## پاریته یک موج تخت چیست؟

## شبه اسکالر چیست؟

## شبه بردار چیست؟

## اگر پاریته و هامیلتونی با هم جابه جا شوند، آیا همواره ویژه تابع مشترک دارند؟

# Symmetry in Quantum Mechanics

Having studied the theory of rotation in detail, we are in a position to discuss, in more general terms, the connection between symmetries, degeneracies, and conservation laws.

We have deliberately postponed this very important topic until now so that we can discuss it using the rotation symmetry of Chapter 3 as an example.

# SYMMETRIES, CONSERVATION LAWS, AND DEGENERACIES

## Symmetries in Classical Physics

We begin with an elementary review of the concepts of symmetry and conservation law in classical physics.

In the Lagrangian formulation of classical mechanics, we start with the Lagrangian L, which is a function of a generalized coordinate $q_i$ and the corresponding generalized velocity $\dot{q}_i$.

If L is unchanged under displacement,

$$q_i \rightarrow q_i + \delta q_i,$$

$$\frac{\partial L}{\partial q_i} = 0.$$

then we must have

$$\frac{dp_i}{dt} = 0,$$

Why?

Because of the Lagrange equation,

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_i}\right) - \frac{\partial L}{\partial q_i} = 0$$

$$p_i = \frac{\partial L}{\partial \dot{q}_i}.$$

$$\frac{dp_i}{dt} = 0,$$

then we have a conserved quantity, the canonical momentum conjugate to $q_i$.

Likewise, in the Hamiltonian formulation based on H regarded as a function of $q_i$ and $p_i$ we have

$$\frac{dp_i}{dt} = 0,$$ whenever $$\frac{\partial H}{\partial q_i} = 0.$$ Why?

$$\left.\begin{aligned} \dot{q}_i &= \frac{\partial H(q_i, p_i)}{\partial p_i} \\ \dot{p}_i &= -\frac{\partial H(q_i, p_i)}{\partial q_i} \end{aligned}\right\} \quad i = 1, 2, \ldots, 3N,$$

So if the Hamiltonian does not explicitly depend on $q_i$, which is another way of saying H has a symmetry under $q_i \text{-->} q_i+\delta q_i$ we have a conserved quantity.

# Symmetry in Quantum Mechanics

In quantum mechanics we have learned to associate a unitary operator, say $\mathscr{S}$ with an operation like translation or rotation.

It has become customary to call $\mathscr{S}$ a symmetry operator regardless of whether the physical system itself possesses the symmetry corresponding to $\mathscr{S}$.

Further, we have learned that for symmetry operations that differ infinitesimally from the identity transformation, we can write

$$\mathscr{S} = 1 - \frac{i\varepsilon}{\hbar} G,$$

where G is the Hermitian generator of the symmetry operator in question.

Let us now suppose that H is invariant under $\mathscr{S}$.

We then have $\mathscr{S}^{\dagger} H \mathscr{S} = H.$

But we had $\mathscr{S} = 1 - \frac{i\varepsilon}{\hbar} G,$

But this is equivalent to $[G, H] = 0.$ Why?

Since $\mathscr{S}\mathscr{S}^{\dagger} \mathbf{H} \mathscr{S} = \mathscr{S} \mathbf{H}$ ➡ $\mathbf{H} \mathscr{S} = \mathscr{S} \mathbf{H}$ **HG=GH**

➡ $\frac{dG}{dt} = 0;$ Why? By virtue of the Heisenberg equation of motion.

$\frac{dG}{dt} = 0;$ ➡ G is a constant of the motion.

For instance, if H is invariant under translation, then momentum is a constant of the motion; if H is invariant under rotation, then angular momentum is a constant of the motion.

It is instructive to look at the connection between [H,G]=0 and conservation of G from the point of view of an eigenket of G when G commutes with H.

Suppose at $t_0$ the system is in an eigenstate of G.

Then the ket at a later time obtained by applying the time-evolution operator

$$|g', t_0; t\rangle = U(t, t_0)|g'\rangle$$

is also an eigenket of G with the same eigenvalue g'.

In other words, once a ket is a G eigenket, it is always a G eigenket with the same eigenvalue.

The proof of this is extremely simple once we realize that [G, H]=0 and dG/dt=0 also imply that G commutes with the time-evolution operator, namely,

$$G\left[U(t,t_0)|g'\rangle\right] = U(t,t_0)G|g'\rangle = g'\left[U(t,t_0)|g'\rangle\right].$$

# Degeneracies

Let us now turn to the concept of degeneracies.

Even though degeneracies may be discussed at the level of classical mechanics—for instance in discussing closed (nonprecessing) orbits in the Kepler problem (Goldstein 1980)—this concept plays a far more important role in quantum mechanics.

Let us suppose that $[H, \mathscr{S}] = 0$ for some symmetry operator.

and also suppose that $|n\rangle$ is an energy eigenket with eigenvalue $E_n$.

Then $\mathscr{S}|n\rangle$ is also an energy eigenket with the same energy, because

$$H(\mathscr{S}|n\rangle) = \mathscr{S}H|n\rangle = E_n(\mathscr{S}|n\rangle)$$

Suppose $|n\rangle$ and $\mathscr{S}|n\rangle$ represent different states.

Then these are two states with the same energy, that is, they are degenerate.

Quite often $\mathscr{S}$ is characterized by continuous parameters, say λ, in which case all states of the form $\mathscr{S}(\lambda)|n\rangle$ have the same energy.

We now consider rotation specifically.

Suppose the Hamiltonian is rotationally invariant, so

$$[\mathscr{D}(R), H] = 0$$

which necessarily implies that

$$[\mathbf{J}, H] = 0, \qquad [\mathbf{J}^2, H] = 0$$

We can then form simultaneous eigenkets of H, $J^2$, and $J_z$, denoted by $|n; j, m\rangle$.

The argument just given implies that all states of the form

$$\mathscr{D}(R)|n; j, m\rangle$$

have the same energy.

We saw in Chapter 3 that under rotation different m-values get mixed up.

In general, $\mathscr{D}(R)|n; j, m\rangle$ is a linear combination of 2j+1 independent states. Explicitly,

$$\mathscr{D}(R)|n; j,m\rangle = \sum_{m'} |n; j,m'\rangle \mathscr{D}^{(j)}_{m'm}(R),$$

and by changing the continuous parameter that characterizes the rotation operator $\mathscr{D}(R)$, we can get different linear combinations of $|n; j,m'\rangle$.

If all states of form $\mathscr{D}(R)|n; j,m\rangle$ with arbitrary $\mathscr{D}(R)$ are to have the same energy, it is then essential that each of $|n; j, m\rangle$ with different m must have the same energy.

So the degeneracy here is $(2j + 1)$-fold, just equal to the number of possible m-values.

This point is also evident from the fact that all states obtained by successively applying $J_{\pm}$, which commutes with H, to $|n; j,m\rangle$ have the same energy.

As an application, consider an atomic electron whose potential is written as $V(r)+V_{LS}(r)\mathbf{L}\bullet\mathbf{S}$.

Because r and **L.S** are both rotationally invariant, we expect a (2j+l)-fold degeneracy for each atomic level.

On the other hand, suppose there is an external electric or magnetic field, say in the z-direction.

The rotational symmetry is now manifestly broken; as a result, the (2j+l)-fold degeneracy is no longer expected and states characterized by different m-values no longer have the same energy.

We will examine how this splitting arises in Chapter 5.

# DISCRETE SYMMETRIES, PARITY, OR SPACE INVERSION

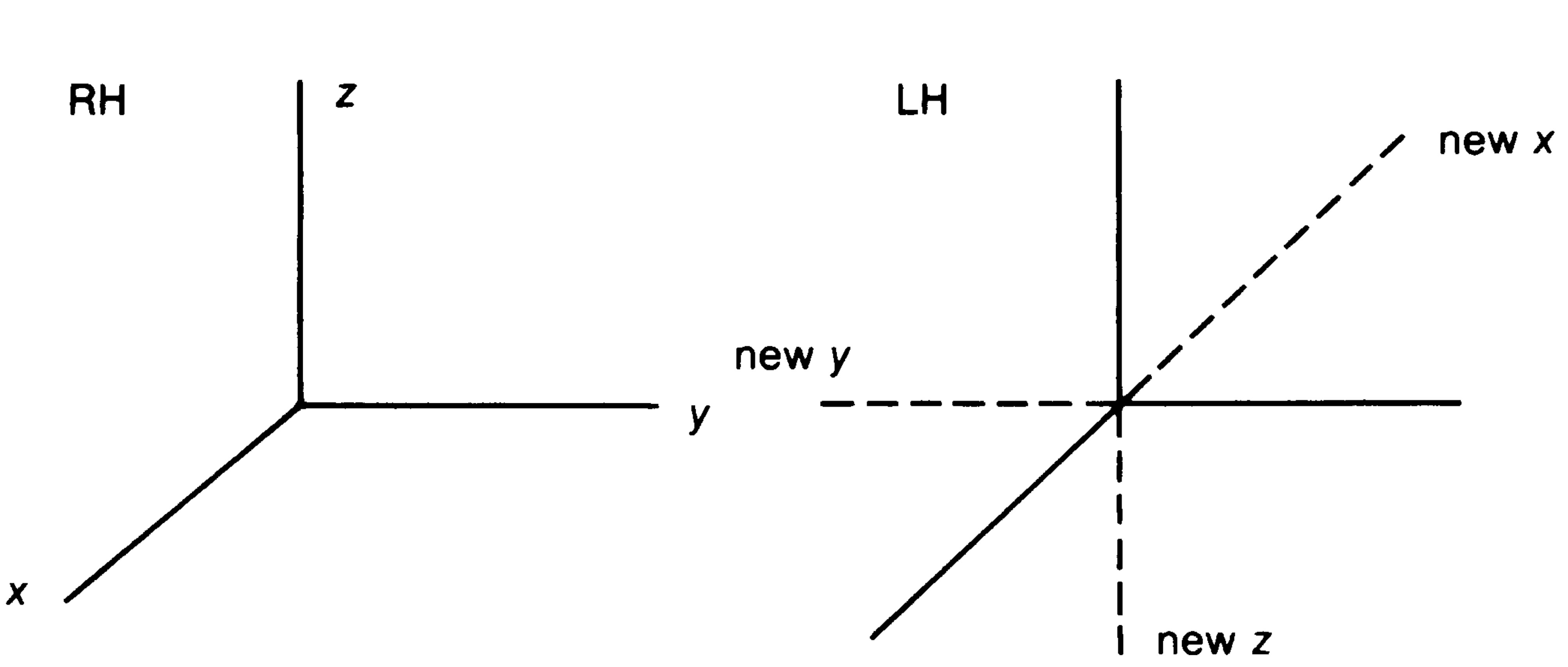
So far we have considered continuous symmetry operators—that is, operations that can be obtained by applying successively infinitesimal symmetry operations.

All symmetry operations useful in quantum mechanics are not necessarily of this form.

In this chapter we consider three symmetry operations that can be considered to be discrete, as opposed to continuous —parity, lattice translation, and time reversal.

The first operation we consider is parity, or space inversion.

The parity operation, as applied to transformation on the coordinate system, changes a right-handed (RH) system into a left-handed (LH) system, as shown in Figure 4.1.



However, in this book we consider a transformation on state kets rather than on the coordinate system.

Given $|\alpha\rangle$, we consider a space-inverted state, assumed to be obtained by applying a unitary operator $\pi$ known as the parity operator, as follows:

$$|\alpha\rangle \rightarrow \pi|\alpha\rangle.$$

We require the expectation value of x taken with respect to the space-inverted state to be opposite in sign.

$$\langle\alpha|\pi^\dagger \mathbf{x}\pi|\alpha\rangle = -\langle\alpha|\mathbf{x}|\alpha\rangle,$$

a very reasonable requirement.

This is accomplished if

$$\pi^{\dagger}\mathbf{x}\pi = -\mathbf{x}$$

or

$$\mathbf{x}\pi = -\pi\mathbf{x},$$

where we have used the fact that π is unitary.

In other words, x and π must anticommute.

How does an eigenket of the position operator transform under parity?

We claim that

$$\pi|\mathbf{x}'\rangle = e^{i\delta}|-\mathbf{x}'\rangle$$

where $e^{i\delta}$ is a phase factor (δ is real).

To prove this assertion let us note that

$$\mathbf{x}\pi|\mathbf{x}'\rangle = -\pi\mathbf{x}|\mathbf{x}'\rangle = (-\mathbf{x}')\pi|\mathbf{x}'\rangle.$$

This equation says that π|x'> is an eigenket of x with eigenvalue -x', so it must be the same as a position eigenket |-x'> up to a phase factor.

It is customary to take $e^{i\delta}=1$ by convention.

Substituting this in $\pi|x'\rangle = e^{i\delta}|-x'\rangle$, we have $\pi^2|x'\rangle=|x'\rangle$; hence, $\pi^2=1$—that is, we come back to the same state by applying $\pi$ twice.

We easily see from $\pi|x'\rangle = e^{i\delta}|-x'\rangle$ that $\pi$ is now not only unitary but also Hermitian:

$$\pi^{-1} = \pi^{\dagger} = \pi.$$

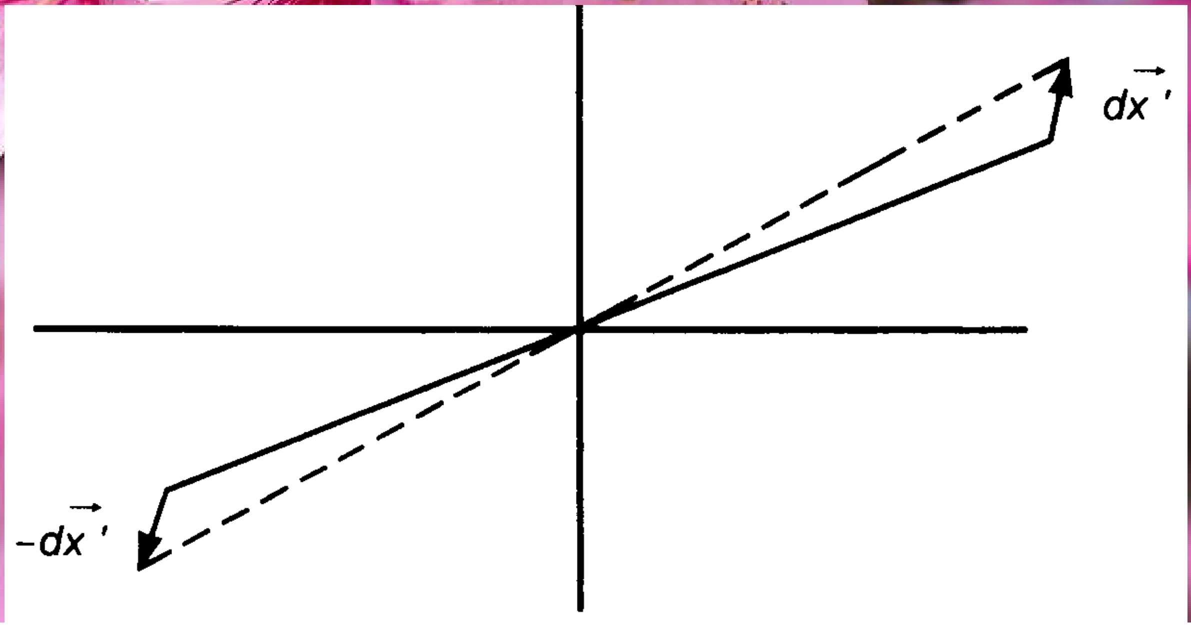
Its eigenvalue can be only +1 or -1.

What about the momentum operator?

The momentum p is like mdx/dt, so it is natural to expect it to be odd under parity, like x.

A more satisfactory argument considers the momentum operator as the generator of translation.

Since translation followed by parity is equivalent to parity followed by translation in the opposite direction, as can be seen from Figure 4.2, then



$$\pi \mathscr{T}(d\mathbf{x}') = \mathscr{T}(-d\mathbf{x}')\pi$$

$$\pi\left(1 - \frac{i\mathbf{p}\cdot d\mathbf{x}'}{\hbar}\right)\pi^\dagger = 1 + \frac{i\mathbf{p}\cdot d\mathbf{x}'}{\hbar},$$

from which follows

$$\{\pi, \mathbf{p}\} = 0 \quad \text{or} \quad \pi^\dagger \mathbf{p} \pi = -\mathbf{p}.$$

We can now discuss the behavior of J under parity.

First, for orbital angular momentum we clearly have

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

because

$$\mathbf{L} = \mathbf{x} \times \mathbf{p},$$

and both x and p are odd under parity.

However, to show that this property also holds for spin, it is best to use the fact that J is the generator of rotation.

For 3x3 orthogonal matrices, we have

$$R^{(\text{parity})} R^{(\text{rotation})} = R^{(\text{rotation})} R^{(\text{parity})},$$

where explicitly

$$R^{(\text{parity})} = \begin{pmatrix} -1 & & 0 \\ & -1 & \\ 0 & & -1 \end{pmatrix};$$

that is, the parity and rotation operations commute.

In quantum mechanics, it is natural to postulate the corresponding relation for the unitary operators, so

$$\pi \mathscr{D}(R) = \mathscr{D}(R)\pi,$$

where $\mathscr{D}(R) = 1 - i\mathbf{J}\cdot\mathbf{n}\varepsilon/\hbar$.

From $\pi \mathscr{D}(R) = \mathscr{D}(R)\pi$ it follows that

$$[\pi, \mathbf{J}] = 0 \quad \text{or} \quad \pi^\dagger \mathbf{J} \pi = \mathbf{J}.$$

This together with $[\pi, \mathbf{L}]=0$ means that the spin operator (given by $\mathbf{J} = \mathbf{L} + \mathbf{S}$) also transforms in the same way as L.

Under rotations, x and J transform in the same way, so they are both vectors, or spherical tensors, of rank 1.

However, **x** (or **p**) is odd under parity [see $\{\pi,\mathbf{x}\}=0$ and $\{\pi,\mathbf{p}\}=0$, while J is even under parity [see $[\pi,\mathbf{J}]=0$.

Vectors that are odd under parity are called **polar vectors**, while vectors that are even under parity are called **axial vectors**, or **pseudovectors**.

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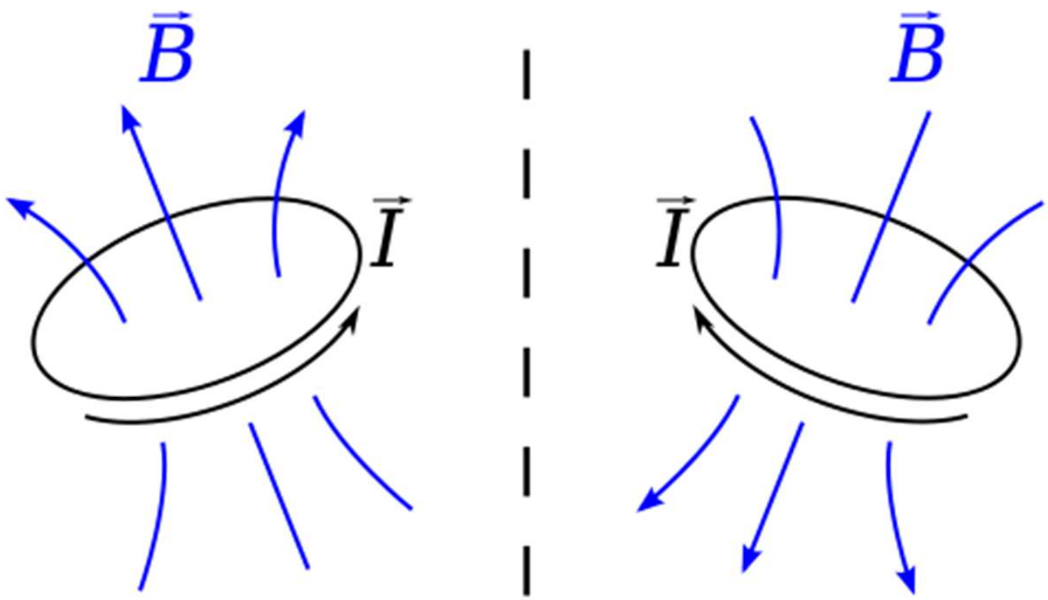
http://myweb.lmu.edu/jphillips/pseudo.pdf




A loop of wire (black), carrying a current, creates a magnetic field (blue). If the position and current of the wire are reflected across the dotted line, the magnetic field it generates would *not* be reflected: Instead, it would be reflected *and reversed*. The position of the wire and its current are vectors, but the magnetic field is a pseudovector.

In physics and mathematics, a **pseudovector** (or **axial vector**) is a quantity that transforms like a vector under a proper rotation, but gains an additional sign flip under an improper rotation such as a reflection. Geometrically it is the opposite, of equal magnitude but in the opposite direction, of its mirror image. This is as opposed to a *true* or *polar* vector (more formally, a contravariant vector), which on reflection matches its mirror image.

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Let us now consider operators like S•x.

Under rotations they transform like ordinary scalars, such as S•L or **x•p**.

Yet under space inversion we have

$$\pi^{-1}\mathbf{S}\cdot\mathbf{x}\pi = -\mathbf{S}\cdot\mathbf{x},$$

while for ordinary scalars we have

$$\pi^{-1}\mathbf{L}\cdot\mathbf{S}\pi = \mathbf{L}\cdot\mathbf{S}$$

and so on.

The operator **S•x** is an example of a **pseudoscalar**.

# Wave Functions Under Parity

Let us now look at the parity property of wave functions.

First, let ψ be the wave function of a spinless particle whose state ket is $|\alpha\rangle$:

$$\psi(\mathbf{x}') = \langle \mathbf{x}'|\alpha\rangle$$

The wave function of the space-inverted state, represented by the state ket $\pi|\alpha\rangle$, is

$$\langle \mathbf{x}'|\pi|\alpha\rangle = \langle -\mathbf{x}'|\alpha\rangle = \psi(-\mathbf{x}')$$

Suppose $|\alpha\rangle$ is an eigenket of parity.

We have already seen that the eigenvalue of parity must be $\pm 1$, so

$$\pi|\alpha\rangle = \pm|\alpha\rangle$$

Let us look at its corresponding wave function,

$$\langle \mathbf{x}'|\pi|\alpha\rangle = \pm\langle \mathbf{x}'|\alpha\rangle$$

But we also have

$$\langle \mathbf{x}'|\pi|\alpha\rangle = \langle -\mathbf{x}'|\alpha\rangle$$

so the state $|\alpha\rangle$ is even or odd under parity depending on whether the corresponding wave function satisfies

$$\psi(-\mathbf{x}') = \pm\,\psi(\mathbf{x}')\begin{cases}\text{even parity,}\\ \text{odd parity.}\end{cases}$$

Not all wave functions of physical interest have definite parities in the sense of $\psi(-x') = \pm\psi(x')\begin{cases} even\ parity \\ odd\ parity\end{cases}.$

Consider, for instance, the momentum eigenket.

The momentum operator anticommutes with the parity operator, so the momentum eigenket is not expected to be a parity eigenket.

Indeed, it is easy to see that the plane wave, which is the wave function for a momentum eigenket, does not satisfy $\psi(-x') = \pm\psi(x') \begin{cases} even\ parity \\ odd\ parity \end{cases}$.

An eigenket of orbital angular momentum is expected to be a parity eigenket because L and $\pi$ commute $[\pi, \mathbf{L}]$=0.

To see how an eigenket of $L^2$ and $L_z$ behaves under parity, let us examine the properties of its wave function under space inversion,

$$\langle \mathbf{x}'|\alpha, lm\rangle = R_\alpha(r) Y_l^m(\theta, \phi)$$

The transformation $x' \rightarrow -x'$ is accomplished by letting

$$r \rightarrow r$$

$$\theta \rightarrow \pi - \theta \qquad (\cos\theta \rightarrow -\cos\theta)$$

$$\phi \rightarrow \phi + \pi \qquad \left(e^{im\phi} \rightarrow (-1)^m e^{im\phi}\right)$$

Using the explicit form of

$$Y_l^m = (-1)^m \sqrt{\frac{(2l+1)(l-m)!}{4\pi(l+m)!}} P_l^m(\cos\theta)e^{im\phi}$$

for positive $m$, with $Y_l^{-m}(\theta,\varphi) = (-1)^m[Y_l^m(\theta,\varphi)]^*$, where

$$P_l^{|m|}(\cos\theta) = \frac{(-1)^{m+l}}{2^l l!}\frac{(l+|m|)!}{(l-|m|)!}\sin^{-|m|}\theta\left(\frac{d}{d(\cos\theta)}\right)^{l-|m|}\sin^{2l}\theta$$

We can easily show that

$$Y_l^m(\pi-\theta,\varphi+\pi) = (-1)^l[Y_l^m(\theta,\varphi)]$$

Therefore, we can conclude that

$$\pi|\alpha,lm\rangle = (-1)^l|\alpha,lm\rangle$$

It is actually not necessary to look at $Y_l^m$; An easier way to obtain the same result is to work with $m$ =0 and note that $L_\pm^r|l,m=0\rangle$ $(r=0,1,\ldots,l)$ must have the same parity because $\pi$ and $(L_\pm)^r$ commute.

Let us now look at the parity properties of energy eigenstates.

We begin by stating a very important theorem.

# *Theorem.*

Suppose $[H, \pi] = 0$ and $|n\rangle$ is a nondegenerate eigenket of H with eigenvalue $E_n$: $H|n\rangle = E_n|n\rangle$ then $|n\rangle$ is also a parity eigenket.

# *Proof:*

We prove this theorem by first noting that $\frac{1}{2}(1 \pm \pi)|n\rangle$ is a parity eigenket with eigenvalues $\pm 1$.

## *Why?*

Just use $\pi^2 = 1$

## *How?*

$$\pi \frac{1}{2}(1 \pm \pi)|n\rangle = \frac{1}{2}(\pi \pm \pi^2)|n\rangle$$

$$= \frac{1}{2}(\pi \pm 1)|n\rangle = \mp \frac{1}{2}(1 \pm \pi)|n\rangle$$

But $\frac{1}{2}(1 \pm \pi)|n\rangle$ is also an energy eigenket with eigenvalues $E_n$ .

***Why?***

$$H\frac{1}{2}(1 \pm \pi)|n\rangle$$

$$= \frac{1}{2}(H \pm H\pi)|n\rangle$$

$$= \frac{1}{2}(H \pm \pi H)|n\rangle$$

$$= \frac{1}{2}(1 \pm \pi)H|n\rangle$$

$$= \frac{1}{2}(1 \pm \pi)E_n|n\rangle$$

$$= E_n\frac{1}{2}(1 \pm \pi)|n\rangle$$

Furthermore $|n\rangle$ and $\frac{1}{2}(1 \pm \pi)|n\rangle$ must represent the same state, otherwise there would be two states with the same energy– a contradiction of our nondegenerate assumption.

It follows that $|n\rangle$, which is the same as $\frac{1}{2}(1 \pm \pi)|n\rangle$ up to a multiplicative constant, must be a parity eigenket with parity $\pm 1$. ■

As an example, let us look at the simple harmonic oscillator (SHO).

The ground state $|0\rangle$ has even parity because its wave function, being Gaussian, is even under $x' \rightarrow -x'$.

The first excited state, $|1\rangle = A = a^{\dagger}|0\rangle$, must have an odd parity because $a^{\dagger}$ is linear in x and p, which are both odd:

$$a = \sqrt{\frac{m\omega}{2\hbar}}\left(x + \frac{ip}{m\omega}\right), \qquad a^{\dagger} = \sqrt{\frac{m\omega}{2\hbar}}\left(x - \frac{ip}{m\omega}\right)$$

In general, the parity of the nth excited state of the simple harmonic operator is given by $(-1)^n$.

It is important to note that the nondegenerate assumption is essential here.

For instance, consider the hydrogen atom in nonrelativistic quantum mechanics.

As is well known, the energy eigenvalues depend only on the principal quantum number n (for example, 2p and 2s states are degenerate) —the Coulomb potential is obviously invariant under parity—yet an energy eigenket $c_p|2p\rangle + c_s|2s\rangle$ is obviously not a parity eigenket.

As another example, consider a momentum eigenket. Momentum anticommutes with parity, so—even though free-particle Hamiltonian $H$ is invariant under parity—the momentum eigenket (though obviously an energy eigenket) is not a parity eigenket. Our theorem remains intact because we have here a degeneracy between $|\mathbf{p}'\rangle$ and $|-\mathbf{p}'\rangle$, which have the same energy. In fact, we can easily construct linear combinations $(1/\sqrt{2})(|\mathbf{p}'\rangle \pm |-\mathbf{p}'\rangle)$, which are parity eigenkets with eigenvalues $\pm 1$. In terms of wave-function language, $e^{i\mathbf{p}'\cdot\mathbf{x}'/\hbar}$ does not have a definite parity, but $\cos \mathbf{p}'\cdot\mathbf{x}'/\hbar$ and $\sin \mathbf{p}'\cdot\mathbf{x}'/\hbar$ do.