G25.2666: Quantum Mechanics II

Notes for Lecture 6

I. SOLUTION OF THE DIRAC EQUATION FOR A FREE PARTICLE

The Dirac Hamiltonian takes the form

$$H = c\,\vec{\alpha}\cdot\mathbf{P} + \beta mc^2$$

where

$$\vec{\alpha} = \begin{pmatrix} 0 & \vec{\sigma} \\ \vec{\sigma} & 0 \end{pmatrix} \qquad \beta = \begin{pmatrix} \mathrm{I} & 0 \\ 0 & -\mathrm{I} \end{pmatrix}$$

Using $\mathbf{P} = (\hbar/i)\nabla$, in the coordinate basis, the Dirac equation for a free particle reads

$$\left[-i\hbar c\,\vec{\alpha}\cdot\nabla + \beta mc^2\right]\Psi(\mathbf{r},) = i\hbar\frac{\partial}{\partial t}\Psi(\mathbf{r},t)$$

Since the operator on the left side is a 4×4 matrix, the wave function $\Psi(\mathbf{r},t)$ is actually a four-component vector of functions of $\mathbf{r}$ and t:

$$\Psi(\mathbf{r},t) = \begin{pmatrix} \Psi_1(\mathbf{r},t) \\ \Psi_2(\mathbf{r},t) \\ \Psi_3(\mathbf{r},t) \\ \Psi_4(\mathbf{r},t) \end{pmatrix}$$

which is called a four-component *Dirac spinor*. In order to generate an eigenvalue problem, we look for a solution of the form

$$\Psi(\mathbf{r},t) = \psi(\mathbf{r})e^{-iEt/\hbar}$$

which, when substituted into the Dirac equation gives the eigenvalue equation

$$\left[-i\hbar c\,\vec{\alpha}\cdot\nabla + \beta mc^2\right]\psi(\mathbf{r}) = E\psi(\mathbf{r})$$

Note that, since H is only a function of $\mathbf{P}$, then $[\mathbf{P},H]=0$ so that the eigenvalues $\mathbf{p}$ of $\mathbf{P}$ can be used to characterize the states. In particular, we look for free-particle (plane-wave) solutions of the form:

$$\psi_{\mathbf{p}}(\mathbf{r}) = u_{\mathbf{p}}e^{i\mathbf{p}\cdot\mathbf{r}/\hbar}$$

where $u_{\mathbf{p}}$ is a four-component vector which satisfies

$$\left[c\,\vec{\alpha}\cdot\mathbf{p} + \beta mc^2\right]u_{\mathbf{p}} = Eu_{\mathbf{p}}$$

Since the matrix on the left is expressible in terms of 2×2 blocks, we look for $u_{\mathbf{p}}$ in the form of a vector composed of two two-component vectors:

$$u_{\mathbf{p}} = \begin{pmatrix} \phi_{\mathbf{p}} \\ \chi_{\mathbf{p}} \end{pmatrix}$$

Therefore, writing the equation in matrix form, we find

$$\begin{pmatrix} mc^2 & c\,\vec{\sigma}\cdot\mathbf{p} \\ c\,\vec{\sigma}\cdot\mathbf{p} & -mc^2 \end{pmatrix}\begin{pmatrix} \phi_{\mathbf{p}} \\ \chi_{\mathbf{p}} \end{pmatrix} = \begin{pmatrix} E & 0 \\ 0 & E \end{pmatrix}\begin{pmatrix} \phi_{\mathbf{p}} \\ \chi_{\mathbf{p}} \end{pmatrix}$$

or

$$\begin{pmatrix} E - mc^2 & -c\,\vec{\sigma}\cdot\mathbf{p} \\ -c\,\vec{\sigma}\cdot\mathbf{p} & E + mc^2 \end{pmatrix} \begin{pmatrix} \phi_{\mathbf{p}} \\ \chi_{\mathbf{p}} \end{pmatrix} = 0$$

which yields two equations

$$\left(E - mc^2\right)\phi_{\mathbf{p}} - c\,\vec{\sigma}\cdot\mathbf{p}\chi_{\mathbf{p}} = 0$$
$$-c\,\vec{\sigma}\cdot\mathbf{p}\phi_{\mathbf{p}} + \left(E + mc^2\right)\chi_{\mathbf{p}} = 0$$

From the second equation:

$$\chi_{\mathbf{p}} = \frac{c\,\vec{\sigma}\cdot\mathbf{p}}{E + mc^2}\phi_{\mathbf{p}}$$

Note, one could also solve the first for $\phi_{\mathbf{p}}$ and obtain

$$\phi_{\mathbf{p}} = \frac{c\,\vec{\sigma}\cdot\mathbf{p}}{E - mc^2}\chi_{\mathbf{p}}$$

Using the first of these, then a single equation for $\phi_{\mathbf{p}}$ can be obtained

$$\left(E - mc^2\right)\left(E + mc^2\right)\phi_{\mathbf{p}} - c^2\left(\vec{\sigma}\cdot\mathbf{p}\right)^2\phi_{\mathbf{p}} = 0$$

However,

$$\left(\vec{\sigma}\cdot\mathbf{p}\right)^2 = \left(\vec{\sigma}\cdot\mathbf{p}\right)\left(\vec{\sigma}\cdot\mathbf{p}\right) = \mathbf{p}\cdot\mathbf{p} + i\,\vec{\sigma}\cdot(\mathbf{p}\times\mathbf{p}) = p^2$$

Hence, we have the condition

$$\left[E^2 - \left((mc^2) + c^2p^2\right)\right]\phi_{\mathbf{p}} = 0$$

Since $\phi_{\mathbf{p}} \neq 0$, the equation is only satisfied if the quantity in the brackets vanishes, which yields the eigenvalues

$$E = E_{\mathbf{p}} = \pm\sqrt{p^2c^2 + m^2c^4}$$

We see that the eigenvalues can be positive or negative. A plot of the energy levels is shown below:

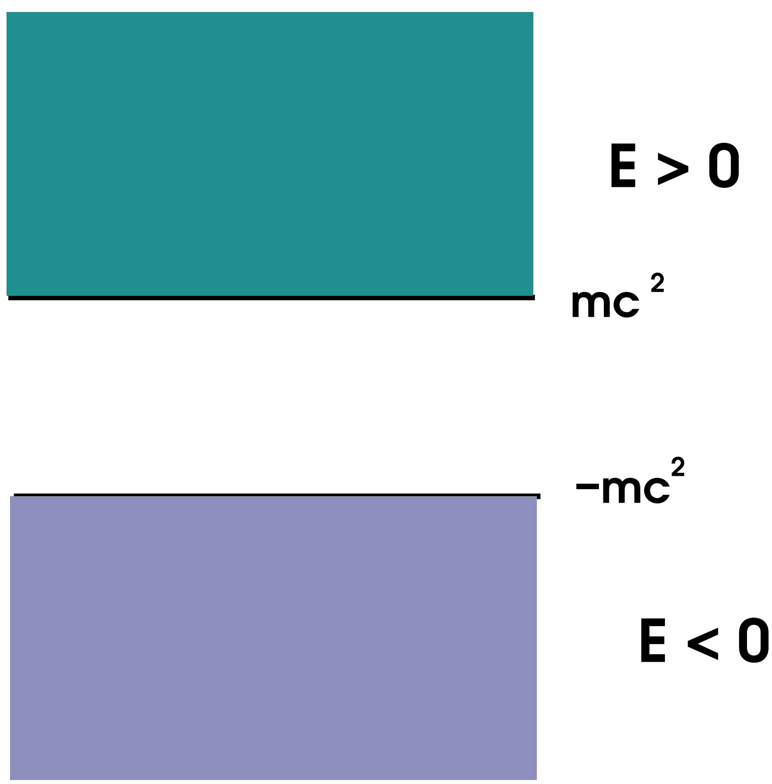

FIG. 1.

There is a continuum for $E_{\mathbf{p}} > mc^2$ (turquoise) and for $E_{\mathbf{p}} < -mc^2$ (periwinkle). There is also a gap between $-mc^2$ and mc^2.

We will show that for $E > 0$, an appropriate solution is to take

$$\phi_{\mathbf{p}} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad \text{or} \qquad \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

If this is the case, then

$$\chi_{\mathbf{p}} = \frac{c\,\vec{\sigma}\cdot\mathbf{p}}{E_{\mathbf{p}} + mc^2}\begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad \text{or} \qquad \frac{c\,\vec{\sigma}\cdot\mathbf{p}}{E_{\mathbf{p}} + mc^2}\begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

However,

$$\vec{\sigma}\cdot\mathbf{p} = \begin{pmatrix} p_z & p_x - ip_y \\ p_x + ip_y & -p_z \end{pmatrix}$$

so that

$$\chi_{\mathbf{p}} = \begin{pmatrix} cp_z/(E_{\mathbf{p}} + mc^2) \\ c(p_x + ip_y)/(E_{\mathbf{p}} + mc^2) \end{pmatrix} \qquad \text{or} \qquad \begin{pmatrix} c(p_x - ip_y)/(E_{\mathbf{p}} + mc^2) \\ -cp_z/(E_{\mathbf{p}} + mc^2) \end{pmatrix}$$

so that the full solution $u_{\mathbf{p}}$ is

$$u_{\mathbf{p}} = \begin{pmatrix} 1 \\ 0 \\ cp_z/(E_{\mathbf{p}} + mc^2) \\ c(p_x + ip_y)/(E_{\mathbf{p}} + mc^2) \end{pmatrix} \qquad \text{or} \qquad \begin{pmatrix} 0 \\ 1 \\ c(p_x - ip_y)/(E_{\mathbf{p}} + mc^2) \\ -cp_z/(E_{\mathbf{p}} + mc^2) \end{pmatrix}$$

Note that when $\mathbf{p} = 0$, the third and fourth components of $u_{\mathbf{p}}$ vanish. In this case, energy is just $E_0 = mc^2$ and the full time-dependent wave function becomes

$$\Psi(t) \longrightarrow \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} e^{-imc^2 t/\hbar} \qquad \text{or} \qquad \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} e^{-imc^2 t/\hbar}$$

which are both forward propagating solutions. These correspond to *particle solutions*, in particular, a spin-1/2 particle propagating forward in time with an energy equal to the rest mass energy.

When $E < 0$, we take

$$\chi_{\mathbf{p}} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad \text{or} \qquad \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

so that

$$\phi_{\mathbf{p}} = \frac{c\,\vec{\sigma}\cdot\mathbf{p}}{E_{\mathbf{p}} - mc^2}\chi_{\mathbf{p}} = \frac{-c\,\vec{\sigma}\cdot\mathbf{p}}{|E_{\mathbf{p}}| + mc^2}\chi_{\mathbf{p}}$$

By the same reasoning, the solution for $u_{\mathbf{p}}$ is

$$u_{\mathbf{p}} = \begin{pmatrix} -cp_z/(|E_{\mathbf{p}}|+mc^2) \\ -c(p_x+ip_y)/(|E_{\mathbf{p}}|+mc^2) \\ 1 \\ 0 \end{pmatrix} \quad \text{or} \quad \begin{pmatrix} -c(p_x-ip_y)/(|E_{\mathbf{p}}|+mc^2) \\ cp_z/(E_{\mathbf{p}}+mc^2) \\ 0 \\ 1 \end{pmatrix}$$

so that in the limit $\mathbf{p} = 0$, and $E_0 = -mc^2$,

$$\Psi(t) \longrightarrow \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} e^{imc^2t/\hbar} \quad \text{or} \quad \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} e^{imc^2t/\hbar}$$

which describes particles moving backward in times. Thus, the interpretation is that the negative energy solutions correspond to anti-particles, the the components, $\phi_{\mathbf{p}}$ and $\chi_{\mathbf{p}}$ of $u_{\mathbf{p}}$ correspond to the particle and anti-particle components, respectively. Thus, the Dirac equation no only describes spin but it also includes particle and the corresponding anti-particle solutions!

In the non-relativistic limit, for $E > 0$, we have

$$E_{\mathbf{p}} \approx mc^2 + \frac{\mathbf{p}^2}{2m}$$

so that

$$\chi_{\mathbf{p}} = \frac{c\,\vec{\sigma}\cdot\mathbf{p}}{2mc^2 + \mathbf{p}^2/2m}\phi_{\mathbf{p}}$$

since $mc^2 \gg \mathbf{p}^2/2m$, it follows that

$$\chi_{\mathbf{p}} \ll \phi_{\mathbf{p}}$$

Neglecting it, and recalling that for $E > 0$,

$$\phi_{\mathbf{p}} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \text{or} \quad \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

the eigenfunctions reduce to

$$\psi_{\mathbf{p}}(\mathbf{r}) = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} e^{i\mathbf{p}\cdot\mathbf{r}/\hbar} \quad \text{or} \quad \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} e^{i\mathbf{p}\cdot\mathbf{r}/\hbar}$$

The lower component has become reduntant, and the eigenfunctions just correspond to those of a free particle with an attached spin eigenfunction $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$ or $\begin{pmatrix} 0 \\ 1 \end{pmatrix}$ for $m_s = \hbar/2$ or $-\hbar/2$, respectively. For $E > 0$, the lower component, $\chi_{\mathbf{p}}$ is called the *minor component* and the upper component $\phi_{\mathbf{p}}$ is called the *major component*.

II. INTRODUCTION TO TOTAL ANGULAR MOMENTUM IN QUANTUM MECHANICS

A. Total orbital angular momentum

In the hydrogen atom or any system with a spherically symmetric potential $V(r)$, we have learned that angular momentum

$$\mathbf{L} = \mathbf{r} \times \mathbf{p}$$

is conserved. The Hamiltonian will be of the form

$$\begin{aligned} H &= -\frac{\hbar^2}{2m}\nabla^2 + V(r) \\ &= -\frac{\hbar^2}{2m}\frac{1}{r}\frac{\partial^2}{\partial r^2}r + \frac{\mathbf{L}^2}{2m\hbar^2 r^2} + V(r) \end{aligned}$$

and will satisfy

$$[\mathbf{L}, H] = 0$$

so that $\mathbf{L}$ is a constant of the motion.

This is illustrated schematically below:

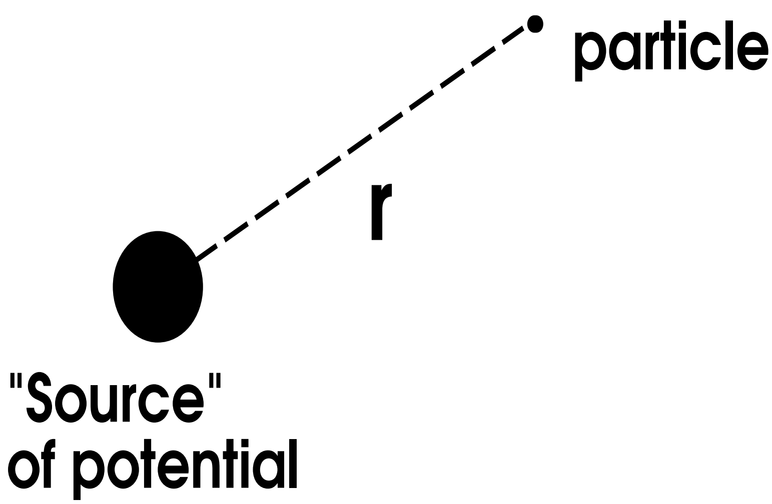

FIG. 2.

This is, however, an idealization because the "nucleus" or source of the spherical potential is assumed not to move and can be, therefore, be held stationary at the origin. Thus, $\mathbf{L}$ corresponds to the angular momentum of the particle in such a potential field. In practice, this is not a bad assumption since the mass of the proton is approximately 2000 time that of the electron.

However, what happens when the "source" of the potential is not so heavy and can move on a time scale similar to that of the particle. An example would be hydrogen with the proton replaced by a particle with positive charge and the same mass of the electron, i.e., a positron. The system, shown below,

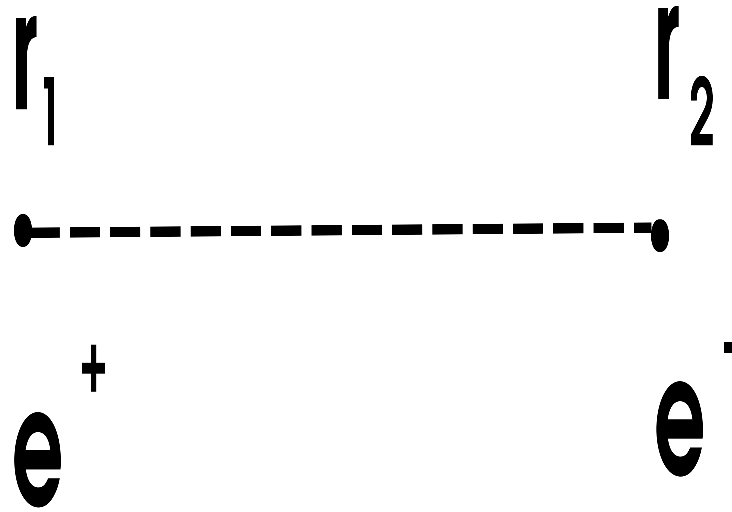

FIG. 3.

is known as *positronium.* It will be described by a Hamiltonian of the form

$$H = -\frac{\hbar^2}{2m}\left(\nabla_1^2 + \nabla_2^2\right) + V(|\mathbf{r}_1 - \mathbf{r}_2|)$$

where

$$\nabla_1 = \frac{\partial}{\partial \mathbf{r}_1} \qquad \nabla_2 = \frac{\partial}{\partial \mathbf{r}_2}$$

and

$$V(|\mathbf{r}_1 - \mathbf{r}_2|) = -\frac{e^2}{|\mathbf{r}_1 - \mathbf{r}_2|}$$

Although this is the specific form of the potential for this example, what we will show will be general for any potential that depends only on $|\mathbf{r}_1 - \mathbf{r}_2|$.

Now, the individual angular momenta

$$\mathbf{L}_1 = \mathbf{r}_1 \times \mathbf{p}_1 \qquad \mathbf{L}_2 = \mathbf{r}_2 \times \mathbf{p}_2$$

are no longer conserved, i.e.,

$$[\mathbf{L}_1, H] \neq 0 \qquad [\mathbf{L}_2, H] \neq 0$$

To see that this is true, consider the z components of the angular momentum operators:

$$L_{1z} = \frac{\hbar}{i}\left(x_1\frac{\partial}{\partial y_1} - y_1\frac{\partial}{\partial x_1}\right) \qquad L_{2z} = \frac{\hbar}{i}\left(x_2\frac{\partial}{\partial y_2} - y_2\frac{\partial}{\partial x_2}\right)$$

It is straightforward to compute the commutators (left as an exercise for the reader) and it is found that

$$\begin{aligned}[L_{1z}, H] &= \frac{\hbar}{i}\left(x_1\frac{\partial V}{\partial y_1} - y_1\frac{\partial V}{\partial x_1}\right)\\ &= \frac{\hbar}{i}\left[x_1 V'(|\mathbf{r}_1 - \mathbf{r}_2|)\frac{y_1 - y_2}{|\mathbf{r}_1 - \mathbf{r}_2|} - y_1 V'(|\mathbf{r}_1 - \mathbf{r}_2|)\frac{x_1 - x_2}{|\mathbf{r}_1 - \mathbf{r}_2|}\right] \neq 0\end{aligned}$$

Similarly,

$$
\begin{aligned}
[L_{2z}, H] &= \frac{\hbar}{i}\left(x_2\frac{\partial V}{\partial y_2} - y_2\frac{\partial V}{\partial x_2}\right) \\
&= \frac{\hbar}{i}\left[x_2 V'(|\mathbf{r}_1-\mathbf{r}_2|)\left(-\frac{y_1-y_2}{|\mathbf{r}_1-\mathbf{r}_2|}\right) - y_2 V'(|\mathbf{r}_1-\mathbf{r}_2|)\left(-\frac{x_1-x_2}{|\mathbf{r}_1-\mathbf{r}_2|}\right)\right] \\
&= -\frac{\hbar}{i}\left[x_2 V'(|\mathbf{r}_1-\mathbf{r}_2|)\frac{y_1-y_2}{|\mathbf{r}_1-\mathbf{r}_2|} - y_2 V'(|\mathbf{r}_1-\mathbf{r}_2|)\frac{x_1-x_2}{|\mathbf{r}_1-\mathbf{r}_2|}\right] \neq 0
\end{aligned}
$$

However, if we add these together, it can be see that

$$
\begin{aligned}
[L_{1z}, H] + [L_{2z}, H] &= [(L_{1z}+L_{2z}), H] \\
&= \frac{\hbar}{i}\left[V'(|\mathbf{r}_1-\mathbf{r}_2|)\frac{(x_1-x_2)(y_1-y_2)}{|\mathbf{r}_1-\mathbf{r}_2|} - V'(|\mathbf{r}_1-\mathbf{r}_2|)\frac{(y_1-y_2)(x_1-x_2)}{|\mathbf{r}_1-\mathbf{r}_2|}\right] = 0
\end{aligned}
$$

Thus, the quantity $L_{1z}+L_{2z}$ is a constant of the motion. The same can be shown to be true for the x and y components. Thus, The quantity

$$\mathbf{L} = \mathbf{L}_1 + \mathbf{L}_2$$

is a constant of the motion. $\mathbf{L} = \mathbf{L}_1 + \mathbf{L}_2$ is known as the *total orbital angular momentum.* It is conserved because the potential only depends on the distance between the two particles.

If we have an N-particle system with a Hamiltonian of the form

$$H = -\hbar^2\sum_{i=1}^{N}\frac{1}{2m_i}\nabla_i^2 + \sum_{i=1}^{N}\sum_{j=i+1}^{N} V(|\mathbf{r}_i-\mathbf{r}_j|)$$

then the total orbital angular momentum

$$\mathbf{L} = \sum_{i=1}^{N}\mathbf{L}_i$$

will be a constant of the motion.

B. Total spin

If the Hamiltonian is independent of spin, then it is clear that the total spin of an N-particle system

$$\mathbf{S} = \sum_{i=1}^{N}\mathbf{S}_i$$

will be a constant of the motion, but so will the individual spins, $\mathbf{S}_i$ of the individual particles.

What happens, however, when the Hamiltonian is spin dependent. Consider the case of the hydrogen atom with relativistic corrections. It can be shown (see problem set # 2) from the Dirac equation that when relativistic corrections are accounted for, a term in the Hamiltonian appears that is explicitly spin dependent and takes the form

$$H_{\rm so} = f(r)\mathbf{L}\cdot\mathbf{S}$$

which is known as the *spin-orbit* coupling.

Let us look at the commutator of this Hamiltonian with the z components of $\mathbf{L}$ and $\mathbf{S}$. First note that

$$H_{\rm so} = f(r)\left(L_xS_x + L_yS_y + L_zS_z\right)$$

Therefore,

$$
\begin{aligned}
[L_z, H_{\rm so}] &= f(r)\left([L_z,L_x]\,S_x + [L_z,L_y]\,S_y + [L_z,L_z]\,S_z\right) \\
&= f(r)\left(i\hbar L_yS_x - i\hbar L_xS_y\right) \neq 0
\end{aligned}
$$

Also,

$$\begin{aligned}[S_z, H_{\text{so}}] &= f(r) \left(L_x [S_z, S_x] + L_y [S_z, S_y] + L_z [S_z, S_z]\right) \\ &= f(r) \left(i\hbar L_x S_y - i\hbar L_y S_x\right) \neq 0\end{aligned}$$

However, if we add these together

$$\begin{aligned}[L_z, H_{\text{so}}] + [S_z, H_{\text{so}}] &= [(L_z + S_z), H_{\text{so}}] \\ &= i\hbar f(r) \left(L_y S_x - L_x S_y + L_x S_y - L_y S_x\right) = 0\end{aligned}$$

Thus, $L_z + S_z$ is a constant of the motion. The same can be shown to be true for the x and y components, thus it follows that

$$\mathbf{J} = \mathbf{L} + \mathbf{S}$$

is a constant of the motion. Recall that $\mathbf{J}$ is the total angular momentum. It is often true for spin-dependent Hamiltonians that the total angular momentum is still conserved.

Thus, we see that total angular orbital angular momentum, total spin, and total angular momentum are all important quantities in quantum mechanics. When $\mathbf{J}$ is conserved, then J^2 and J_z are good quantum numbers. In general, it remains to discuss how to derive a set of basis vectors appropriate for total angular momenta of any type. We expect that they can be composed of tensor products of the basis vectors of the corresponding individual angular momenta but will not be equal to them. We will show that they are equal to in the next lecture.