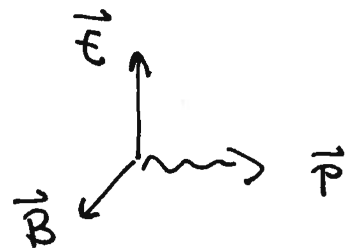
February 27

Spin

In the previous lecture, we derived the commutation relations of angular momentum and the action of the angular momentum generators on Schrödinger wavefunctions. In this lecture, I will discuss some additional important aspects of this theory.

To begin, I should explain that, while the theory of the previous lecture applies to idealized structureless particles described completely by the Schrödinger wavefunction, it does not actually apply to most of the real particles that we observe in nature. In particular, we need to augment this theory to describe photons, protons, and electrons. Let me begin by describing the quantum state of a photon.

A photon is the quantum of an electromagnetic wave that contains perpendicular $\vec{E}$ and $\vec{B}$ fields.



For this reason, a photon has not only a spatial wavefunction but also a vector (called the *polarization vector* that gives the direction in which the $\vec{E}$ field points. A photon interacts with an atom by shaking the electrons in the direction of the $\vec{E}$ field; thus, the polarization vector plays a key role in describing the interactions of photons with matter. (This statement is also true for the interaction of classical radiation with matter.) A typical wavefunction for a photon is

$$|\hat{n}, \vec{p}\rangle = \hat{n}\, e^{+i\vec{p}\cdot\vec{x}/\hbar}$$

where $\vec{p}$ is the photon momentum and $\hat{n}$, a unit vector, is the direction of polarization.

A rotation acts on this state as follows: First, it must rotate the wavefunction as we saw in the previous lecture

$$\psi(\vec{x}) \rightarrow \psi(\vec{R}^{-1}(\vec{\alpha})\vec{x})$$

But, also, it must rotate the polarization vector

$$\hat{n} \longrightarrow R(\vec{\alpha})\,\hat{n}$$

In all

$$U(\vec{\alpha})\,|\hat{n},\vec{p}\rangle = R(\vec{\alpha})\,\hat{n}\; e^{i\vec{p}\cdot\vec{R}^{-1}(\vec{\alpha})\vec{x}/\hbar}$$

Using $\vec{p}\cdot R^{-1}(\vec{\alpha})\vec{x} = R(\vec{\alpha})\vec{p}\cdot\vec{x}$, we can rewrite this expression as

$$R(\vec{\alpha})\,\hat{n}\; e^{i R(\vec{\alpha})\vec{p}\cdot\vec{x}/\hbar} = |R(\vec{\alpha})\hat{n}, R(\vec{\alpha})\vec{p}\rangle$$

The infinitesimal form of the transformation is

$$\hat{n}\, e^{i\vec{p}\cdot\vec{x}/\hbar} \rightarrow \left(1 - i\vec{\alpha}\cdot\underset{\sim}{\vec{S}} - i\vec{\alpha}\,\frac{\vec{L}}{\hbar}\right)\hat{n}\, e^{i\vec{p}\cdot\vec{x}/\hbar} + O(\alpha^2)$$

so we write

$$\vec{J} = \vec{L} + \vec{\mathcal{S}} \qquad\qquad \vec{\mathcal{S}} = \hbar\vec{S}$$

where $\vec{J}$ is the complete angular momentum of the photon, the sum of its orbital and *spin* angular momentum. The spin is an intrinsic angular momentum carried, somehow, inside the quantum particle.

We have now encountered *scalar particles*, which are described by Schrödinger wavefunctions with are complex-valued and *vector particles*, which are described by Schrödinger wavefunctions that whose values are complex 3-vectors. Pi mesons in nuclear physics are examples of scalar particles. Photons are examples of vector particles. It is interesting to ask whether there are other possible kinds of quantum particles beyond these. A typical wavefunction of some other type of particle would be

$$\chi_a \, e^{i\vec{p}\cdot\vec{x}/\hbar}$$

where χ_a is a vector in some Hilbert space that transforms in a natural way under rotations. What are the possibilities for χ_a? To answer this question, or even to pose it properly, we need some additional concepts.

To enter this subject, I need to define a *group* and a *group representation*. A group G is a set of abstract elements $\{g_i\}$ with a definite multiplication law

$$g_i \cdot g_j = g_k \in G$$

The group multiplication law must satisfy three axioms: Multiplication must be associative, the group must contain an inverse 1 such that $g_i \cdot 1 = 1 \cdot g_i = g_i$ for all i, and each element g_i must have an inverse g_i^{-1} such that $g_i \cdot g_i^{-1} = 1$.

The simplest group is Z_2, the group that has the multiplication law of the numbers $\{1, -1\}$. There are many other groups with a discrete set of elements, for example, the group of permutations of n objects.

The set of all rotations in 3-dimensional space is a larger group with an infinite set of elements. The rotation group $SO(3)$ is rather special in that all group elements are build up from infinitesimal group transformations. Such a group is called a *Lie group*. The commutator algebra of the generators is called the *Lie algebra*. I argued in the previous lecture that this commutator algebra completely determines the multiplication law of the associated Lie group.

In quantum mechanics, a group will act on vectors in a Hilbert space. The action is implemented by a set of unitary matrices $U(g_i)$ with the multiplication law of the group.

$$g_1 \cdot g_2 = g_3 \quad \Rightarrow \quad U(g_1)U(g_2) = U(g_3)$$

Such a set of matrices is called a *unitary representation* of the group. If

$$[U(g_i), H] = 0$$

for all i, we say that G is a *symmetry* of the quantum mechanical problem.

Symmetry groups arise naturally in many quantum mechanical problems. For example, if a potential is invariant under the tranformation $x \to -x$,

$$V(x) = +V(-x)$$

then the operations

$$U(1)\,\psi(x) = \psi(x) \qquad U(-1)\,\psi(x) = \psi(-x)$$

are unitary transformations that commute with the Hamiltonian for a particle in this potential. The operators $U(1)$ and $U(-1)$ provide a unitary representation of the group Z_2. Normally, we call

$$U(1) = 1 \qquad U(-1) = P \quad \text{(parity)}$$

Since $[P, H] = 0$, we can find a basis for the Hilbert space in which all states are simultaneously eigenstates of P and H. For example, in the basis of eigenstates of the harmonic oscillator Hamiltonian,

$$H = \frac{\hbar\Omega}{2} + \hbar\Omega \begin{pmatrix} 0 & & & \\ & 1 & & \\ & & 2 & \\ & & & 3 & \\ & & & & \ddots \end{pmatrix} \qquad P = \begin{pmatrix} 1 & & & \\ & -1 & & \\ & & 1 & \\ & & & -1 & \\ & & & & \ddots \end{pmatrix}$$

In this basis, the action of P is very simple; P multiplies each wavefunction by $+1$ or -1. In other words, we can *reduce* the action of P to transformations within 1-dimensional spaces.

More generally, we define a *reducible representation of G* as a representation in which, for all elements g of G, there is a change of basis that brings the unitary matrices $U(g)$ into the block-diagonal form

$$U(g) = \left(\begin{array}{c|c} U_1(g) & 0 \\ \hline 0 & U_2(g) \end{array}\right)$$

We have then reduced the original representation to a sum of the representations $U_1(g)$ and $U_2(g)$, acting on orthogonal Hilbert spaces. The representation of Z_2 written above is reduced, in the basis of harmonic oscillator wavefunctions, to a sum of 1-dimensional representations.

A representation of G is *irreducible* if there is <u>no</u> unitary matrix V that, for all g, reduces $U(g)$ to block diagonal form

$$V^{+} U(g) V = \left(\begin{array}{c|c} & 0 \\ \hline 0 & \end{array}\right)$$

The irreducible representations are the building blocks of all unitary representations of G.

These definitions give us an appropriate language to address the question: What are all possible ways in which a Hilbert space vector can transform under 3-dimensional rotations? We can ask, more precisely: What are all possible finite-dimensional irreducible representations of the rotation group $SO(3)$?

Since the multiplication law of $SO(3)$ is determined by the commutation relations of angular momentum

$$[\mathcal{S}^i, \mathcal{S}^j] = i\hbar\, \epsilon^{ijk} \mathcal{S}^k$$

we can recast this question as the following one, which is easier to solve: What are all possible sets of finite-dimensional irreducible Hermitian matrices that have the commutation relations of angular momentum? Given any set of such matrices, we can construct an irreducible unitary representation of the rotation group by writing

$$U(\vec{\alpha}) = e^{-i\vec{\alpha}\cdot\vec{\mathcal{S}}/\hbar}$$

We have already encountered two solutions to this problem. The first is trivial

$$\mathcal{S}^k = 0$$

This the *scalar* representation of $SO(3)$ and the theory of a scalar Schrödinger particle. Here

$$U(\vec{\alpha}) = 1$$

Next, we can set

$$\mathcal{S}^k = \hbar S^k$$

where S^x, S^y, S^z are the 3×3 matrices defined in the previous lecture. This gives the *vector* representation of $SO(3)$ and the theory of a vector particle. There is one more solution that is of great importance in atomic physics. This is the *spinor* representation of $SO(3)$; I will describe it now.

Define the *Pauli sigma matrices* σ^i, for $i = x, y, z$, by

$$\sigma^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \sigma^y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad \sigma^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

These matrices are Hermitian and obey the identities

$$\sigma^x\sigma^y = -\sigma^y\sigma^x = i\sigma^z$$
$$\sigma^y\sigma^z = -\sigma^z\sigma^y = i\sigma^x$$
$$\sigma^z\sigma^x = -\sigma^x\sigma^z = i\sigma^y$$

and

$$(\sigma^i)^2 = 1 \qquad \text{for } i = x, y, z$$

A consequence of these relations is

$$\left[\frac{\sigma^i}{2}, \frac{\sigma^j}{2} \right] = i\epsilon^{ijk} \frac{\sigma^k}{2}$$

Thus

$$\mathcal{S}^k = \hbar \frac{\sigma^k}{2}$$

is a representation of the angular momentum commutation relations. The corresponding representation of the elements of $SO(3)$ is

$$\mathcal{U}(\vec{\alpha}) = e^{-i\vec{\alpha}\cdot\vec{\sigma}/2}$$

Because of the special properties of the sigma matrices, they obey

$$(\vec{\alpha}\cdot\vec{\sigma})^2 = |\vec{\alpha}|^2$$

Then it is straightforward to expand the exponential $\mathcal{U}(\vec{\alpha})$ compute, each term, and resum. We find

$$\mathcal{U}(\vec{\alpha}) = 1 - i\frac{\vec{\alpha}\cdot\vec{\sigma}}{2} + \frac{(-i\vec{\alpha}\vec{\sigma})^2}{2!\,2^2} + \frac{(-i\vec{\alpha}\vec{\sigma})^3}{3!\,2^3} + \cdots$$

$$= 1 - i\hat{\alpha}\vec{\sigma}\cdot\left(\frac{|\vec{\alpha}|}{2}\right) - \frac{|\alpha|^2}{2!\,2^2} + i\hat{\alpha}\vec{\sigma}\,\frac{|\alpha|^3}{3!\,2^3} + \cdots$$

and so

$$\mathcal{U}(\vec{\alpha}) = \cos\frac{|\vec{\alpha}|}{2} - i\,\hat{\alpha}\cdot\vec{\sigma}\,\sin\frac{|\vec{\alpha}|}{2}$$

The $\mathcal{U}(\vec{\alpha})$ are 2×2 matrices that act on 2-component complex vectors, called *spinors*. It is surprising that the complete action of the group of rotations in 3 dimensions can be realized on a 2-component vector, but it is true.

If we attach spinors to Schrödinger wavefunctions, we obtain the theory of a *spinor particle*. A typical wavefunction of a spinor particle is

$$|\xi, \vec{p}\rangle = \begin{pmatrix}\xi_1\\ \xi_2\end{pmatrix}\cdot e^{+i\vec{p}\cdot\vec{x}/\hbar}$$

Under a rotation, this state transforms according to

$$\mathcal{U}(\vec{\alpha})\begin{pmatrix}\xi_1\\ \xi_2\end{pmatrix}\cdot e^{+i\vec{p}\cdot R^{-1}(\vec{\alpha})\vec{x}} = |\,\mathcal{U}(\vec{\alpha})\xi,\ R(\vec{\alpha})\vec{p}\,\rangle$$

Electrons, protons, neutrons, and quarks are spinor particles. To understand the properties of these particles, we must understand the properties of spinors under rotations. The total angular momentum of an electron or other spinor particle takes the form

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

where

$$\vec{L} = \vec{X}\times\vec{P} \qquad \vec{S} = \hbar\frac{\vec{\sigma}}{2}$$

There is a deep reason why all of the particles that compose matter are spinor particles. It follows from the principles of local relativistic quantum field theory that scalar and vector particles obey *Bose-Einstein statistics.* Bose-Einstein particles of the same type are absolutely identical, but an arbitrary number of them can be put into the same Schrödinger wavefunction. These principles also imply that spinor particles obey *Fermi-Dirac statistics.* Fermi-Dirac particles of the same type are absolutely identical, but only one particle can occupy a given Schrödinger wavefunction. This latter statement is the Pauli exclusion principle that is responsible for the rigidity of atoms. If electrons were vector or scalar particles, a Uranium atom would collapse down to a situation with all of the electrons in the 1S state.

To understand the properties of spinors, it is instructive to construct the eigenstates of the components of $\vec{S}$. Begin with S^z

$$S^z = \frac{\hbar}{2}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}$$

Its eigenvectors and eigenvalues are

$$\begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad S^z = +\frac{\hbar}{2} \qquad\qquad \begin{pmatrix} 0 \\ 1 \end{pmatrix} \quad S^z = -\frac{\hbar}{2}$$

These states are called the *spin up* and *spin down* states of the electron and are often notated $|\uparrow\rangle$ and $|\downarrow\rangle$. We know that

$$[S^2, S^z] = 0$$

so S^2 should be diagonal in the same basis as S^z. In fact,

$$S^2 = \frac{\hbar^2}{4}\left[(\sigma^x)^2 + (\sigma^y)^2 + (\sigma^z)^2\right] = \frac{3}{4}\hbar^2 \cdot 1$$

It is very tempting to notate the eigenvalues of S^z as

$$S^z = \hbar m$$

where

$$m = -\tfrac{1}{2}, \tfrac{1}{2}$$

Then the eigenvalue of S^2 can be written

$$S^2 = \hbar^2 j(j+1)$$

where j is the largest possible value of m. This is the same structure that we found in the solution for the spherical harmonics, except that here m is a half-integer, not an integer.

In the next lecture, I will show that all finite-dimensional irreducible representations of the angular momentum algebra have this structure. The eigenvalues of $\mathcal{S}^z$ are

$$\mathcal{S}^z = \hbar m \qquad m = -j, -j+1, \cdots j-1, j$$

with j an integer or half-integer

$$j = 0, \tfrac{1}{2}, 1, \tfrac{3}{2}, 2, \cdots$$

The total number of states in the representation is

$$(2j+1)$$

the value of $\mathcal{S}^2$ in the representation is

$$\mathcal{S}^2 = \hbar^2 j(j+1)$$

This is called the spin j representation of $SO(3)$. The scalar, spinor, and vector representations are the three simplest cases, spin 0, spin $\frac{1}{2}$, and spin 1, respectively. It can be shown that a quantum particle of spin j obeys Bose-Einstein statistics if j is integer and Fermi-Dirac statistics if j is half-integer.

For spinors, the eigenstates of S^x and S^y are

$$S^x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad S^x = +\frac{\hbar}{2} : \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix} \qquad S^x = -\frac{\hbar}{2} : \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

$$S^y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad S^y = +\frac{\hbar}{2} : \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ i \end{pmatrix} \qquad S^y = -\frac{\hbar}{2} : \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -i \end{pmatrix}$$

The Hilbert space of spinors is 2-dimensional, so all of these states are linear combinations of $|\uparrow\rangle$ and $|\downarrow\rangle$. For example,

$$\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix} = \frac{1}{\sqrt{2}}\left[\, |\uparrow\rangle + |\downarrow\rangle \,\right]$$

This equation leads to some very counterintuitive behavior for electrons that I will describe in next week's lectures.

A very odd property of the spinor representation, and of all spin j representations with j a half-integer, is that a rotation by 360° does not bring the state back to its original starting point. A 2π rotation transforms an eigenstate of S^z according to

$$|S^z = \hbar m\rangle \quad \rightarrow \quad e^{i 2\pi \cdot m} \cdot |S^z = \hbar m\rangle$$

For m a half-integer, this reads

$$|\hbar m\rangle \quad \longrightarrow \quad (-1) \cdot |\hbar m\rangle$$

so the state comes back to itself with an extra phase factor (-1). This is exceedingly odd, but it is required by many experiments on the electron and other spinor particles. For neutrons, this phase was actually observed directly by Werner, Collela, Overhauser, and Eagen (Phys. Rev. Lett. 35, 1053 (1975)). These authors took the wave function of neutrons, split them into to pieces using a thin piece of silicon as a diffraction grating, rotated the neutron on one side by precession in a magnetic field, and then brought the two parts of the wave back together and observed the interference effect. With the magnetic field off, the relative phase of the waves was 1; with the magnetic field on, the relative phase of the waves was -1.