A$

using $\boldsymbol{\sigma}\cdot\boldsymbol{a}\;\boldsymbol{\sigma}\cdot\boldsymbol{b} = \boldsymbol{a}\cdot\boldsymbol{b} + i\boldsymbol{\sigma}\left[\boldsymbol{a}\times\boldsymbol{b}\right]$.

$$\left(E^2 - m^2c^4\right) u_A = c^2 \boldsymbol{p}^2 u_A$$

Therefore, we get four eigenvalues:

$$E_+ = +\sqrt{m^2c^4 + c^2p^2} \quad (twice)$$
$$E_- = -\sqrt{m^2c^4 + c^2p^2} \quad (twice).$$

Plane wave solutions of the Dirac equation

We can get the same result by expanding $\begin{pmatrix} mc^2 I & c\boldsymbol{\sigma}\cdot\boldsymbol{p} \\ c\boldsymbol{\sigma}\cdot\boldsymbol{p} & -mc^2 I \end{pmatrix}\begin{pmatrix} u_A \\ u_B \end{pmatrix} = E\begin{pmatrix} u_A \\ u_B \end{pmatrix}$

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$\boldsymbol{\sigma}\cdot\boldsymbol{p} = \sigma_x p_x + \sigma_y p_y + \sigma_z p_z = \begin{pmatrix} p_z & p_x - ip_y \\ p_x + ip_y & -p_z \end{pmatrix}$$

$$\begin{pmatrix} mc^2 - E & 0 & cp_z & c\left(p_x - ip_y\right) \\ 0 & mc^2 - E & c\left(p_x + ip_y\right) & -cp_z \\ cp_z & c\left(p_x - ip_y\right) & -mc^2 - E & 0 \\ c\left(p_x + ip_y\right) & -cp_z & 0 & -mc^2 - E \end{pmatrix}\begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \end{pmatrix} = 0$$

Plane wave solutions of the Dirac equation

The corresponding determinant is $E^2 - m^2c^4 - c^2p^2 = 0$.

```
> with(LinearAlgebra):
> A := Matrix([[m*c^2-E,0,c*pz,c*px-I*c*py],
[0,m*c^2-E,c*px+I*c*py,-c*pz],[c*pz,c*px-I*c*py,-m*c^2-E,0],
[c*px+I*c*py,-c*pz,0,-m*c^2-E]]);
```

$$A := \begin{bmatrix} m\,c^2 - E & 0 & c\,pz & c\,px - c\,py\,I \\ 0 & m\,c^2 - E & c\,px + c\,py\,I & -c\,pz \\ c\,pz & c\,px - c\,py\,I & -m\,c^2 - E & 0 \\ c\,px + c\,py\,I & -c\,pz & 0 & -m\,c^2 - E \end{bmatrix}$$

```
> B:=factor(Determinant(A));
```

$$B := (-c^2\,px^2 - c^2\,py^2 - c^2\,pz^2 - m^2\,c^4 + E^2)^2$$

So we get the same results, as expected: $E_+ = +\sqrt{m^2c^4 + c^2p^2} \quad (twice)$

$$E_- = -\sqrt{m^2c^4 + c^2p^2} \quad (twice).$$

Plane wave solutions of the Dirac equation

We note that if $E^2 - m^2c^4 - c^2p^2 = 0$ holds, then the determinant is of rank 2 (all 3x3 minors vanish). Therefore, there are two linearly independent solutions corresponding to E_+.

$$u^{(1)} = N\begin{pmatrix} \alpha^{(1)} \\ \dfrac{c\,\boldsymbol{\sigma}\cdot\boldsymbol{p}}{E_+ + mc^2}\alpha^{(1)} \end{pmatrix} \qquad u^{(2)} = N\begin{pmatrix} \alpha^{(2)} \\ \dfrac{c\,\boldsymbol{\sigma}\cdot\boldsymbol{p}}{E_+ + mc^2}\alpha^{(2)} \end{pmatrix} \qquad \alpha^{(1)} = \begin{pmatrix} 1 \\ 0 \end{pmatrix},\ \alpha^{(2)} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

The general solution is given by a linear combination $u_+ = au^{(1)} + bu^{(2)}$.

Solutions corresponding to E_ are

$$u^{(3)} = N\begin{pmatrix} -\dfrac{c\,\boldsymbol{\sigma}\cdot\boldsymbol{p}}{-E_- + mc^2}\alpha^{(1)} \\ \alpha^{(1)} \end{pmatrix} \qquad u^{(4)} = N\begin{pmatrix} -\dfrac{c\,\boldsymbol{\sigma}\cdot\boldsymbol{p}}{-E_- + mc^2}\alpha^{(2)} \\ \alpha^{(2)} \end{pmatrix}.$$

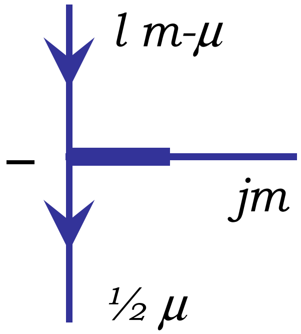
Spherical spinors

$h_D\varphi = E\varphi,$ in atomic units $h_D = c\,\boldsymbol{\alpha}\cdot\mathbf{p} + \beta c^2 + V(r)$

Total angular momentum is given by $\boldsymbol{J}=\boldsymbol{L}+\boldsymbol{S}$.
$\boldsymbol{J}$ commutes with the Dirac Hamiltonian $h_{D.}$ Therefore, we may classify the eigenstates of h_D according to the eigenvalues of energy, J^2 and J_z. The eigenstates of J^2 and J_z are spherical spinors $\Omega_{\kappa m}(\theta,\phi)$.

We combine spherical harmonics, which are eigenstates of L^2 and L_z and spinors, which are eigenstates of S^2 and S_z to form eigenstates of J^2 and J_z (refereed to as spherical spinors $\Omega_{jlm}(\theta,\phi)$).

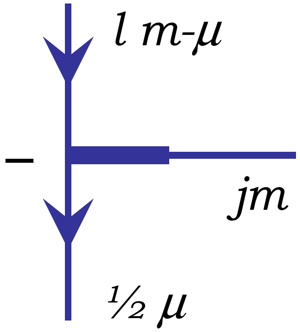
$$\Omega_{jlm}(\theta,\phi) = \sum_{\mu}$$



$$Y_{l,m-\mu}(\theta,\phi)\chi_{\mu}$$

Spherical spinors

$$\Omega_{jlm}(\theta,\phi)=\sum_{\mu}$$



$$Y_{l,m-\mu}(\theta,\phi)\chi_{\mu}$$

$$\boxed{j=l\pm1/2}$$

$j=l+1/2$

$$\Omega_{l+1/2\,lm}(\theta,\phi)=\begin{pmatrix}\sqrt{\dfrac{l+m+1/2}{2l+1}}\;Y_{l,m-1/2}(\theta,\phi)\\ \sqrt{\dfrac{l-m+1/2}{2l+1}}\;Y_{l,m+1/2}(\theta,\phi)\end{pmatrix}$$

$j=l-1/2$

$$\Omega_{l-1/2\,lm}(\theta,\phi)=\begin{pmatrix}-\sqrt{\dfrac{l-m+1/2}{2l+1}}\;Y_{l,m-1/2}(\theta,\phi)\\ \sqrt{\dfrac{l+m+1/2}{2l+1}}\;Y_{l,m+1/2}(\theta,\phi)\end{pmatrix}$$

Spherical spinors

Spherical spinors are eigenfunctions of $\boldsymbol{\sigma}\cdot\boldsymbol{L}$ and, therefore, of $K=-1-\boldsymbol{\sigma}\cdot\boldsymbol{L}$
The eigenvalue for K is

$$K\Omega_{jlm}(\theta,\phi)=\kappa\,\Omega_{jlm}(\theta,\phi) \qquad \kappa=\begin{cases}-l-1 & j=l+1/2\\ l & j=l-1/2\end{cases}$$

Note that the κ (which is referred to as *relativistic angular momentum quantum number*) uniquely defines the orbital with l and j
so we can use designations $\Omega_{\kappa m}(\theta,\phi)$.

s	$l=0$	$j=1/2$	$\kappa=-1$
$p_{1/2}$	$l=1$	$j=1/2$	$\kappa=\ \ 1$
$p_{3/2}$	$l=1$	$j=3/2$	$\kappa=-2$
$d_{3/2}$	$l=2$	$j=3/2$	$\kappa=\ \ 2$
$d_{5/2}$	$l=2$	$j=3/2$	$\kappa=-3$

Dirac equation for a central potential

$h_D\varphi = E\varphi$, in atomic units $h_D = c\,\boldsymbol{\alpha}\cdot\mathbf{p} + \beta c^2 + V(r)$

Total angular momentum is given by ***J*=*L*+*S***.
J commutes with the Dirac Hamiltonian $h_{D.}$ Therefore, we may classify the eigenstates of h_D according to the eigenvalues of energy, J^2 and J_z.
The eigenstates of J^2 and J_z are spherical spinors $\Omega_{\kappa m}(\theta,\phi)$.

We seek solutions in a form $\varphi_k(\mathbf{r}) = \frac{1}{r}\begin{pmatrix} iP_\kappa(r)\,\Omega_{\kappa m}(\theta,\phi) \\ Q_\kappa(r)\,\Omega_{-\kappa m}(\theta,\phi) \end{pmatrix}$.

The resulting equations for the radial functions are

$$\left[c^2 + V(r)\right]P_\kappa(r) + c\left[\frac{d}{dr} - \frac{\kappa}{r}\right]Q_\kappa(r) = E\,P_\kappa(r)$$

$$-c\left[\frac{d}{dr} + \frac{\kappa}{r}\right]P_\kappa(r) + \left[V(r) - c^2\right]Q_\kappa(r) = E\,Q_\kappa(r).$$

Hydrogen-like systems: Dirac energy levels

$$\left[c^2 + V(r)\right]P_\kappa(r) + c\left[\frac{d}{dr} - \frac{\kappa}{r}\right]Q_\kappa(r) = E\,P_\kappa(r)$$

$$\boxed{V(r) = -\frac{Z}{r}}$$

$$-c\left[\frac{d}{dr} + \frac{\kappa}{r}\right]P_\kappa(r) + \left[V(r) - c^2\right]Q_\kappa(r) = E\,Q_\kappa(r)$$

Dirac energy levels: $E_{n\kappa} = \dfrac{c^2}{\sqrt{1 + \dfrac{\alpha^2 Z^2}{\left(\gamma + n + |\kappa|\right)}}}, \quad \gamma = \sqrt{\kappa^2 - \alpha^2 Z^2}$

The non-relativistic energy levels depends only on the principal quantum number n. When relativistic effects are taken into accounts the non-relativistic energy level will split into n different Dirac energy levels (fine structure splitting). Note that the energy above depends only on the values of n and $|\kappa|=j+1/2$, therefore the levels with the same n and l but different j, for example levels $2p_{1/2}$ and $2p_{3/2}$ will have different energies. The energy difference between such levels is called the fine-structure interval.

Hydrogen-like systems: Dirac energy levels

Dirac energy levels: $E_{n\kappa} = \dfrac{c^2}{\sqrt{1+\dfrac{\alpha^2 Z^2}{\left(\gamma+n+|\kappa|\right)}}}, \quad \gamma = \sqrt{\kappa^2 - \alpha^2 Z^2}$

The levels the same n and *j* but different *l* will have the same energies, for example levels $2s_{1/2}$ and $2p_{1/2}$. The experimentally observed energy difference between these levels is called the Lamb shift and is explained by quantum electrodynamics (QED) effects, known as radiative corrections. The expansion of the formula above in powers of αZ will give (in atomic units)

$$E_{n\kappa} = c^2 - \frac{Z^2}{2n^2} - \underbrace{\frac{\alpha^2 Z^4}{2n^3}\left[\frac{1}{|\kappa|} - \frac{3}{4n}\right] + \ldots}$$

Electron's rest energy (mc^2)

Non-relativistic Coulomb-field binding energy

Leading fine-structure correction