Lecture 22 (Nov. 27, 2017)

22.1 Parity

22.1.1 Some Standard Terminology

When we refer to a *scalar*, we mean an observable that is invariant under rotations and even under parity. Examples include $\boldsymbol{x}^2$ and $\boldsymbol{p}^2$. There is a different type of object, called a *pseudoscalar*, that is invariant under rotations, but odd under parity. An example of a pseudoscalar is the product $\boldsymbol{S} \cdot \boldsymbol{x}$; this is invariant under rotations, but odd under parity because $\boldsymbol{S}$ is parity even and $\boldsymbol{x}$ is parity odd.

A *vector* is an object that transforms as a vector under rotations and is odd under parity. Examples are $\boldsymbol{x}$ and $\boldsymbol{p}$. A *pseudovector* is an object that transforms as a vector under rotations, but is even under parity. Examples of pseudovectors are $\boldsymbol{L}$, $\boldsymbol{S}$, and $\boldsymbol{J}$.

22.1.2 Wavefunctions Under Parity

Eigenstates of parity satisfy

$$\Pi|\psi\rangle = \pm|\psi\rangle\,, \tag{22.1}$$

as we know that Π has eigenvalues ± 1 only. If we take the matrix element with a position ket, then we find

$$\langle \boldsymbol{x}|\Pi|\psi\rangle = \pm\langle \boldsymbol{x}|\psi\rangle = \pm\psi(\boldsymbol{x})\,. \tag{22.2}$$

On the other hand, we can have the parity operator act on the position ket, giving

$$\langle \boldsymbol{x}|\Pi|\psi\rangle = \langle -\boldsymbol{x}|\psi\rangle = \psi(-\boldsymbol{x})\,. \tag{22.3}$$

Thus, wavefunctions of parity eigenstates satisfy

$$\psi(-\boldsymbol{x}) = \pm\psi(\boldsymbol{x})\,. \tag{22.4}$$

We refer to such wavefunctions as *even* (+) or *odd* (−).

22.1.3 Momentum and Angular Momentum

As we have seen, $[\boldsymbol{p}, \Pi] \neq 0$. Thus, we cannot simultaneously diagonalize the momentum and parity operators, i.e., momentum eigenstates are not, in general, parity eigenstates.

As an example, consider the free particle

$$H = \frac{p^2}{2m}\,. \tag{22.5}$$

The energy eigenstates

$$\frac{1}{\sqrt{2\pi\hbar}} e^{ipx/\hbar} \tag{22.6}$$

are not parity eigenstates. However, $[\Pi, H] = 0$, which means that we can choose energy eigenstates that are also parity eigenstates in this case. Because the two states

$$|\pm p\rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{\pm ipx/\hbar} \tag{22.7}$$

are degenerate, we can choose

$$|\pm_p\rangle = \frac{|p\rangle \pm |-p\rangle}{\sqrt{2}} \tag{22.8}$$

as energy eigenstates. These are energy and parity eigenstates, but are not momentum eigenstates.

By contrast, $[\boldsymbol{L}, \Pi] = 0$, so we can simultaneously diagonalize both orbital angular momentum and parity. Under a parity operation, the spherical angles (θ, ϕ) are sent to

$$(\theta, \phi) \to (\pi - \theta, \phi + \pi)\,. \tag{22.9}$$

This tells us that states with a definite angular position transform as

$$\Pi|\theta, \phi\rangle = |\pi - \theta, \phi + \pi\rangle\,. \tag{22.10}$$

We can write the orbital angular momentum eigenstates $|\ell, m\rangle$ in terms of these states using the matrix elements

$$\langle\theta, \phi|\ell, m\rangle := Y_{\ell,m}(\theta, \phi)\,, \tag{22.11}$$

which are known as *spherical harmonics*.

The spherical harmonic $Y_{0,0}$ is a constant, meaning that

$$\Pi|\ell = 0, m = 0\rangle = |\ell = 0, m = 0\rangle\,. \tag{22.12}$$

The $\ell = 1$ states transform together as a vector, i.e., as linear combinations of x, y, z. In particular, the $\ell = 1, m = +1$ state transforms like $x + iy$; the $\ell = 1, m = -1$ states transforms like $x - iy$; and the $\ell = 1, m = 0$ state transforms like z. Because vectors are odd under parity, this tells us that

$$\Pi|\ell = 1, m\rangle = -|\ell = 1, m\rangle\,, \tag{22.13}$$

or equivalently,

$$Y_{\ell,m}(\pi - \theta, \phi + \pi) = -Y_{\ell,m}(\theta, \phi)\,. \tag{22.14}$$

In general, $Y_{\ell,m}$ has parity $(-1)^\ell$.

22.1.4 Selection Rules

Let $\mathcal{O}$ be an operator with definite parity, i.e.

$$\Pi\mathcal{O}\Pi = \lambda\mathcal{O}\,, \tag{22.15}$$

with $\lambda = \pm 1$. Consider the matrix elements $\langle\psi|\mathcal{O}|\psi'\rangle$ of this operator with two parity eigenstates $|\psi\rangle$ and $|\psi'\rangle$, such that

$$\Pi|\psi\rangle = s|\psi\rangle\,, \quad \Pi|\psi'\rangle = s'|\psi'\rangle\,, \tag{22.16}$$

with $s, s' = \pm 1$. We then have

$$\begin{aligned} \langle\psi|\mathcal{O}|\psi'\rangle &= \langle\psi|\Pi\Pi\mathcal{O}\Pi\Pi|\psi'\rangle \\ &= \lambda s s' \langle\psi|\mathcal{O}|\psi'\rangle\,, \end{aligned} \tag{22.17}$$

where in the first step we have used $\Pi^2 = \mathbb{1}$. This implies that $\langle\psi|\mathcal{O}|\psi'\rangle = 0$ unless $\lambda s s' = 1$. Thus, if $\mathcal{O}$ is even under parity ($\lambda = +1$), then $|\psi\rangle$ and $|\psi'\rangle$ must have the same parity for the matrix element to be nonzero; similarly, if $\mathcal{O}$ is odd under parity ($\lambda = -1$), then $|\psi\rangle$ and $|\psi'\rangle$ must have opposite parity for the matrix element to be nonzero. This is a selection rule.

For example, $\langle\psi|\boldsymbol{x}|\psi'\rangle \neq 0$ only when $|\psi\rangle$ and $|\psi'\rangle$ have opposite parity. As a corollary, we see that the expectation value of $\boldsymbol{x}$ in any parity eigenstate must be zero.

22.2 Time Reversal

Classical physics is time-reversal invariant: Newton's law

$$m\ddot{\boldsymbol{x}} = -\nabla V(\boldsymbol{x}) \tag{22.18}$$

is invariant under $t \to -t, \boldsymbol{x} \to \boldsymbol{x}$. Thus, if $\boldsymbol{x}(t)$ is a valid solution to Newton's equation, then so is $\boldsymbol{x}(-t)$.

Consider now the Schrödinger equation,

$$i\hbar\frac{\partial\psi}{\partial t} = \left(-\frac{\hbar^2}{2m}\nabla^2 + V(\boldsymbol{x})\right)\psi(\boldsymbol{x},t)\,. \tag{22.19}$$

If we let $t \to -t$, we see that we can get a solution if we take

$$\psi(\boldsymbol{x},t) \to \psi^*(\boldsymbol{x},-t) \tag{22.20}$$

for some solution $\psi(\boldsymbol{x},t)$. This suggests that we should take the time reversal operator Θ to be anti-unitary. (Recall that an anti-unitary operator A can be written in the form $A = KU$, where K is complex conjugation and U is some unitary operator.) Thus, we have

$$\theta(a|\alpha\rangle + b|\beta\rangle) = a^*\theta|\alpha\rangle + b^*\theta|\beta\rangle \tag{22.21}$$

for any $a, b \in \mathbb{C}$ and $|\alpha\rangle, |\beta\rangle \in \mathcal{H}$.

We now consider combinations of time reversal and time translation operations. Assuming that time reversal is a symmetry, we require that

$$|\psi(-\delta t)\rangle = \theta|\psi(\delta t)\rangle\,, \quad |\psi(0)\rangle = \theta|\psi(0)\rangle\,. \tag{22.22}$$

By using forward and backward time translations from $t = 0$, we see that

$$\begin{aligned} |\psi(-\delta t)\rangle &= \left(1 + \frac{iH}{\hbar}\delta t\right)|\psi(0)\rangle\,, \\ |\psi(\delta t)\rangle &= \left(1 - \frac{iH}{\hbar}\delta t\right)|\psi(0)\rangle\,, \end{aligned} \tag{22.23}$$

so the statements $|\psi(-\delta t)\rangle = \theta|\psi(\delta t)\rangle$ and $|\psi(0)\rangle = \theta|\psi(0)\rangle$ imply that

$$iH\theta|\psi(0)\rangle = \theta(-iH)|\psi(0)\rangle\,. \tag{22.24}$$

Thus, we have

$$iH\theta = \theta(-iH) \tag{22.25}$$

as an operator equation. Because θ is anti-unitary, this tells us that $[H,\theta] = 0$, exactly as expected of a symmetry of the Hamiltonian.

As usual, operators transform under time reversal as $\mathcal{O} \to \theta\mathcal{O}\theta^{-1}$. An operator $\mathcal{O}$ is even/odd under time reversal if

$$\theta\mathcal{O}\theta^{-1} = \pm\mathcal{O}\,. \tag{22.26}$$

We require that

$$\theta\boldsymbol{x}\theta^{-1} = \boldsymbol{x}\,, \quad \theta\boldsymbol{p}\theta^{-1} = -\boldsymbol{p}\,. \tag{22.27}$$

There are two ways to see that $\boldsymbol{p}$ must be odd under time reversal: first, we could consider the position space representation $\boldsymbol{p} \to -i\hbar\nabla$, and use that fact that θ is anti-unitary; alternatively, we can use the fact that time reversal should preserve the commutation algebra $[x_i, p_j] = i\hbar\delta_{ij}$, which requires that $\boldsymbol{p}$ be odd because $\boldsymbol{x}$ is even and the right-hand side contains a factor of i.

Similarly, in order to preserve the commutation algebra $[J_i, J_j] = i\hbar\epsilon_{ijk}J_k$, we need

$$\theta\boldsymbol{J}\theta^{-1} = -\boldsymbol{J}\,, \tag{22.28}$$

meaning that $\boldsymbol{L} \to -\boldsymbol{L}$ and $\boldsymbol{S} \to -\boldsymbol{S}$ under parity. Note that $\boldsymbol{L}^2 \to \boldsymbol{L}^2$, so this tells us that $\theta|\ell, m\rangle \propto |\ell, -m\rangle$. In particular,

$$\theta|\ell, m\rangle = (-1)^m|\ell, -m\rangle\,. \tag{22.29}$$

Here, the phase factor $(-1)^m$ is a convention choice built into the definition of the spherical harmonics,

$$Y^*_{\ell,m}(\theta, \phi) = (-1)^m Y_{\ell,-m}(\theta, \phi)\,. \tag{22.30}$$

22.2.1 Time Reversal and Spin

We find interesting outcomes when acting on spin-$\frac{1}{2}$ systems (or systems with other half-integer spin) with time reversal. The statement

$$\theta J_z\theta^{-1} = -J_z \tag{22.31}$$

implies for a spin-$\frac{1}{2}$ particle that

$$J_z\theta|+\rangle = -\theta J_z|+\rangle = -\frac{\hbar}{2}\theta|+\rangle\,. \tag{22.32}$$

Thus, we see that $\theta|+\rangle \propto |-\rangle$. In general, there can be some phase η, so that

$$\theta|+\rangle = \eta|-\rangle\,. \tag{22.33}$$

We can write this equation in the form

$$\theta|+\rangle = \eta e^{-i\pi S_y/\hbar}|+\rangle\,. \tag{22.34}$$

We could have similarly chosen S_x instead of S_y, or indeed any spin operator in the x, y-plane. Based on this statement, we write

$$\theta = \eta e^{-i\pi S_y/\hbar}K\,, \tag{22.35}$$

where we have included K because θ is anti-unitary. We then have

$$\theta|-\rangle = \eta e^{-i\pi S_y/\hbar}K|-\rangle = -\eta|+\rangle\,. \tag{22.36}$$

From this, we see that

$$\theta^2|+\rangle = \theta(\eta|-\rangle) = \eta^*\theta|-\rangle = -|\eta|^2|+\rangle = -|+\rangle\,, \tag{22.37}$$

where we have used the fact that $|\theta|^2 = 1$ because θ is purely a phase. Similarly, $\theta^2|-\rangle = -|-\rangle$. This means that

$$\theta^2 = -\mathbb{1} \tag{22.38}$$

holds as an operator equation for a spin-$\frac{1}{2}$ system. This is true for any system with half-integer spin. There is a standard phase choice for spin-$\frac{1}{2}$, which is to take $\eta = i$, which gives

$$\theta = ie^{-i\pi S_y/\hbar}K\,. \tag{22.39}$$