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Now parity. Parity begins life as an operation P on ordinary 3D space, the spatial inversion operator,

$$P\vec{r} = -\vec{r}$$

or as a matrix,

$$P = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix} = -I.$$

P is an improper rotation. P satisfies the following properties:

$$P^2 = I, \qquad PRP^{-1} = R, \qquad \text{any } R \in SO(3).$$

The latter property is trivial, since P commutes with all 3×3 matrices.

We seek a representation of P by means of an operator π that acts on the Hilbert space of our quantum system. Just as we found representations of ordinary rotations $R \in SO(3)$,

$$R \longrightarrow U(R)$$

we now seek

$$P \longrightarrow \pi.$$

We postulate that π should satisfy:

1. $\pi^\dagger \pi = 1$ (π is unitary)
2. $\pi^2 = 1$ (rep. of $P^2 = I$)
3. $\pi U(R) \pi^\dagger = U(R)$ (rep of $PRP^{-1} = R$).

Property 3 is equivalent to $\boxed{\pi \vec{J} \pi^\dagger = \vec{J}}$.

These properties do not uniquely determine π, but they do restrict the possibilities considerably.

First take case of spinless particle in 3D, where ket space is $\mathcal{E} = \text{span}\{|\vec{r}_0\rangle\}$ and wave functions are $\psi(\vec{r})$.

For rotations (proper), we guessed the definition,

$$U(R)\,|\vec{r}_0\rangle = |R\vec{r}_0\rangle,$$

and that worked, so now we guess

$$\pi\,|\vec{r}_0\rangle = |-\vec{r}_0\rangle = |P\vec{r}_0\rangle.$$

This leads to some consequences. Consider the operator $\pi\vec{r}\pi^\dagger$ ($\vec{r}$ = position operator, $\vec{r}_0$ = c-number eigenvalues). Then

$$\pi\vec{r}\pi^\dagger|\vec{r}_0\rangle = \pi\vec{r}\pi|\vec{r}_0\rangle \qquad (\text{since } \pi = \pi^\dagger = \pi^{-1})$$

$$= \pi\vec{r}\,|-\vec{r}_0\rangle \qquad (\text{defn of } \pi)$$

$$= -\vec{r}_0\,\pi|-\vec{r}_0\rangle \qquad (\vec{r} \text{ brings out eigenvalue}).$$

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or, since $|\vec{r}_0\rangle$ is arbitrary,

$$\boxed{\pi\vec{r}\pi^\dagger = -\vec{r}}$$

Similarly we find

$$\boxed{\pi \vec{p}\, \pi^+ = -\vec{p}}$$

These two imply

$$\boxed{\pi \vec{L}\, \pi^+ = +\vec{L}}$$

since $\vec{L} = \vec{r} \times \vec{p}$ and there are 2 sign changes. Since $\vec{L} = \vec{J}$ for this system, this agrees with postulate 3. So this defn of π is satisfactory. Note effect of rotations and parity on wave functions:

$$\big(U(R)\psi\big)(\vec{r}) = \psi(R^{-1}\vec{r})$$

$$(\pi\, \psi)(\vec{r}) = \psi(-\vec{r}).$$

Above transformation laws (for $\vec{r}, \vec{p}, \vec{L}$) ~~is~~ are examples of how operators can be classified by their transformation laws under parity. This is an extension of the transformation laws (scalar, vector, irreducible tensor, etc.) under proper rotation.

Let K be a scalar (invariant under proper rotations). Then we say, if

$$\pi K \pi^+ = \begin{cases} +K, & \text{true-scalar} \\ -K, & \text{pseudo-scalar}. \end{cases}$$

Sim., let $\vec{V}$ = a vector operator (under proper rotations). Then 11/8/05

$$\pi \vec{V} \pi^+ = \begin{cases} -\vec{V}, & \text{true vector} \\ +\vec{V}, & \text{pseudo vector.} \end{cases}$$

For example, $\vec{r}, \vec{p}$ = true vectors, $\vec{L} = \vec{r} \times \vec{p}$ = pseudo-vector.

Now consider a particle in 3D with spin. Ket space is

$$\mathcal{E} = \text{span} \{ |\vec{r}_0, m\rangle = |\vec{r}_0\rangle |m\rangle \}.$$

We know what π does to $|\vec{r}_0\rangle$. What does it do to $|m\rangle$? (This is $|m\rangle = |sm\rangle$, s = spin of particle). One can show that without loss of generality, the action of π on $|m\rangle$, consistent with the postulates, is

$$\pi |m\rangle = |m\rangle.$$

Notice that since $\pi \vec{J} \pi^+ = \vec{J}$, and $\vec{J} = \vec{L} + \vec{S}$, and fact (already shown) that $\pi \vec{L} \pi^+ = \vec{L}$, we must have $\pi \vec{S} \pi^+ = \vec{S}$.

Thus parity does nothing to spin; it is a <u>purely</u> <u>orbital</u> <u>operator</u>. (This only applies in the nonrelativistic theory, as we will see.)

Parity is important because it is a fundamental space-time symmetry (not always respected in nature, however). Also, for almost all low-energy problems (atomic, molecular, nuclear, to a very high accuracy

CM physics) parity is conserved in isolated systems. That 11/8/05

is, if H is the Hamiltonian for an isolated system, then

$$[\pi, H] = 0$$

to a very high accuracy. The only reason it is not exactly true is because of the weak interactions. The strong and electromagnetic interactions conserve parity. The weak interactions are not easy to detect in low-energy physics, even if you are looking for them. (Their most obvious manifestation is in the β-decay of nuclei, a process that must be regarded as relativistic since it involves the creation and annihilation of particles, including massive particles.)

If a system is not isolated (if it is interacting with external fields) then parity invariance can be broken.

Look at some examples. In 1D, if $H = \frac{p^2}{2m} + V(x)$, then

$$\pi H \pi^+ = \frac{p^2}{2m} + V(-x) = H \quad \text{if} \quad V(x) = V(-x).$$

The momentum p changes sign under π, but since the K.E. goes like p^2, it commutes with π. Similarly, in 3D if $H = \frac{\vec{p}^2}{2m} + V(\vec{r})$, then

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$$\pi H \pi^+ = \frac{p^2}{2m} + V(-\vec{r}) = H \quad \text{if} \quad V(\vec{r}) = V(-\vec{r}).$$

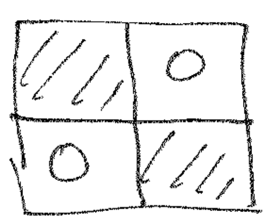
Here $V(\vec{r})$ means $V(x,y,z)$. A central force potential depends only on $r = |\vec{r}|$, so in that case H always commutes with π.

In 1D, the bound states of H are always nondegenerate (proven earlier in semester). But ~~since~~ if $[H,\pi]=0$, then by Theorem 1.5 in the notes, every eigenstate of H is also an eigenstate of π. That is, energy eigenstates in a symmetric potential $V(x)=V(-x)$ are always either even or odd under parity,

$$(\pi \psi_n)(x) = \begin{cases} +\psi_n(-x) \\ -\psi_n(-x) \end{cases}$$

for 1D energy eigenfns in a symm. potential. You can see an example of this in the case of the harmonic oscillator.

Parity is an excuse to talk about the practical effects of symmetry on a Hamiltonian. The first remark is the advantage of block-diagonal matrices. The work to diagonalize a matrix (Householder algorithm) goes like N^3, where N is the size of a matrix. Suppose an $N\times N$ matrix is block-diagonal, with 2 blocks of size $N/2$.



Then to diagonalize the two sub-blocks requires work

$$2 \times \left(\frac{N}{2}\right)^3 = \frac{N^3}{4},$$

only 1/4 as much work as diagonalizing ~~the origin~~ a full $N \times N$ matrix. So if you can find a basis for a quantum problem that leads to a block diagonal matrix, then it will simplify diagonalization.

In the case of parity, if $[\pi, H] = 0$, then π and H possess simultaneous eigenstates. So if you want to diagonalize H, it's good to use a basis that is already an eigenbasis of parity. For example, for the quartic oscillator in 1D, $V(x) = x^4$, you might want to use a harmonic oscillator basis, segregated into even and odd basis wavefunctions.

Suppose (in the general case, not nec. 1D) that $[H, \pi] = 0$, and suppose we set up a set of basis states $\{ |\pm k\rangle \}$ $k = 0, 1, \ldots$ that are eigenstates of parity:

$$\pi |\pm k\rangle = \pm |\pm k\rangle.$$

(ignore this, will say it better.)

Then H is block-diagonal in this basis, because

$$\langle +k | H | -k' \rangle$$

$$= \langle +k | \pi^+ H \pi | -k' \rangle = - \langle +k | H | -k' \rangle = 0.$$