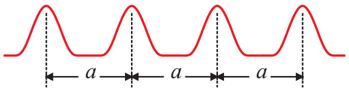
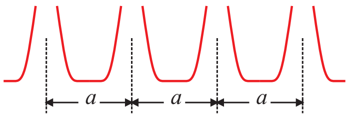
Lattice translations

We consider a particle in the one dimensional periodic potential

$$V(x \pm a) = V(x).$$



(a)



(b)

For example electron in a solid state system (a chrystal of positive ions)
The Hamiltonian of the system is not in general invariant under translations

$$\tau^\dagger(l)x\tau(l) = x + l, \quad \tau(l)|x'\rangle = |x' + l\rangle.$$

However, when l is exactly equal to the period of the lattice a we have

$$\tau^\dagger(a)V(x)\tau(a) = V(x + a) = V(x).$$

Because the operator corresponding to the kinetic energy in the Hamiltonian is translationally invariant the whole Hamiltonian H satisfies the condition

$$\tau^\dagger(a)H\tau(a) = H,$$

which, due to the unitarity of the translation operator can be written as

$$[H, \tau(a)] = 0.$$

The operators H and $\tau(a)$ have thus common eigenstates.
Note The operator $\tau(a)$ is unitary (but not hermitian) and hence its eigenvalues need not be real.
Let us suppose that the potential barrier between the lattice points is infinitely high. Let $|n\rangle$ be the state localized in the lattice cell n, i.e.

$$\langle x'|n\rangle \neq 0 \text{ only if } x' \approx na.$$

Obviously $|n\rangle$ is a stationary state. Because all lattice cells are exactly alike we must have

$$H|n\rangle = E_0|n\rangle, \ \forall n.$$

Thus the system has countably infinite number of ground states
$|n\rangle, \ n = -\infty, \ldots, \infty.$
Now

$$\tau(a)|n\rangle = |n + 1\rangle,$$

so the state $|n\rangle$ is not an eigenstate of the translation $\tau(a)$.
We want to find the simultaneous eigenkets of H and $\tau(a)$
Let's try

$$|\theta\rangle \equiv \sum_{-\infty}^{\infty} e^{in\theta}|n\rangle,$$

where θ is a real parameter and

$$-\pi \leq \theta \leq \pi.$$

Obviously we have

$$H|\theta\rangle = E_0|\theta\rangle.$$

Furthermore we get

$$\begin{aligned}\tau(a)|\theta\rangle &= \sum_{n=-\infty}^{\infty} e^{in\theta}|n+1\rangle = \sum_{n=-\infty}^{\infty} e^{i(n-1)\theta}|n\rangle \\ &= e^{-i\theta}|\theta\rangle.\end{aligned}$$

This is simultaneous eigenstate of H and $\tau(a)$ and the energy eigenvalues E_0 are independent on θ , i.e. the ground state of the system is infinitely degenerate.
Let us suppose further that

- $|n\rangle$ is a state localized at the point n so that

$$\tau(a)|n\rangle = |n+1\rangle,$$

- $\langle x'|n\rangle \neq 0$ (but small), when $|x' - na| > a$.

Due to the translation symmetry the diagonal elements of the Hamiltonian H in the base $\{|n\rangle\}$ are all equal to eachother:

$$\langle n|H|n\rangle = E_0.$$

Let us suppose now that

$$\langle n'|H|n\rangle \neq 0 \text{ only if } n' = n \text{ or } n' = n \pm 1.$$

We are dealing with the so called *tight binding approximation.*
Physically this means that the particle can tunnel through the (high but not infinite) potential barrier.
When we define

$$\Delta = -\langle n \pm 1|H|n\rangle,$$

we can write

$$H|n\rangle = E_0|n\rangle - \Delta|n+1\rangle - \Delta|n-1\rangle,$$

where we have exploited the orthonormality of the basis $\{|n\rangle\}$. Thus the state $|n\rangle$ is not an energy eigen state.

Let us look again at the trial

$$|\theta\rangle = \sum_{n=-\infty}^{\infty} e^{in\theta}|n\rangle.$$

Like before we have

$$\tau(a)|\theta\rangle = e^{-i\theta}|\theta\rangle.$$

Furthermore

$$\begin{aligned} H & \sum e^{in\theta}|n\rangle \\ &= E_0 \sum e^{in\theta}|n\rangle - \Delta \sum e^{in\theta}|n+1\rangle \\ &\quad -\Delta \sum e^{in\theta}|n-1\rangle \\ &= E_0 \sum e^{in\theta}|n\rangle - \Delta \sum (e^{in\theta - i\theta} + e^{in\theta + i\theta})|n\rangle \\ &= (E_0 - 2\Delta\cos\theta) \sum e^{in\theta}|n\rangle. \end{aligned}$$

The earlier degeneracy will be lifted if $\Delta \neq 0$ and

$$E_0 - 2\Delta \leq E \leq E_0 + 2\Delta.$$

Energy levels form a continuous band as Δ increases.

Bloch's theorem

Let us consider the wave function $\langle x'|\theta\rangle$. In the translated state $\tau(a)|\theta\rangle$ the wave function is

$$\langle x'|\tau(a)|\theta\rangle = \langle x' - a|\theta\rangle$$

when the operator $\tau(a)$ acts on left. When it acts on right we get

$$\langle x'|\tau(a)|\theta\rangle = e^{-i\theta}\langle x'|\theta\rangle,$$

so we have

$$\langle x' - a|\theta\rangle = \langle x'|\theta\rangle e^{-i\theta}.$$

This equation can be solved by substituting

$$\langle x'|\theta\rangle = e^{ikx'}u_k(x')$$

when $\theta = ka$ and $u_k(x')$ is a periodic function with the period a.

$$\begin{aligned} \langle x' - a|\theta\rangle &= \langle x'|\theta\rangle e^{-i\theta} \\ \mathrm{e}^{ik(x'-a)}u_k(x'-a) &= \mathrm{e}^{ikx'}u_k(x')e^{-ika} \end{aligned}$$

We have derived a theorem known as the *Bloch theorem*:

Theorem 1 *The wave function of the eigenstate $|\theta\rangle$ of the translation operator $\tau(a)$ can be written as the procuct of the plane wave $e^{ikx'}$ and a function with the period a.*
Note When deriving the theorem we exploited only the fact that $|\theta\rangle$ an eigenstate of the operator $\tau(a)$ belonging to the eigenvalue $e^{i\theta}$. Thus it is valid for all periodic systems (whether the tight binding approximation holds or not) With the help of the Bloch theorem the dispersion relation of the energy in the tight binding model can be written as

$$E(k) = E_0 - 2\Delta \cos ka, \; -\frac{\pi}{a} \leq k \leq \frac{\pi}{a}$$

Above does not depend explicitly on the shape of potential as long as tight binding approx holds.
The degeneracy is removed and this continuum of the energies is known as the *Brillouin zone*.
We have been dealing with a single electron. In case of many electrons, being fermions, they start filling the energy levels from bottom. From this (translation invariance + exclusion principle), features of metals and semiconductors will follow.

Time reversal (reversal of motion)

The Newton equations of motion are invariant under the transformation $t \longrightarrow -t$: if $\boldsymbol{x}(t)$ is a solution of the equation

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

then also $\boldsymbol{x}(-t)$ is a solution.
At the moment $t = 0$ let there be a particle at the point $\boldsymbol{x}(t = 0)$ with the momentum $\boldsymbol{p}(t = 0)$. Then a particle at the same point but with the momentum $-\boldsymbol{p}(t = 0)$ follows the trajectory $\boldsymbol{x}(-t)$.
In the quantum mechanical Schrödinger equation

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

due to the first derivative with respect to the time, $\psi(\boldsymbol{x}, -t)$ is not a solution eventhough $\psi(\boldsymbol{x}, t)$ were, but $\psi^*(\boldsymbol{x}, -t)$ is. In quantum mechanics the time reversal has obviously something to do with the complex conjugation.
Let us consider the symmetry operation

$$|\alpha\rangle \longrightarrow |\tilde{\alpha}\rangle, \quad |\beta\rangle \longrightarrow |\tilde{\beta}\rangle.$$

We require that the absolute value of the inner product is invariant under that operation:

$$|\langle\tilde{\beta}|\tilde{\alpha}\rangle| = |\langle\beta|\alpha\rangle|.$$

There are two possibilities to satisfy this condition:

1. $\langle\tilde{\beta}|\tilde{\alpha}\rangle = \langle\beta|\alpha\rangle$, so the corresponding symmetry operator is unitary, that is
$$\langle\beta|\alpha\rangle \longrightarrow \langle\beta|U^\dagger U|\alpha\rangle = \langle\beta|\alpha\rangle.$$
The symmetries treated earlier have obeyed this condition.
2. $\langle\tilde{\beta}|\tilde{\alpha}\rangle = \langle\beta|\alpha\rangle^* = \langle\alpha|\beta\rangle$, so the symmetry operator cannot be unitary.

We define the *antiunitary* operator θ so that
$$\begin{aligned}\langle\tilde{\beta}|\tilde{\alpha}\rangle &= \langle\beta|\alpha\rangle^* \\ \theta(c_1|\alpha\rangle + c_2|\beta\rangle) &= c_1^*\theta|\alpha\rangle + c_2^*\theta|\beta\rangle,\end{aligned}$$
where
$$|\alpha\rangle \longrightarrow |\tilde{\alpha}\rangle = \theta|\alpha\rangle, \quad |\beta\rangle \longrightarrow |\tilde{\beta}\rangle = \theta|\beta\rangle$$
If the operator satisfies only the last condition it is called *antilinear*.
We define the complex conjugation operator K so that
$$Kc|\alpha\rangle = c^*K|\alpha\rangle.$$
We present the state $|\alpha\rangle$ in the base $\{|a'\rangle\}$. The effect of the operator K is then
$$\begin{aligned}|\alpha\rangle &= \sum_{a'}|a'\rangle\langle a'|\alpha\rangle \xrightarrow{K} |\tilde{\alpha}\rangle = \sum_{a'}\langle a'|\alpha\rangle^* K|a'\rangle \\ &= \sum_{a'}\langle a'|\alpha\rangle^*|a'\rangle.\end{aligned}$$
The fact that the operator K does not change the base states can be justified like:
The state $|a'\rangle$ represented in the base $\{|a'\rangle\}$ maps to the column vector
$$|a'\rangle \mapsto \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 0 \\ 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix},$$
which is unaffected by the complex conjugation.
Note The effect of the operator K depends thus on the choice of the basis states.
Example: let us work in $|S_z;\uparrow\rangle, |S_z;\downarrow\rangle$ basis. In this case the eigenkets of S_z stay the same while eigenkets of S_y change as
$$K\frac{1}{\sqrt{2}}\Big(|1\rangle \pm i|2\rangle\Big) \rightarrow \frac{1}{\sqrt{2}}\Big(|1\rangle \mp i|2\rangle\Big)$$

If U is a unitary operator then the operator $\theta = UK$ is antiunitary.
Proof: Firstly

$$\begin{aligned}
\theta(c_1|\alpha\rangle + c_2|\beta\rangle) &= UK(c_1|\alpha\rangle + c_2|\beta\rangle) \\
&= (c_1^* UK|\alpha\rangle + c_2^* UK|\beta\rangle) \\
&= (c_1^* \theta|\alpha\rangle + c_2^* \theta|\beta\rangle),
\end{aligned}$$

so θ is antiliniear. Secondly, expanding the states $|\alpha\rangle$ and $|\beta\rangle$ in a complete basis $\{|a'\rangle\}$ we get

$$\begin{aligned}
|\alpha\rangle \xrightarrow{\theta} |\tilde{\alpha}\rangle &= \sum_{a'} \langle a'|\alpha\rangle^* UK|a'\rangle \\
&= \sum_{a'} \langle a'|\alpha\rangle^* U|a'\rangle \\
&= \sum_{a'} \langle \alpha|a'\rangle U|a'\rangle
\end{aligned}$$

and

$$|\tilde{\beta}\rangle = \sum_{a'} \langle a'|\beta\rangle^* U|a'\rangle \leftrightarrow \langle\tilde{\beta}| = \sum_{a'} \langle a'|\beta\rangle\langle a'|U^\dagger.$$

Thus the scalar product is

$$\begin{aligned}
\langle\tilde{\beta}|\tilde{\alpha}\rangle &= \sum_{a''}\sum_{a'} \langle a''|\beta\rangle\langle a''|U^\dagger U|a'\rangle\langle\alpha|a'\rangle \\
&= \sum_{a'} \langle\alpha|a'\rangle\langle a'|\beta\rangle = \langle\alpha|\beta\rangle \\
&= \langle\beta|\alpha\rangle^*.
\end{aligned}$$

The operator θ is thus indeed antiunitary. ■

Time-reversal operator
Let Θ be the time-reversal operator. We consider the transformation

$$|\alpha\rangle \longrightarrow \Theta|\alpha\rangle,$$

where $\Theta|\alpha\rangle$ is the time reversed (motion reversed) state.
If $|\alpha\rangle$ is the momentum eigenstate $|\boldsymbol{p}'\rangle$, we should have

$$\Theta|\boldsymbol{p}'\rangle = e^{i\varphi}|-\boldsymbol{p}'\rangle.$$

Let the system be at the moment $t = 0$ in the state $|\alpha\rangle$. At a slightly later moment $t = \delta t$ it is in the state

$$|\alpha, t_0 = 0; t = \delta t\rangle = \left(1 - \frac{iH}{\hbar}\delta t\right)|\alpha\rangle.$$

We apply now, at the moment $t = 0$, the time reversal operator Θ and let the system evolve under the Hamiltonian H. Then at the moment δt the system is in the state

$$\left(1 - \frac{iH}{\hbar}\delta t\right)\Theta|\alpha\rangle.$$

If the motion of the system is invariant under time reversal this state should be the same as

$$\Theta|\alpha, t_0 = 0; -\delta t\rangle,$$

i.e. we first look at the state at the earlier moment $-\delta t$ and then reverse the direction of the momentum $\boldsymbol{p}$. Mathematically this condition can be expressed as

$$\left(1 - \frac{iH}{\hbar}\delta t\right)\Theta|\alpha\rangle = \Theta\left(1 - \frac{iH}{\hbar}(-\delta t)\right)|\alpha\rangle.$$

Thus we must have

$$-iH\Theta|\rangle = \Theta iH|\rangle,$$

where $|\rangle$ stands for an arbitrary state vector.
If Θ were linear we would obtain the anticommutator relation

$$H\Theta = -\Theta H.$$

If now $|n\rangle$ is an energy eigenstate corresponding to the eigenvalue E_n then, according to the anticommutation rule

$$H\Theta|n\rangle = -\Theta H|n\rangle = (-E_n)\Theta|n\rangle,$$

and the state $\Theta|n\rangle$ is an energy eigenstate corresponding to the eigenvalue $-E_n$. Thus most systems (those, whose energy spectrum is not bounded) would not have any ground state.
Thus the operator Θ must be antilinear, and, in order to be a symmetry operator, it must be antiunitary. Using the antilinearity for the right hand side of the condition

$$-iH\Theta|\rangle = \Theta iH|\rangle$$

we can write it as

$$\Theta iH|\rangle = -i\Theta H|\rangle.$$

So, we see that the operators commute:

$$\Theta H = H\Theta.$$

Note We have not defined the Hermitean conjugate of the antiunitary operator θ nor have we defined the meaning of the expression $\langle\beta|\theta$. That being, we let the time reversal operator Θ to operate always on the right and with the matrix element $\langle\beta|\Theta|\alpha\rangle$ we mean the expression $(\langle\beta|)\cdot(\Theta|\alpha\rangle)$.
Let $\otimes$ be an arbitrary linear operator. We define

$$|\gamma\rangle \equiv \otimes^\dagger|\beta\rangle,$$

so that

$$\langle\beta|\otimes = \langle\gamma|$$

and

$$\begin{aligned}\langle\beta|\otimes|\alpha\rangle &= \langle\gamma|\alpha\rangle = \langle\tilde{\alpha}|\tilde{\gamma}\rangle \\ &= \langle\tilde{\alpha}|\Theta\otimes^{\dagger}|\beta\rangle = \langle\tilde{\alpha}|\Theta\otimes^{\dagger}\Theta^{-1}\Theta|\beta\rangle \\ &= \langle\tilde{\alpha}|\Theta\otimes^{\dagger}\Theta^{-1}|\tilde{\beta}\rangle.\end{aligned}$$

In partcular, for a Hermitean observable A we have

$$\langle\beta|A|\alpha\rangle = \langle\tilde{\alpha}|\Theta A\Theta^{-1}|\tilde{\beta}\rangle.$$

We say that the observable A is even or odd under time reversal depending on wheter in the equation

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

the upper or the lower sign holds. This together with the equation

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

imposes certain conditions on the phases of the matrix elements of the operator A between the time reversed states. Namely, they has to satisfy

$$\langle\beta|A|\alpha\rangle = \pm\langle\tilde{\beta}|A|\tilde{\alpha}\rangle^{*}.$$

In particular, the expectation value satisfies the condition

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

Example The expectation value of the momentum operator $\boldsymbol{p}$.
We require that

$$\langle\alpha|\boldsymbol{p}|\alpha\rangle = -\langle\tilde{\alpha}|\boldsymbol{p}|\tilde{\alpha}\rangle,$$

so $\boldsymbol{p}$ is odd, or

$$\Theta\boldsymbol{p}\Theta^{-1} = -\boldsymbol{p}.$$

The momentum eigenstates satisfy

$$\begin{aligned}\boldsymbol{p}\Theta|\boldsymbol{p}'\rangle &= -\Theta\boldsymbol{p}\Theta^{-1}\Theta|\boldsymbol{p}'\rangle \\ &= (-\boldsymbol{p}')\Theta|\boldsymbol{p}'\rangle,\end{aligned}$$

i.e. $\Theta|\boldsymbol{p}'\rangle$ is the momentum eigenstates correponding to the eigenvalue $-\boldsymbol{p}'$:

$$\Theta|\boldsymbol{p}'\rangle = e^{i\varphi}|-\boldsymbol{p}'\rangle.$$

Similarly we can derive for the position operator $\boldsymbol{x}$ the expressions

$$\begin{aligned}\Theta\boldsymbol{x}\Theta^{-1} &= \boldsymbol{x} \\ \Theta|\boldsymbol{x}'\rangle &= |\boldsymbol{x}'\rangle\end{aligned}$$

when we impose the physically sensible condition

$$\langle\alpha|\boldsymbol{x}|\alpha\rangle = \langle\tilde{\alpha}|\boldsymbol{x}|\tilde{\alpha}\rangle.$$

We consider the basic commutation relations

$$[x_i, p_j]|\rangle = i\hbar\delta_{ij}|\rangle.$$

Now

$$\Theta[x_i, p_j]\Theta^{-1}\Theta|\rangle = \Theta i\hbar\delta_{ij}|\rangle,$$

from which, using the antilinearity and the time reversal properties of the operators $\boldsymbol{x}$ and $\boldsymbol{p}$ we get

$$[x_i, (-p_j)]\Theta|\rangle = -i\hbar\delta_{ij}\Theta|\rangle.$$

We see thus that the commutation rule

$$[x_i, p_j]|\rangle = i\hbar\delta_{ij}|\rangle$$

remains invariant under the time reversal.
Correspondingly, the requirement of the invariance of the commutation rule

$$[J_i, J_j] = i\hbar\epsilon_{ijk}J_k$$

leads to the condition

$$\Theta\boldsymbol{J}\Theta^{-1} = -\boldsymbol{J}.$$

This agrees with transformation properties of the orbital angular momentum $\boldsymbol{x}\times\boldsymbol{p}$.

Wave functions
We expand the state $|\alpha\rangle$ with the help of position eigenstates:

$$|\alpha\rangle = \int d^3x'\,|\boldsymbol{x}'\rangle\langle\boldsymbol{x}'|\alpha\rangle.$$

Now

$$\begin{aligned}\Theta|\alpha\rangle &= \int d^3x'\,\Theta|\boldsymbol{x}'\rangle\langle\boldsymbol{x}'|\alpha\rangle^* \\ &= \int d^3x'\,|\boldsymbol{x}'\rangle\langle\boldsymbol{x}'|\alpha\rangle^*,\end{aligned}$$

so under the time reversal the wave function

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

transforms like

$$\psi(\boldsymbol{x}') \longrightarrow \psi^*(\boldsymbol{x}').$$

If in particular we have

$$\psi(\boldsymbol{x}') = R(r)Y_l^m(\theta,\phi),$$

we see that

$$Y_l^m(\theta,\phi) \longrightarrow Y_l^{m*}(\theta,\phi) = (-1)^m Y_l^{-m}(\theta,\phi).$$

Because Y_l^m is the wave function belonging to the state $|lm\rangle$ we must have

$$\Theta|lm\rangle = (-1)^m|l,-m\rangle.$$

The probability current

$$\mathbf{j}(x,t) = \Big(\frac{\hbar}{m}\Big) Im(\psi^*\nabla\psi)$$

corresponding to the wave function $R(r)Y_l^m$ seems to turn clockwise when looked at from the direction of the positive z-axis and $m > 0$. The probability current of the corresponding time reversed state on the other hand turns counterclockwise because m changes its sign under the operation.
The spinles particles obey
Theorem 2 *If the Hamiltonian H is invariant under the time reversal and the energy eigenstate $|n\rangle$ nondegenerate then the corresponding energy eigenfunction is real (or more generally a real function times a phase factor independent on the coordinate $\boldsymbol{x}'$).*

$$H\Theta|n\rangle = \Theta H|n\rangle = E_n\Theta|n\rangle,$$

so the states $|n\rangle$ and $\Theta|n\rangle$ have the same energy. Because the state $|n\rangle$ was supposed to be nondegenerate they must represent the same state. The wave function of the state $|n\rangle$ is $\langle\boldsymbol{x}'|n\rangle$ and the one of the state $\Theta|n\rangle$ correspondingly $\langle\boldsymbol{x}'|n\rangle^*$. These must be same (or more accurately, they can differ only by a phase factor which does not depend on the coordinate $\boldsymbol{x}'$), i.e.

$$\langle\boldsymbol{x}'|n\rangle = \langle\boldsymbol{x}'|n\rangle^* \quad \blacksquare$$

For example the wave function of a nondegenerate groundstate is always real.
For a spinles particle in the state $|\alpha\rangle$ we get

$$\begin{aligned}\Theta|\alpha\rangle &= \Theta\int d\boldsymbol{x}'\,\langle\boldsymbol{x}'|\alpha\rangle|\boldsymbol{x}'\rangle\\ &= \int d\boldsymbol{x}'\,\langle\boldsymbol{x}'|\alpha\rangle^*|\boldsymbol{x}'\rangle = K|\alpha\rangle,\end{aligned}$$

i.e. the time reversal is equivalent to the complex conjugation.
On the other hand, in the momentum space we have

$$\begin{aligned}\Theta|\alpha\rangle &= \int d^3p'\,|-\boldsymbol{p}'\rangle\langle\boldsymbol{p}'|\alpha\rangle^*\\ &= \int d^3p'\,|\boldsymbol{p}'\rangle\langle-\boldsymbol{p}'|\alpha\rangle^*,\end{aligned}$$

because

$$\Theta|\boldsymbol{p}'\rangle = |-\boldsymbol{p}'\rangle.$$

The momentum space wave function transform thus under time reversal like

$$\phi(\boldsymbol{p}') \longrightarrow \phi^*(-\boldsymbol{p}').$$

We consider a spin $\frac{1}{2}$ particle the spin of which is oriented along $\hat{\boldsymbol{n}}$. The corresponding state is obtained by rotating the state $|S_z;\uparrow\rangle$:

$$|\boldsymbol{n};\uparrow\rangle = e^{-iS_z\alpha/\hbar}e^{-iS_y\beta/\hbar}|S_z;\uparrow\rangle,$$

where α and β are the direction angles of the vector $\hat{\boldsymbol{n}}$. Because

$$\Theta\boldsymbol{J}\Theta^{-1} = -\boldsymbol{J}.$$

we see that

$$\Theta|\boldsymbol{n};\uparrow\rangle = e^{-iS_z\alpha/\hbar}e^{-iS_y\beta/\hbar}\Theta|S_z;\uparrow\rangle.$$

Furthermore, due to the oddity of the angular momentum, it follows that

$$J_z\Theta|S_z;\uparrow\rangle = -\frac{\hbar}{2}\Theta|S_z;\uparrow\rangle,$$

so we must have

$$\Theta|S_z;\uparrow\rangle = \eta|S_z;\downarrow\rangle,$$

where η is an arbitrary phase factor. So we get

$$\Theta|\boldsymbol{n};\uparrow\rangle = \eta|\boldsymbol{n};\downarrow\rangle.$$

On the other hand we have

$$|\boldsymbol{n};\downarrow\rangle = e^{-i\alpha S_z/\hbar}e^{-i(\pi+\beta)S_y/\hbar}|S_z;\uparrow\rangle,$$

so

$$\begin{aligned}
\eta|\boldsymbol{n};\downarrow\rangle &= \Theta|\boldsymbol{n};\uparrow\rangle = e^{-iS_z\alpha/\hbar}e^{-iS_y\beta/\hbar}\Theta|S_z;\uparrow\rangle \\
&= \eta e^{-i\alpha S_z/\hbar}e^{-i(\pi+\beta)S_y/\hbar}|S_z;\uparrow\rangle.
\end{aligned}$$

Writing

$$\Theta = UK,\ U \text{ unitary}$$

and recalling that the complex conjugation K has no effect on the base states we see that

$$\Theta = \eta e^{-i\pi S_y/\hbar}K = -i\eta\left(\frac{2S_y}{\hbar}\right)K.$$

Now

$$\begin{aligned}
e^{-i\pi S_y/\hbar}|S_z;\uparrow\rangle &= +|S_z;\downarrow\rangle \\
e^{-i\pi S_y/\hbar}|S_z;\downarrow\rangle &= -|S_z;\uparrow\rangle,
\end{aligned}$$

so the effect of the time reversal on a general spin $\frac{1}{2}$ state is

$$\Theta(c_\uparrow|S_z;\uparrow\rangle + c_\downarrow|S_z;\downarrow\rangle) = +\eta c_\uparrow^*|S_z;\downarrow\rangle - \eta c_\downarrow^*|S_z;\uparrow\rangle.$$

Applying the operator Θ once again we get

$$\begin{aligned}&\Theta^2(c_\uparrow|S_z;\uparrow\rangle + c_\downarrow|S_z;\downarrow\rangle)\\ &\quad = -|\eta|^2 c_\uparrow|S_z;\uparrow\rangle - |\eta|^2 c_\downarrow|S_z;\downarrow\rangle\\ &\quad = -(c_\uparrow|S_z;\uparrow\rangle + c_\downarrow|S_z;\downarrow\rangle),\end{aligned}$$

i.e. for an arbitrary spin orientation we have

$$\Theta^2 = -1.$$

From the relation

$$\Theta|lm\rangle = (-1)^m|l,-m\rangle$$

we see that for spinles particles we have

$$\Theta^2 = 1.$$

In general, one can show that

$$\begin{aligned}\Theta^2|j \text{ half integer}\rangle &= -|j \text{ half integer}\rangle\\ \Theta^2|j \text{ integer}\rangle &= +|j \text{ integer}\rangle.\end{aligned}$$

Generally we can write

$$\Theta = \eta e^{-i\pi J_y/\hbar}K.$$

Now

$$e^{-2i\pi J_y/\hbar}|jm\rangle = (-1)^{2j}|jm\rangle,$$

so

$$\begin{aligned}\Theta^2|jm\rangle &= \Theta\left(\eta e^{-i\pi J_y/\hbar}|jm\rangle\right)\\ &= |\eta|^2 e^{-2i\pi J_y/\hbar}|jm\rangle\\ &= (-1)^{2j}|jm\rangle.\end{aligned}$$

Thus we must have

$$\Theta^2 = (-1)^{2j}.$$

Often one chooses

$$\Theta|jm\rangle = i^{2m}|j,-m\rangle.$$

Spherical tensors

Let us suppose that the operator A is either even or odd, i.e.

$$\Theta A\Theta^{(-1)} = \pm A.$$

We saw that then we have

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

In an eigenstate of the angular momentum we have thus

$$\langle\alpha, jm|A|\alpha, jm\rangle = \pm\langle\alpha, j, -m|A|\alpha, j, -m\rangle.$$

Let now A be a component of a Hermitian spherical tensor:

$$A = T_q^{(k)}.$$

According to the Wigner-Eckart theorem it is sufficient to consider only the component $q = 0$.
We define $T^{(k)}$ to be even/odd under the time reversal if

$$\Theta T_{q=0}^{(k)}\Theta^{-1} = \pm T_{q=0}^{(k)}.$$

Then we have

$$\langle\alpha, jm|T_0^{(k)}|\alpha, jm\rangle = \pm\langle\alpha, j, -m|T_0^{(k)}|\alpha, j, -m\rangle.$$

The state $|\alpha, j, -m\rangle$ is obtained by rotating the state $|\alpha, jm\rangle$:

$$\mathcal{D}(0, \pi, 0)|\alpha, jm\rangle = e^{i\varphi}|\alpha, j, -m\rangle.$$

On the other hand, due to the definition of the spherical tensor

$$\mathcal{D}^\dagger(R)T_q^{(k)}\mathcal{D}(R) = \sum_{q'=-k}^{k} \mathcal{D}_{qq'}^{(k)^*}(R)T_{q'}^{(k)},$$

we get

$$\mathcal{D}^\dagger(0, \pi, 0)T_0^{(k)}\mathcal{D}(0, \pi, 0) = \sum_q \mathcal{D}_{0q}^{(k)}(0, \pi, 0)T_q^{(k)}.$$

Now

$$\mathcal{D}_{00}^{(k)}(0, \pi, 0) = P_k(\cos\pi) = (-1)^k,$$

so we have

$$\begin{aligned}&\mathcal{D}^\dagger(0, \pi, 0)T_0^{(k)}\mathcal{D}(0, \pi, 0)\\ &\quad = (-1)^k T_0^{(k)} + (q \neq 0 \text{ components}).\end{aligned}$$

Furthermore

$$\langle\alpha, jm|T_{q\neq 0}^{(k)}|\alpha, jm\rangle = 0,$$

since the m selection rule would require $m = m + q$. So we get

$$\begin{aligned}&\langle\alpha, jm|T_0^{(k)}|\alpha, jm\rangle\\ &\quad = \pm\langle\alpha, jm|\mathcal{D}^\dagger(0, \pi, 0)T_0^{(k)}\mathcal{D}(0, \pi, 0)|\alpha, jm\rangle\\ &\quad = \pm(-1)^k\langle\alpha, jm|T_0^{(k)}|\alpha, jm\rangle.\end{aligned}$$

Note Unlike under other symmetries the invariance of the Hamiltonian under the time reversal

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

does not lead to any conservation laws. This is due to the fact that the time evolution operator is not invariant:

$$\Theta U(t, t_0) \neq U(t, t_0)\Theta.$$

Time reversal and degeneracy
Let us suppose that

$$[\Theta, H] = 0.$$

Then the energy eigenstates obey

$$\begin{aligned} H|n\rangle &= E_n|n\rangle \\ H\Theta|n\rangle &= E_n\Theta|n\rangle. \end{aligned}$$

If we now had

$$\Theta|n\rangle = e^{i\delta}|n\rangle,$$

then, reapplying the time reversal we would obtain

$$\Theta^2|n\rangle = e^{-i\delta}\Theta|n\rangle = |n\rangle,$$

or

$$\Theta^2 = 1.$$

This is, however, impossible if the system j is half integer, because then $\Theta^2 = -1$. In systems of this kind $|n\rangle$ and $\Theta|n\rangle$ are degenerate.
Example Electon in electromagnetic field
If a particle is influenced by an external static electric field

$$V(\boldsymbol{x}) = e\phi(\boldsymbol{x}),$$

then clearly the Hamiltonian

$$H = \frac{\boldsymbol{p}^2}{2m} + V(\boldsymbol{x})$$

is invariant under the time reversal:

$$[\Theta, H] = 0.$$

If now there are odd number of electrons in the system the total j is half integer. Thus, in a system of this kind there is at least twofold degeneracy, so called *Kramers' degeneracy*.
In the magnetic field

$$\boldsymbol{B} = \nabla \times \boldsymbol{A}$$

the Hamiltonian of an electron contains such terms as

$$\boldsymbol{S} \cdot \boldsymbol{B}, \quad \boldsymbol{p} \cdot \boldsymbol{A} + \boldsymbol{A} \cdot \boldsymbol{p}.$$

The magnetic field $\boldsymbol{B}$ is external, independent on the system, so

$$[\Theta, \boldsymbol{B}] = 0 \text{ ja } [\Theta, \boldsymbol{A}] = 0.$$

On the other hand, $\boldsymbol{S}$ and $\boldsymbol{p}$ are odd, or

$$\Theta \boldsymbol{S} \Theta^{-1} = -\boldsymbol{S} \text{ ja } \Theta \boldsymbol{p} \Theta^{-1} = -\boldsymbol{p},$$

so

$$[\Theta, H] \neq 0.$$

We say that magnetic field breaks the time reversal symmetry and lifts the Kramers degeneracy.
For example, for a spin-$\frac{1}{2}$ system in external magnetic field, the $|S_z; \uparrow\rangle$ and $|S_z; \downarrow\rangle$ have different energies.