Discrete symmetries: Parity and Time reversal

March 3, 2017

A discrete transformation is still a symmetry if it leaves the Hamiltonian invariant,

$$\hat{\mathcal{U}}\hat{H}\hat{\mathcal{U}}^{\dagger}=\hat{H}$$

so discrete symmetries are constants of the motion. However, for discrete symmetries we cannot expand infinitesimally, and a different approach is required. We study the cases of parity and time reversal invariance.

1 Discrete symmetry: Parity

1.1 Parity in classical physics

We first consider parity, or space inversion. Classically, parity is the reflection of position vectors through the origin,

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

Any vector which transforms in this way is said to be *odd* under parity. Since time is unchanged by the parity transformation, momentum is also of odd parity,

$$\begin{aligned}\pi\mathbf{p} &= \pi\left(m\frac{d\mathbf{x}}{dt}\right)\\ &= m\frac{d\left(\pi\mathbf{x}\right)}{dt}\\ &= -\mathbf{p}\end{aligned}$$

On the other hand, angular momentum is even,

$$\begin{aligned}\pi\mathbf{L} &= \pi\left(\mathbf{x}\times\mathbf{p}\right)\\ &= (-\mathbf{x})\times(-\mathbf{p})\\ &= \mathbf{L}\end{aligned}$$

We now need to represent these relations quantum mechanically.

1.2 Parity of quantum operators

Define the parity operator by its action on the position basis,

$$\hat{\pi}\left|\mathbf{x}\right\rangle = \left|-\mathbf{x}\right\rangle$$

Notice that a second application of $\hat{\pi}$ returns us to the original state, so $\hat{\pi}$ is its own inverse.

We may find the effect of parity on the position operator by letting $\hat{\mathbf{X}}$ act on a parity transformed state, $\hat{\pi}\left|\mathbf{x}\right\rangle$,

$$\hat{\mathbf{X}}\hat{\pi}\left|\mathbf{x}\right\rangle=\hat{\mathbf{X}}\left|-\mathbf{x}\right\rangle=-\mathbf{x}\left|-\mathbf{x}\right\rangle$$

Now act on both sides with $\hat{\pi}^{\dagger}=\hat{\pi}^{-1}=\hat{\pi}$:

$$\begin{aligned}
\hat{\pi}^{\dagger}\hat{\mathbf{X}}\hat{\pi}\left|\mathbf{x}\right\rangle &= -\mathbf{x}\hat{\pi}^{\dagger}\left|-\mathbf{x}\right\rangle \\
&= -\mathbf{x}\hat{\pi}\left|-\mathbf{x}\right\rangle \\
&= -\mathbf{x}\left|\mathbf{x}\right\rangle \\
&= -\hat{\mathbf{X}}\left|\mathbf{x}\right\rangle
\end{aligned}$$

Since the $\left|\mathbf{x}\right\rangle$ states are complete, this proves the operator relationship,

$$\hat{\pi}^{\dagger}\hat{\mathbf{X}}\hat{\pi}=-\hat{\mathbf{X}}$$

Using unitarity, $\hat{\pi}^{\dagger}=\hat{\pi}^{-1}$ we may write this as

$$\hat{\mathbf{X}}\hat{\pi}+\hat{\pi}\hat{\mathbf{X}}\equiv\left\{\hat{\mathbf{X}},\hat{\pi}\right\}=0$$

so that the parity operator and the position operators *anticommute*.

Next, consider the action of the parity operator $\hat{\pi}$ on momentum. Begin with the translation operator,

$$\hat{\mathcal{T}}\left(\mathbf{a}\right)=\exp\left(-\frac{i}{\hbar}\mathbf{a}\cdot\hat{\mathbf{P}}\right)$$

which has the effect

$$\hat{\mathcal{T}}\left(\mathbf{a}\right)\left|\mathbf{x}\right\rangle = \left|\mathbf{x}+\mathbf{a}\right\rangle$$

Transforming the translation operator with parity, $\hat{\mathcal{T}}\left(\mathbf{a}\right)\rightarrow\hat{\pi}^{\dagger}\hat{\mathcal{T}}\left(\mathbf{a}\right)\hat{\pi}$, consider the action on a position eigenket,

$$\begin{aligned}
\hat{\pi}^{\dagger}\hat{\mathcal{T}}\left(\mathbf{a}\right)\hat{\pi}\left|\mathbf{x}\right\rangle &= \hat{\pi}^{\dagger}\hat{\mathcal{T}}\left(\mathbf{a}\right)\left|-\mathbf{x}\right\rangle \\
&= \hat{\pi}^{\dagger}\left|-\mathbf{x}+\mathbf{a}\right\rangle \\
&= \hat{\pi}\left|-\mathbf{x}+\mathbf{a}\right\rangle \\
&= \left|\mathbf{x}-\mathbf{a}\right\rangle \\
&= \hat{\mathcal{T}}\left(-\mathbf{a}\right)\left|\mathbf{x}\right\rangle
\end{aligned}$$

from which we see that

$$\hat{\pi}^{\dagger}\hat{\mathcal{T}}\left(\mathbf{a}\right)\hat{\pi}=\hat{\mathcal{T}}\left(-\mathbf{a}\right)$$

For the case of an infinitesimal translation, $\hat{\mathcal{T}}\left(\boldsymbol{\varepsilon}\right)=\hat{1}-\frac{i}{\hbar}\boldsymbol{\varepsilon}\cdot\hat{\mathbf{P}}$, this becomes

$$\begin{aligned}
\hat{\pi}^{\dagger}\left(\hat{1}-\frac{i}{\hbar}\boldsymbol{\varepsilon}\cdot\hat{\mathbf{P}}\right)\hat{\pi} &= \hat{1}+\frac{i}{\hbar}\boldsymbol{\varepsilon}\cdot\hat{\mathbf{P}} \\
\hat{1}-\frac{i}{\hbar}\boldsymbol{\varepsilon}\cdot\hat{\pi}^{\dagger}\hat{\mathbf{P}}\hat{\pi} &= \hat{1}+\frac{i}{\hbar}\boldsymbol{\varepsilon}\cdot\hat{\mathbf{P}} \\
-\boldsymbol{\varepsilon}\cdot\hat{\pi}^{\dagger}\hat{\mathbf{P}}\hat{\pi} &= \boldsymbol{\varepsilon}\cdot\hat{\mathbf{P}}
\end{aligned}$$

and since $\boldsymbol{\varepsilon}$ is arbitrary, we see that the momentum operator is odd,

$$\hat{\pi}^{\dagger}\hat{\mathbf{P}}\hat{\pi}=-\hat{\mathbf{P}}$$

Now, writing the angular momentum in components, $\hat{\mathbf{L}}=\hat{\mathbf{X}}\times\hat{\mathbf{P}}$,

$$\begin{aligned}
\hat{\pi}^{\dagger}\hat{L}_i\hat{\pi} &= \hat{\pi}^{\dagger}\left(\varepsilon_{ijk}\hat{X}_j\hat{P}_k\right)\hat{\pi} \\
&= \varepsilon_{ijk}\hat{\pi}^{\dagger}\hat{X}_j\left(\hat{\pi}\hat{\pi}^{\dagger}\right)\hat{P}_k\hat{\pi} \\
&= \varepsilon_{ijk}\left(\hat{\pi}^{\dagger}\hat{X}_j\hat{\pi}\right)\left(\hat{\pi}^{\dagger}\hat{P}_k\hat{\pi}\right) \\
&= \varepsilon_{ijk}\left(-\hat{X}_j\right)\left(-\hat{P}_k\right) \\
&= L_i
\end{aligned}$$

and we find the as in the classical case, angular momentum is even,

$$\hat{\pi}^{\dagger}\hat{\mathbf{L}}\hat{\pi} = \hat{\mathbf{L}}$$

1.3 Parity of the wave function

Now consider a state, in the coordiante basis,

$$\psi(\mathbf{x}) = \langle \mathbf{x} \mid \psi \rangle$$

If we transform the state

$$\hat{\pi} |\psi\rangle$$

then the wave function becomes

$$P\psi(\mathbf{x}) = \langle \mathbf{x}| \hat{\pi} |\psi\rangle$$

Using $\hat{\pi}^{\dagger} = \hat{\pi}^{-1} = \hat{\pi}$ this becomes

$$\begin{aligned} P\psi(\mathbf{x}) &= \langle \mathbf{x}| (\hat{\pi} |\psi\rangle) \\ &= \left(\langle \mathbf{x}| \hat{\pi}^{\dagger}\right) |\psi\rangle \\ &= \langle -\mathbf{x} \mid \psi\rangle \\ &= \psi(-\mathbf{x}) \end{aligned}$$

1.4 Conservation of parity

Suppose $|\psi\rangle$ is an eigenstate of parity, with eigenvalue π. Then $\hat{\pi}^2 = \hat{1}$ implies

$$\begin{aligned} \hat{\pi}^2 |\psi\rangle &= \hat{1} |\psi\rangle \\ \pi^2 |\psi\rangle &= |\psi\rangle \end{aligned}$$

and the eigenvalues must be $\pi = \pm 1$. Now, if $\hat{\pi}$ commutes with the Hamiltonian then any solution of the stationary state Schrodinger equation

$$\hat{H} |E\rangle = E |E\rangle$$

may be made a simultaneous eigenket of parity, $|E, \pi\rangle$.

Let $u_E(\mathbf{x}) = \langle \mathbf{x} \mid E\rangle$ be a stationary state solution with energy E, but *not* an eigenstate of parity.

$$\begin{aligned} \langle \mathbf{x}| \hat{\pi} |E\rangle &= \langle -\mathbf{x} \mid E\rangle \\ &= u_E(-\mathbf{x}) \\ &\neq \pi u_E(\mathbf{x}) \end{aligned}$$

so that the energy eigenstates are degenerate, i.e., there are two distinct states, $|E\rangle, \hat{\pi}|E\rangle$, (or in a coordinate basis, $u_E(\mathbf{x}), u_E(-\mathbf{x})$) with energy E. Call these states $|E\rangle = |E, 1\rangle$ and $\hat{\pi}|E\rangle = |E, 2\rangle$. They have the property that

$$\hat{\pi} |E, 1\rangle = |E, 2\rangle$$

and since $\hat{\pi}^2 = \hat{1}$,

$$\hat{\pi} |E, 2\rangle = |E, 1\rangle$$

Therefore, we may construct simultaneous eigenkets,

$$\begin{aligned} |E, +\rangle &= \frac{1}{\sqrt{2}} (|E, 1\rangle + |E, 2\rangle) \\ |E, -\rangle &= \frac{1}{\sqrt{2}} (|E, 1\rangle - |E, 2\rangle) \end{aligned}$$

such that

$$\hat{\pi} |E, \pm\rangle = \pm |E, \pm\rangle$$

Exercises:

1. Verify that $\hat{\pi}\,|E,\pm\rangle = \pm\,|E,\pm\rangle$.
2. Let a free particle state be given by

$$\langle \mathbf{x} \mid \psi\rangle = \frac{Ae^{i\mathbf{k}\cdot\mathbf{x}}}{a^2+\mathbf{x}^2}$$

   for fixed A, a and $\mathbf{k}$. Find the parity eigenstates.

3. Consider the symmetric infinite square well,

$$V(x) = \begin{cases} \infty & x < -\frac{L}{2} \\ 0 & -\frac{L}{2} < x < \frac{L}{2} \\ \infty & x > \frac{L}{2} \end{cases}$$

   (a) Show that $\left[\hat{H},\hat{\pi}\right] = 0$.

   (b) Find the simultaneous energy and parity eigenstates. Are the energies degenerate? Do there exist energy eigenstates which are *not* also eigenstates of parity?

2 Time reversal

Our picture of symmetries as unitary transformations runs into a difficulty when we try to formulate time reversal invariance, $\Theta t = -t$.

2.1 Time reversal in classical physics

In classical physics, Newton's second law has this symmetry since it contains two time derivatives

$$\mathbf{F} = m\frac{d^2\mathbf{x}}{dt^2}$$

so for a time-independent force, $\Theta\mathbf{F} = \mathbf{F}$,

$$\begin{aligned} \Theta\mathbf{F} &= \Theta m\frac{d^2\mathbf{x}}{dt^2} \\ \mathbf{F} &= m\left(-\frac{d}{dt}\right)\left(-\frac{d}{dt}\right)\mathbf{x} \\ &= m\frac{d^2\mathbf{x}}{dt^2} \end{aligned}$$

and the equation of motion is invariant. For Maxwell's equations,

$$\begin{aligned} \boldsymbol{\nabla}\cdot\mathbf{E} &= 4\pi\rho \\ \boldsymbol{\nabla}\cdot\mathbf{B} &= 0 \\ \boldsymbol{\nabla}\times\mathbf{B} - \frac{1}{c^2}\frac{\partial\mathbf{E}}{\partial t} &= \frac{4\pi}{c}\mathbf{J} \\ \boldsymbol{\nabla}\times\mathbf{E} + \frac{\partial\mathbf{B}}{\partial t} &= 0 \end{aligned}$$

time reversal changes the equations to

$$\begin{aligned} \boldsymbol{\nabla}\cdot\Theta\mathbf{E} &= 4\pi\rho \\ \boldsymbol{\nabla}\cdot\Theta\mathbf{B} &= 0 \\ \boldsymbol{\nabla}\times\Theta\mathbf{B} + \frac{1}{c^2}\frac{\partial\Theta\mathbf{E}}{\partial t} &= -\frac{4\pi}{c}\mathbf{J} \\ \boldsymbol{\nabla}\times\Theta\mathbf{E} - \frac{\partial\Theta\mathbf{B}}{\partial t} &= 0 \end{aligned}$$

where we expect that time reversal changes the direction of the current

$$\Theta \mathbf{J} = -\mathbf{J}$$

Gauss's law shows that we need $\Theta \mathbf{E} = \mathbf{E}$, while Ampere's law applied to a current carrying wire show that $\Theta \mathbf{B} = -\mathbf{B}$, since time reversal will reverse the direction of flow of the current and therefore reverse the magnetic field.

2.2 The problem with time reversal operator

For a quantum system, we consider the time evolution of a state, $|\alpha\rangle$. We will see soon in detail that there exists a time translation operator such that

$$|\alpha, t\rangle = \hat{\mathcal{U}}(t)\,|\alpha, 0\rangle$$

where the infinitesimal generator of time translations is proportional to the Hamiltonian. Now, suppose $\hat{\mathcal{U}}$ is unitary and consider its action on a time reversed state,

$$\begin{aligned} \hat{\Theta}\,|\alpha, t\rangle &= \hat{\Theta}\hat{\mathcal{U}}(t)\,|\alpha, 0\rangle \\ |\alpha, -t\rangle &= \hat{\Theta}\hat{\mathcal{U}}(t)\,\hat{\Theta}^{\dagger}\hat{\Theta}\,|\alpha, 0\rangle \\ |\alpha, -t\rangle &= \hat{\Theta}\hat{\mathcal{U}}(t)\,\hat{\Theta}^{\dagger}\,|\alpha, 0\rangle \end{aligned}$$

This means that

$$\hat{\Theta}\hat{\mathcal{U}}(t)\,\hat{\Theta}^{\dagger} = \hat{\mathcal{U}}(-t)$$

There is a problem, however. If we expand the time translation operator infinitesimally,

$$\begin{aligned} \hat{\Theta}\hat{\mathcal{U}}(t) &= \hat{\mathcal{U}}(-t)\,\hat{\Theta} \\ \hat{\Theta}\left(\hat{1} - \frac{i}{\hbar}\hat{H}t\right) &= \left(\hat{1} + \frac{i}{\hbar}\hat{H}t\right)\hat{\Theta} \end{aligned}$$

and therefore,

$$-\hat{\Theta} i \hat{H} = i \hat{H} \hat{\Theta} \tag{1}$$

So far, this is correct, but if $\hat{\Theta}$ is unitary it means that

$$\hat{\Theta}\hat{H} = -\hat{H}\hat{\Theta}$$

so that for a system with unitary time reversal symmetry, time reversal anticommutes with the Hamiltonian

$$\left\{\hat{\Theta}, \hat{H}\right\} = 0$$

This is the result we found for parity and momentum, but if $|E\rangle$ is an energy eigenket with energy $E > 0$ then

$$\begin{aligned} \hat{H}\hat{\Theta}\,|E\rangle &= -\hat{\Theta}\hat{H}\,|E\rangle \\ &= -E\hat{\Theta}\,|E\rangle \end{aligned}$$

so that the time reversed state $\hat{\Theta}\,|E\rangle$ is also an energy eigenket, but with energy $-E$. Therefore, simultaneous eigenkets give negative energies.

Additionally, in order for $\hat{\Theta}$ to be a symmetry, we require $\left[\hat{\Theta}, \hat{H}\right] = 0$, and this together with the anticommutation relation implies

$$\hat{\Theta}\hat{H} = 0$$

and since $\hat{\Theta}$ is necessarily invertible, vanishing Hamiltonian, $\hat{H} = 0$.

Negative energies are a problem because quantum systems enter all available states in proportion to their abundance (entropy increases!). Suppose the quantum harmonic oscillator had energy eigenstates, $|E_n\rangle$, for negative E_n as well as positive. Then every state $|E_n\rangle$ would have a probability of a transition to $|E_{n-1}\rangle + \textit{photon}$, and the latter is more abundant because the phase space available to a photon is large since there are many, many states available to a given photon. This process would continue as the oscillator dropped to lower and lower energies, emitting more and more photons.

There are different ways of reconciling this problem, including:

1. Introduce *antiunitary operators*, with the property that $\hat{\Theta} i = -i\hat{\Theta}$. Then eq.(1) gives only $\left[\hat{\Theta}, \hat{H}\right] = 0$, which we require for a symmetry anyway.

2. Weaken the condition $\hat{H} = 0$ by requiring only that the Hamiltonian vanish when acting on *physical* states. In a gauge theory, this means that the Hamiltonian may still be built from purely gauge-dependent terms, and this can give satisfactory results.

3. Invoke the Stückelberg-Feynman interpretation, which reinterprets the negative energy, time reversed states as antiparticles of positive energy traveling forward in time. This view is widely accepted in quantum field theory.

In relativistic theories, it is not possible to simply replace $t \to -t$ to define time reversal. Elapsed time is not universal – proper time increases differently along different world-lines. The problem is simplified in quantum mechanics because time is a parameter just as in classical mechanics. This allows us to avoid this problem in quantum mechanics by defining *antiunitary* operators. When we introduce time reversal as an antiunitary operator, we avoid the negative energies. The situation is different in quantum field theory, where the negative energy states are reinterpreted as antiparticles.

We continue with the introduction of an antiunitary time reversal operator.

2.3 Antiunitary operators and Wigner's theorem

We define an *antiunitary operator* to be one which satisfies

$$\begin{aligned}\left\langle \tilde{\beta} \mid \tilde{\alpha} \right\rangle &= \langle \beta \mid \alpha \rangle^* \\ \hat{\Theta}\left(c_1 |\alpha\rangle + c_2 |\beta\rangle\right) &= c_1^* |\tilde{\alpha}\rangle + c_2^* \left|\tilde{\beta}\right\rangle\end{aligned}$$

where $|\tilde{\alpha}\rangle \equiv \hat{\Theta} |\alpha\rangle$ an $\left|\tilde{\beta}\right\rangle \equiv \hat{\Theta} |\beta\rangle$ are the transformed states. If we take $c_1 = i$ and $c_2 = 0$ we have

$$\hat{\Theta} i |\alpha\rangle = -i |\tilde{\alpha}\rangle = -i\hat{\Theta} |\alpha\rangle$$

and therefore, $\hat{\Theta} i = -i\hat{\Theta}$.

Suppose:

1. $\hat{\Theta} i = -i\hat{\Theta}$

2. Real numbers commute with $\hat{\Theta}$

3. $\hat{\Theta}$ is distributive over addition, $\hat{\Theta}\left(c_1 |\alpha\rangle + c_2 |\beta\rangle\right) = \hat{\Theta}\left(c_1 |\alpha\rangle\right) + \hat{\Theta}\left(c_2 |\beta\rangle\right)$

Then for every complex numbers $c_1 = a_1 + ib_1, c_2 = a_2 + ib_2$,

$$\begin{aligned}\hat{\Theta}\left(c_1 |\alpha\rangle + c_2 |\beta\rangle\right) &= \hat{\Theta}\left(\left(a_1 + ib_1\right) |\alpha\rangle\right) + \hat{\Theta}\left(\left(a_2 + ib_2\right) |\beta\rangle\right) \\ &= \left(a_1 - ib_1\right) \hat{\Theta} |\alpha\rangle + \left(a_2 - ib_2\right) \hat{\Theta} |\beta\rangle \\ &= c_1^* |\tilde{\alpha}\rangle + c_2^* \left|\tilde{\beta}\right\rangle\end{aligned}$$

Suppose $\hat{\Theta}$ is any antiunitary operator and $\hat{\mathcal{U}}$ is any unitary operator. Let $\hat{\Psi} \equiv \hat{\Theta}\hat{\mathcal{U}}$. Then letting $\left|\tilde{\beta}\right\rangle = \hat{\Psi}\left|\beta\right\rangle$ we have

$$\begin{aligned}
\left\langle \tilde{\beta} \mid \tilde{\alpha} \right\rangle &= \left(\langle\beta|\,\hat{\Psi}^\dagger\right)\left(\hat{\Psi}\,|\alpha\rangle\right) \\
&= \left(\langle\beta|\hat{\mathcal{U}}^\dagger\right)\hat{\Theta}^\dagger\hat{\Theta}\left(\hat{\mathcal{U}}\,|\alpha\rangle\right) \\
&= \left(\langle\beta|\hat{\mathcal{U}}^\dagger\hat{\mathcal{U}}\,|\alpha\rangle\right)^* \\
&= \langle\beta \mid \alpha\rangle^*
\end{aligned}$$

and for the second condition,

$$\begin{aligned}
\hat{\Psi}\left(c_1\,|\alpha\rangle + c_2\,|\beta\rangle\right) &= \hat{\Theta}\hat{\mathcal{U}}\left(c_1\,|\alpha\rangle\right) + \hat{\Theta}\hat{\mathcal{U}}\left(c_2\,|\beta\rangle\right) \\
&= \hat{\Theta}\left(c_1\hat{\mathcal{U}}\,|\alpha\rangle\right) + \hat{\Theta}\left(c_2\hat{\mathcal{U}}\,|\beta\rangle\right) \\
&= c_1^*\hat{\Theta}\hat{\mathcal{U}}\,|\alpha\rangle + c_2^*\hat{\Theta}\hat{\mathcal{U}}\,|\beta\rangle \\
&= c_1^*\,|\tilde{\alpha}\rangle + c_2^*\left|\tilde{\beta}\right\rangle
\end{aligned}$$

so that $\hat{\Psi}$ is also antiunitary. Now let $\hat{\Psi}$ and $\hat{\Theta}$ be any two antiunitary operators. Then their product satisfies

$$\begin{aligned}
\left\langle \tilde{\beta} \mid \tilde{\alpha} \right\rangle &= \left(\langle\beta|\,\hat{\Theta}^\dagger\hat{\Psi}^\dagger\right)\left(\hat{\Psi}\hat{\Theta}\,|\alpha\rangle\right) \\
&= \left(\langle\beta|\,\hat{\Theta}^\dagger\right)\hat{\Psi}^\dagger\hat{\Psi}\left(\hat{\Theta}\,|\alpha\rangle\right) \\
&= \left(\langle\beta|\,\hat{\Theta}^\dagger\hat{\Theta}\,|\alpha\rangle\right)^* \\
&= \left(\langle\beta \mid \alpha\rangle^*\right)^* \\
&= \langle\beta \mid \alpha\rangle
\end{aligned}$$

and

$$\begin{aligned}
\hat{\Psi}\hat{\Theta}\left(c_1\,|\alpha\rangle + c_2\,|\beta\rangle\right) &= \hat{\Psi}\left(c_1^*\hat{\Theta}\,|\alpha\rangle + c_2^*\hat{\Theta}\,|\beta\rangle\right) \\
&= c_1\hat{\Psi}\hat{\Theta}\,|\alpha\rangle + c_2\hat{\Psi}\hat{\Theta}\,|\beta\rangle \\
&= c_1\,|\tilde{\alpha}\rangle + c_2\left|\tilde{\beta}\right\rangle
\end{aligned}$$

so the product is some unitary operator,

$$\hat{\mathcal{U}} = \hat{\Psi}\hat{\Theta}$$

Inverting $\hat{\Psi}$, we see that $\hat{\Psi}^{-1}\hat{\mathcal{U}} = \hat{\Theta}$. Choose the complex conjugation operator, $\hat{K}$, where $\hat{K}i = -i\hat{K}$, $\hat{\Psi}^{-1}$. Then for any other antiunitary operator $\hat{\Theta}$ there is a unitary operator $\hat{\mathcal{U}}$ such that

$$\hat{\Theta} = \hat{K}\hat{\mathcal{U}}$$

We see that every antiunitary operator may be decomposed into the product, $\hat{\mathcal{U}}\hat{K}$, of a unitary operator, $\hat{\mathcal{U}}$, times the complex conjugation operator.

There are several properties to note, which we quote without proof:

1. Clearly, antiunitary operators preserve probabilities, since $\left\langle \tilde{\beta} \mid \tilde{\alpha} \right\rangle = \langle\beta \mid \alpha\rangle^*$ immediately implies $\left|\left\langle \tilde{\beta} \mid \tilde{\alpha} \right\rangle\right|^2 = \left|\langle\beta \mid \alpha\rangle\right|^2$. The converse to this is *Wigner's theorem*: Every invertible operator which preserves transition probabilities is either unitary or antiunitary.

2. We only define the action of $\hat{K}$ on kets, not bras, $|\tilde{\alpha}\rangle = \hat{K}|\alpha\rangle$.

3. The charge conjugation operator does *not* change base kets. Therefore, if we expand $|\alpha\rangle = \sum_a |a\rangle \langle a \mid \alpha\rangle = \sum_a \langle a \mid \alpha\rangle |a\rangle$, we have

$$\begin{aligned} |\tilde{\alpha}\rangle &= \hat{K}|\alpha\rangle \\ &= \hat{K}\sum_a \langle a \mid \alpha\rangle |a\rangle \\ &= \sum_a \langle a \mid \alpha\rangle^* \hat{K}|a\rangle \\ &= \sum_a \langle a |\tilde{\alpha}\rangle^* |a\rangle \end{aligned}$$

The last requirment makes the definition of $\hat{K}$ dependent on the basis, since another basis may be defined by a complex linear combination, $|b\rangle = \sum_a c_{ba}|a\rangle$. To find the form of $\hat{K}$ in a new basis, let the change of basis given by a unitary transformation $\hat{U}$,

$$|b\rangle = \hat{U}|a\rangle$$

Given the form of $\hat{K}$ which leaves the$|a\rangle$ basis invariant, and letting $\hat{\tilde{K}}|b\rangle = |b\rangle$ we find

$$\begin{aligned} \hat{\tilde{K}}|b\rangle &= |b\rangle \\ \hat{\tilde{K}}\hat{U}|a\rangle &= \hat{U}|a\rangle \\ &= \hat{U}\hat{K}|a\rangle \\ \hat{\tilde{K}}\hat{U} &= \hat{U}\hat{K} \\ \hat{\tilde{K}} &= \hat{U}\hat{K}\hat{U}^\dagger \end{aligned}$$

so the new form of $\hat{K}$ is given by a similarity transformation.

2.4 Time reversal

Now, revisit the infinitesimal time translation operator. We had reached the conclusion that

$$-\hat{\Theta}i\hat{H} = i\hat{H}\hat{\Theta}$$

so that, continuing with $\hat{\Theta}$ antiunitary, we have

$$i\hat{\Theta}\hat{H} = i\hat{H}\hat{\Theta}$$

and the Hamiltonian commutes with time reversal.

With a bit of work, we may classify states by their behavior under time reversal. Let $\hat{A}$ be a linear operator, and

$$\begin{aligned} |\tilde{\alpha}\rangle &= \hat{\Theta}|\alpha\rangle \\ \left|\tilde{\beta}\right\rangle &= \hat{\Theta}|\beta\rangle \end{aligned}$$

Define an intermediate state,

$$|\gamma\rangle = \hat{A}^\dagger|\beta\rangle$$

and its dual,

$$\langle\gamma| = \langle\beta|\hat{A}$$

Then

$$\langle\beta|\,\hat{A}\,|\alpha\rangle = \langle\gamma\mid\alpha\rangle$$

and since

$$\langle\gamma\mid\alpha\rangle = \langle\alpha\mid\gamma\rangle^* = \langle\tilde{\alpha}\mid\tilde{\gamma}\rangle$$

for an antiunitary operator, we have

$$\begin{aligned}\langle\beta|\,\hat{A}\,|\alpha\rangle &= \langle\tilde{\alpha}\mid\tilde{\gamma}\rangle \\ &= \langle\tilde{\alpha}|\,\hat{\Theta}\,|\gamma\rangle \\ &= \langle\tilde{\alpha}|\,\hat{\Theta}\hat{A}^\dagger\,|\beta\rangle \\ &= \langle\tilde{\alpha}|\,\hat{\Theta}\hat{A}^\dagger\hat{\Theta}^{-1}\hat{\Theta}\,|\beta\rangle \\ &= \langle\tilde{\alpha}|\,\hat{\Theta}\hat{A}^\dagger\hat{\Theta}^{-1}\left|\tilde{\beta}\right\rangle\end{aligned}$$

This shows the effect of an antiunitary similarity transformation on an operator, $\hat{A}^\dagger$. If $\hat{A}$ is Hermitian, then

$$\langle\beta|\,\hat{A}\,|\alpha\rangle = \langle\tilde{\alpha}|\,\hat{\Theta}\hat{A}\hat{\Theta}^{-1}\left|\tilde{\beta}\right\rangle$$

We define an operator as even or odd under time reversal if

$$\hat{\Theta}\hat{A}\hat{\Theta}^{-1} = \pm\hat{A}$$

For an even or odd Hermitian operator,

$$\langle\alpha|\,\hat{A}\,|\alpha\rangle = \pm\langle\tilde{\alpha}|\,\hat{A}\,|\tilde{\alpha}\rangle$$

so that expectation values in the time reversed state result in a factor of ± 1.

Under time reversal, we require the momentum operator to be odd just as for the classical variable:

$$\langle\alpha|\,\hat{\mathbf{P}}\,|\alpha\rangle = -\langle\tilde{\alpha}|\,\hat{\mathbf{P}}\,|\tilde{\alpha}\rangle$$

Comparing the two relations

$$\begin{aligned}\langle\alpha|\,\hat{\mathbf{P}}\,|\alpha\rangle &= \langle\tilde{\alpha}|\,\hat{\Theta}\hat{\mathbf{P}}\hat{\Theta}^{-1}\,|\tilde{\alpha}\rangle \\ \langle\alpha|\,\hat{\mathbf{P}}\,|\alpha\rangle &= -\langle\tilde{\alpha}|\,\hat{\mathbf{P}}\,|\tilde{\alpha}\rangle\end{aligned}$$

we see that

$$\hat{\Theta}\hat{\mathbf{P}}\hat{\Theta}^{-1} = -\hat{\mathbf{P}}$$

We require expectation values of the position operator to be even,

$$\langle\alpha|\,\hat{\mathbf{X}}\,|\alpha\rangle = \langle\tilde{\alpha}|\,\hat{\mathbf{X}}\,|\tilde{\alpha}\rangle$$

and therefore,

$$\hat{\Theta}\hat{\mathbf{X}}\hat{\Theta}^{-1} = \hat{\mathbf{X}}$$

From these we see that the commutator of $\hat{\mathbf{X}}$ with $\hat{\mathbf{P}}$ satisfies

$$\begin{aligned}\hat{\Theta}\left[\hat{X}_i,\hat{P}_j\right]\hat{\Theta}^{-1} &= \hat{\Theta}\left(\hat{X}_i\hat{P}_j - \hat{P}_j\hat{X}_i\right)\hat{\Theta}^{-1} \\ &= \hat{\Theta}\hat{X}_i\hat{\Theta}^{-1}\hat{\Theta}\hat{P}_j\hat{\Theta}^{-1} - \hat{\Theta}\hat{P}_j\hat{\Theta}^{-1}\hat{\Theta}\hat{X}_i\hat{\Theta}^{-1} \\ &= -\hat{X}_i\hat{P}_j + \hat{P}_j\hat{X}_i \\ &= -\left[\hat{X}_i,\hat{P}_j\right]\end{aligned}$$

which agrees with the right hand side of the commutator,

$$\begin{aligned}\hat{\Theta}\left[\hat{X}_i, \hat{P}_j\right]\hat{\Theta}^{-1} &= \hat{\Theta} i\hbar\delta_{ij}\hat{\Theta}^{-1} \\ &= -i\hbar\delta_{ij}\hat{\Theta}\hat{\Theta}^{-1} \\ &= -i\hbar\delta_{ij}\end{aligned}$$

so the commutator is preserved.

By considering the fundamental commutator for angular momentum, we see that

$$\hat{\Theta}\left[\hat{J}_i, \hat{J}_j\right]\hat{\Theta}^{-1} = \hat{\Theta} i\hbar\varepsilon_{ijk}\hat{J}_k\hat{\Theta}^{-1}$$

is only consistent if $\hat{\Theta}\hat{\mathbf{J}}\hat{\Theta}^{-1} = -\hat{\mathbf{J}}$, so $\hat{\mathbf{J}}$ is odd under time reversal.