Time reversal operator

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The time-reversal invariance is the only one that can be discussed within the framework of classical theory. A symmetric principle or a conservation law is a result of an invariance property of the theory under a certain transformation group. Some correspondences between invariance properties of a system and the conservation laws resulting from them are:

Transformation group	Conservation law
translation in time	energy
translation in space	momentum
rotation	angular momentum

The time reversal transformation is the only discontinuous transformation appearing in classical theory. (K. Nishijima, Fundamental particles W.A. Benjamin, 1963, p.20).

For example, we consider the motion of a charged particle of charge q and mass m in an electric field $\boldsymbol{E}(t)$,

$$m\frac{d^2}{dt^2}\boldsymbol{r}(t) = q\boldsymbol{E}(t)\,. \qquad (1)$$

If $\boldsymbol{r}(t)$ is a solution of this equations, then so is $\boldsymbol{r}(-t)$ as follows easily from the fact that the equations are second order in time, so that the two changes of sign coming from $t \to -t$ cancel. In other words, if we take a movie of a motion which is physically allowed according to Eq. (.1) and run it backwards, the reversed motion is also physically allowed. However, this property does not hold for magnetic forces, in which case the equations of motion include first order time derivatives:

$$m\frac{d^2}{dt^2}\boldsymbol{r}(t) = \frac{q}{c}\frac{d}{dt}\boldsymbol{r}(t)\times\boldsymbol{B}(t)\,, \qquad (2)$$

In these equations, the left-hand side is invariant under $t \to -t$, while the right-hand side changes sign. For example, in a constant magnetic field, the sense of the circular motion of a charged particle (clockwise or counterclockwise) is determined by the charge of the particle, not the initial conditions, and the time-reversed motion $\boldsymbol{r}(-t)$ has the wrong sense. We note, however, that if we make the replacement $\boldsymbol{B} \to -\boldsymbol{B}$ as well as $t \to -t$, then time-reversal invariance is restored to Eq.(.2). In other words, the time reversed motion is physically allowable in the reversed magnetic field.

1. Classical mechanics

The time reversal is an odd kind of symmetry. It suggests that a motion picture of a physical event could be run without the viewer being able to tell something is wrong. Application of the time reversal operation classically requires reversing all velocities and letting time proceed in the reverse direction so that a system runs back through its past history. That this is a classically allowed symmetry follows from the fact that ***F*** = *m**a*** involves only a second derivative with respect to time. A similar situation holds in quantum mechanics provided that *H* is real, as it is expected to be, since it represents energy (Tinkham, Group theory and quantum mechanics).

We consider a set *S* of dynamical variables - a point in phase space- which specifies the state of a dynamical system. For the case of a single particle, the point *S* is described by the particle co-ordinate and the momentum.

$$S = S(x, p)\,.$$

Suppose the system to be initially in the state $S_i(x_i, p_i)$, and after a time *T* in the state $S_f(x_f, p_f)$,

$$S_i \xrightarrow{\quad\quad T \quad\quad} S_f$$

The system is said to be reversible if there exists a transformation *R*, on the collection of states *S*, with the property that to every state *S* there corresponds one and only one state S^R, such that

$$S_f^R \xrightarrow{\quad\quad T \quad\quad} S_i^R$$

Thus *R* is seen to be a mapping of the phase space on itself, as illustrated in Fig. If *R* does not exist, the system is said to be irreversible.

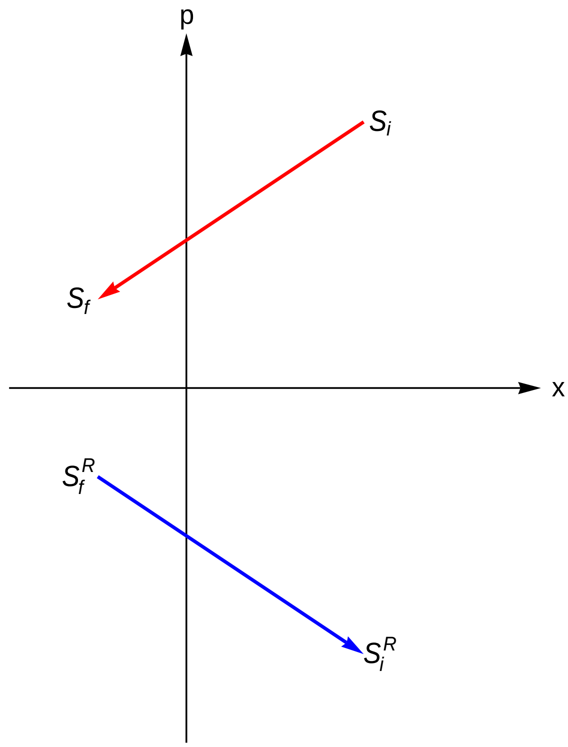


Fig. The mapping $S \to S_R$ in the phase space (x, p) for a reversible system.

For example, we consider the circular motion of a particle in the presence of a certain force field. The particle moves from the point A to the point B after time T. Let the particle reverse its motion at the point B. Then the particle traverses backward along the same trajectory from the point B to the point A after time T.

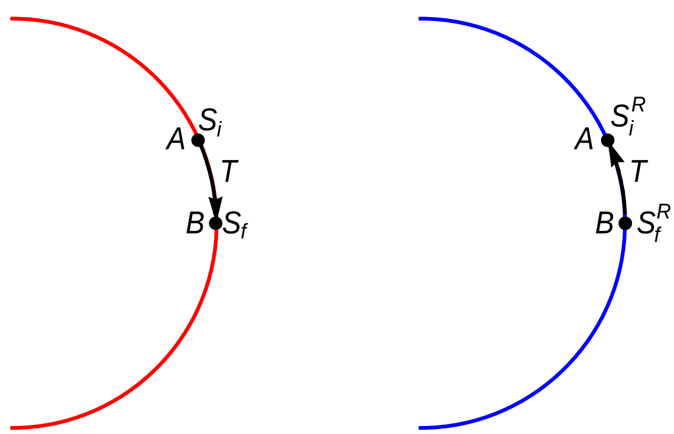


Fig. Classical trajectory of a particle undergoing the circular motion.

Symbolically, we describe this fact by saying

$$S_i(r_A,p_i) \xrightarrow{T} S_f(r_B,p_f)$$

and

$$S_f^R(r_B,-p_f) \xrightarrow{T} S_i^R(r_A,-p_i)$$

The operation *R*, called the time-reversal operation, is defined by

$$\boldsymbol{r} \to \boldsymbol{r}^R = \boldsymbol{r}, \quad \text{and} \quad \boldsymbol{p} \to \boldsymbol{p}^R = -\boldsymbol{p}$$

We define the time-reversed state as one which the position is the same but the momentum is reversed.

(a)

$$\boldsymbol{p}^R = -\boldsymbol{p}, \qquad (R\text{: time reversal}).$$

$$H^R = H,$$

and

$$\boldsymbol{r}^R = \boldsymbol{r}.$$

Hamiltonian *H* and $\boldsymbol{r}$ are invariant under the time reversal.

In addition to the rule (a), we also a set of rules of the *R*-operation.

(b) Physical quantities that are not dynamical variables are not changed by the R operation, e.g., mass, charge, etc.

(c) If *F* is a function of the dynamical variables A, ..., then

$$F(A,B,...)^R = F(A^R,B^R,...).$$

Here we also have the following theorems (the proof is given in K. Nishijima, Fundamental particles W.A. Benjamin, 1963 p.20).

((**Theorem-1**))
If *Q* is an arbitrary dynamical variable, then

$$\{Q,H\}^R + \{Q^R,H\} = 0$$

where { } denotes the Poisson bracket.

((**Theorem-2**))

$$\{F,G\}^R = -\{F^R, G^R\} = 0 .$$

((**Theorem-3**))

$$\left(\frac{dQ}{dt}\right)^R = -\frac{dQ^R}{dt} .$$

((**Theorem-4**))

$$L^R = L .$$

where L is the Lagrangian of the system.

From these three rules and four theorems, we can develop the theory of time reversal in classical physics.

2. Approach from the Electromagnetic theory

(i) Hamiltonian in the presence of *E* and *B*

The Hamiltonian of a charged particle with mass m and charge q is given by

$$H = \frac{1}{2m}[\boldsymbol{p} - \frac{q}{c}\boldsymbol{A}(\boldsymbol{r})]^2 + q\phi(\boldsymbol{r}) ,$$

where $\boldsymbol{A}$ and ϕ are the usual potentials of the electromagnetic field. Since $\boldsymbol{p}^R = -\boldsymbol{p}$, $H^R = H$,and $\boldsymbol{r}^R = \boldsymbol{r}$, we have

$$\boldsymbol{A}(\boldsymbol{r})^R = -\boldsymbol{A}(\boldsymbol{r}),$$

and

$$\phi(\mathbf{r})^R = \phi(\mathbf{r}).$$

Noting that

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

$$\boldsymbol{E} = -\frac{1}{c}\frac{\partial \boldsymbol{A}}{\partial t} - \nabla\phi .$$

then we have

$\boldsymbol{E}^R = \boldsymbol{E}$,

$\boldsymbol{B}^R = -\boldsymbol{B}$.

(ii) Maxwell's equation

Maxwell's equation is given by

$$\begin{cases} \nabla \cdot \boldsymbol{E} = 4\pi\rho \\ \nabla \times \boldsymbol{E} = -\dfrac{1}{c}\dfrac{\partial \boldsymbol{B}}{\partial t} \\ \nabla \cdot \boldsymbol{B} = 0 \\ \nabla \times \boldsymbol{B} = \dfrac{4\pi}{c}\boldsymbol{j} + \dfrac{1}{c}\dfrac{\partial \boldsymbol{E}}{\partial t} \end{cases},$$

From this, we get the expressions

$\rho^R = \rho$,

and

$\boldsymbol{j}^R = -\boldsymbol{j}$,

(iii) Lorentz force on a particle of charge *q*

The Lorentz force is given by

$$\boldsymbol{F} = q(\boldsymbol{E} + \frac{1}{c}\boldsymbol{v} \times \boldsymbol{B})$$

Then we get

$$\begin{aligned} \boldsymbol{F}^R &= q(\boldsymbol{E}^R + \frac{1}{c}\boldsymbol{v}^R \times \boldsymbol{B}^R) \\ &= q(\boldsymbol{E} + \frac{1}{c}\boldsymbol{v} \times \boldsymbol{B}) \\ &= \boldsymbol{F} \end{aligned}$$

which means that $\boldsymbol{F}$ is invariant under the time reversal, where we use

$$\boldsymbol{v}^R = \left(\frac{d\boldsymbol{r}}{dt}\right)^R = -\frac{d\boldsymbol{r}^R}{dt} = -\frac{d\boldsymbol{r}}{dt} = -\boldsymbol{v}$$

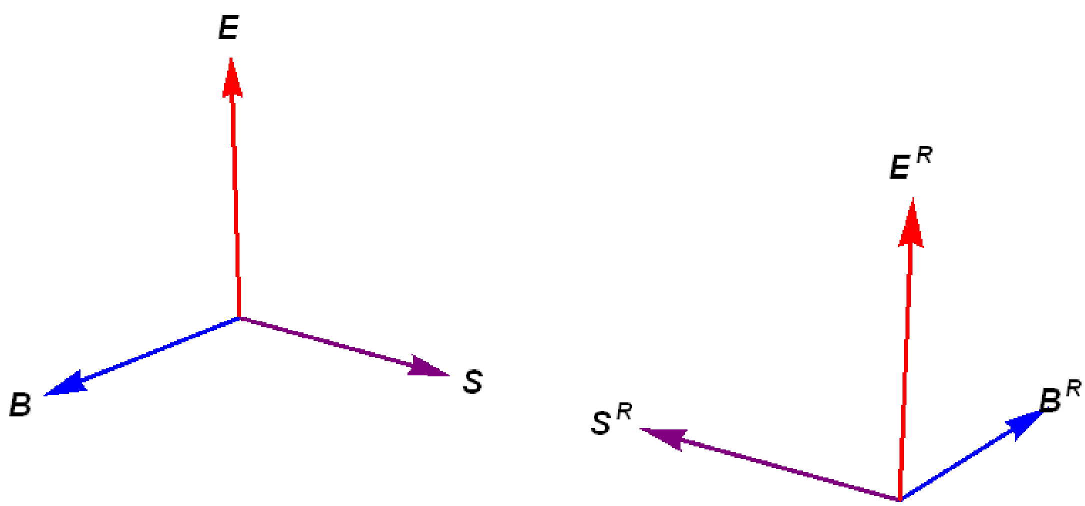
(iv) The poynting vector *S*

$$\boldsymbol{S} = \frac{c}{4\pi} \boldsymbol{E} \times \boldsymbol{B} .$$

So we get

$$\boldsymbol{S}^R = \frac{c}{4\pi} \boldsymbol{E}^R \times \boldsymbol{B}^R = -\frac{c}{4\pi} \boldsymbol{E} \times \boldsymbol{B} = -\boldsymbol{S} ,$$

under *R*. Under the time-reversal *R* an electromagnetic wave reverses its direction of propagation leaving the polarization vector ($\boldsymbol{E}^R = \boldsymbol{E}$) unchanged.



3. Summary

In summary, there are two kinds of operators.

(i) Even: Classical variables which do not change upon time reversal include:

r, the position of a particle in three-space
a, the acceleration of the particle
F, the force on the particle
H, the energy of the particle
ϕ, the electric potential (voltage)
E, the electric field
D, the electric displacement
ρ, the density of electric charge
P, the electric polarization
All masses, charges, coupling constants, and other physical constants, except those associated with the weak force

(ii) Odd: Classical variables which are negated by time reversal include:

t, the time when an event occurs
v, the velocity of a particle
p, the linear momentum of a particle
L, the angular momentum of a particle (both orbital and spin)
A, the electromagnetic vector potential
B, the magnetic induction
H, the magnetic field
J, the density of electric current
M, the magnetization
S, Poynting vector

4. Irreversible case

If an equation is not invariant, then the system is irreversible.

A simple example is given by Ohm's law;

$\boldsymbol{j} = \sigma \boldsymbol{E}$: irreversible on time reversal.

because $\boldsymbol{j}^R = -\boldsymbol{j}$ and $\boldsymbol{E}^R = \boldsymbol{E}$, where σ is the conductivity. In this case Joule heat is produced so that the system is not reversible.

5. Time-reversal in quantum mechanics

A system is said to exhibit symmetry under the time reversal if, at least in principle, its time development may be reversed and all physical processes run backwards, with initial and final states interchanged. Symmetry between the two directions of motion in time implies that to every state $|\psi\rangle$ there corresponds a time-reversed state $\Theta|\psi\rangle$ and that the transformation Θ preserves the value of all probabilities, thus leaving invariant the absolute value of any inner product between states.

We start with the Schrödinger equation given by

$$i\hbar \frac{\partial}{\partial t}\psi(t) = H\psi(t) .$$

Suppose that $\psi(t)$ is a solution. We can easily verify that $\psi(-t)$ is not a solution because of the first-order time derivative. However,

$$-i\hbar \frac{\partial}{\partial t}\psi^*(t) = H^*\psi^*(t) = H\psi^*(t) .$$

Here we use the reality of *H*. When $t \to -t$

$$i\hbar \frac{\partial}{\partial t}\psi^*(-t) = H\psi^*(-t) .$$

This means that $\psi^*(-t)$ is a solution of the Schrödinger equation. The time reversal state is defined by

$$\Theta\psi(t) = \psi^*(-t).$$

If we consider a stationary state,

$$\psi(t) = e^{-\frac{i}{\hbar}Et}\psi(0),$$

$$\psi^*(-t) = e^{-\frac{i}{\hbar}Et}\psi^*(0),$$

$$\Theta\psi(t) = \Theta[e^{-\frac{i}{\hbar}Et}\psi(0)] = e^{-\frac{i}{\hbar}Et}\psi^*(0),$$

or

$$\Theta e^{-\frac{i}{\hbar}Et}\psi(0) = e^{-\frac{i}{\hbar}Et}\psi^*(0).$$

((**Note**))

As a simple example, we consider the plane wave propagating with the momentum $\hbar\boldsymbol{k}$.

$$\psi(t) = e^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)} = e^{-i\omega t}\psi(0),$$

with $\psi(0) = e^{i\mathbf{k}\cdot\mathbf{r}}$. Then we get

$$\psi^*(-t) = [e^{i(\boldsymbol{k}\cdot\boldsymbol{r}+\omega t)}]^* = e^{i(-\boldsymbol{k}\cdot\boldsymbol{r}-\omega t)} = e^{-i\omega t}\psi^*(0),$$

implying that the $\psi^*(-t)$ is the plane wave propagating with the momentum $-\hbar\boldsymbol{k}$.

$$\Theta\psi(0) = \psi^*(0) = K\psi(0),$$

where K is an operator which takes the complex conjugate. We note that

$$\Theta[i\psi(0)] = -i\psi^*(0) = -i\Theta\psi(0),$$

or

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

6. Orbital and spin angular momentum operators

We now consider the wave function of the hydrogen atom

$$\psi(0) = R_{nl}(r) Y_l^m(\theta,\phi),$$

$$K\psi(0) = R_{nl}(r)^* Y_l^m(\theta,\phi)^* = (-1)^m R_{nl}(r)^* Y_l^{-m}(\theta,\phi),$$

where,

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

for $m \geq 0$ and $Y_l^{-m}(\theta,\phi)$ is defined by

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

Thus we have

$$\Theta\psi(0) = K\psi(0) = (-1)^m R_{nl}^*(r) Y_l^{-m}(\theta,\phi).$$

This means that

$$\hat{L}_z|l,m\rangle = m\hbar|l,m\rangle, \tag{1}$$

$$\hat{\Theta}|l,m\rangle = (-1)^m|l,-m\rangle,$$

and

$$\hat{L}_z\hat{\Theta}|l,m\rangle = -m\hbar(-1)^m|l,-m\rangle, \tag{2}$$

From Eqs.(1) and (2), we have

$$\hat{\Theta}\hat{L}_z|l,m\rangle = m\hbar\hat{\Theta}|l,m\rangle = m\hbar(-1)^m|l,-m\rangle = -\hat{L}_z\hat{\Theta}|l,m\rangle$$

$$\hat{\Theta}\hat{L}_z\hat{\Theta}^{-1}\hat{\Theta}|l,m\rangle = -\hat{L}_z\hat{\Theta}|l,m\rangle$$

Thus we have

$$\hat{\Theta}\hat{L}_z\hat{\Theta}^{-1} = -\hat{L}_z$$

More generally

$$\hat{\Theta}\hat{\boldsymbol{L}}\hat{\Theta}^{-1} = -\hat{\boldsymbol{L}}$$

$\hat{\boldsymbol{L}}$ is odd under time reversal. It is natural to consider that for spin angular momentum,

$$\hat{\Theta}\hat{\boldsymbol{S}}\hat{\Theta}^{-1} = -\hat{\boldsymbol{S}}$$

The spin operator is odd under the time reversal.

7. Position and momentum operators

Similar relation is valid for $\hat{\boldsymbol{p}}$,

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

$\hat{\boldsymbol{p}}$ is an odd under time reversal. This implies that

$$\hat{\boldsymbol{p}}\hat{\Theta}|\boldsymbol{p}\rangle = -\hat{\Theta}\hat{\boldsymbol{p}}\hat{\Theta}^{-1}\hat{\Theta}|\boldsymbol{p}\rangle = -\hat{\Theta}\hat{\boldsymbol{p}}|\boldsymbol{p}\rangle = -\boldsymbol{p}\hat{\Theta}|\boldsymbol{p}\rangle$$

Thus the state $\hat{\Theta}|\boldsymbol{p}\rangle$ is the momentum eigenket of $\hat{\boldsymbol{p}}$ with the eigenvalue (-$\boldsymbol{p}$).

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

Similarly, we have the relation for $\hat{\boldsymbol{r}}$,

$$\hat{\Theta}\hat{\boldsymbol{r}}\hat{\Theta}^{-1} = \hat{\boldsymbol{r}}.$$

This implies that

$$\hat{\boldsymbol{r}}\hat{\Theta}|\boldsymbol{r}\rangle = \hat{\Theta}\hat{\boldsymbol{r}}\hat{\Theta}^{-1}\hat{\Theta}|\boldsymbol{r}\rangle = \hat{\Theta}\hat{\boldsymbol{r}}|\boldsymbol{r}\rangle = \boldsymbol{r}\hat{\Theta}|\boldsymbol{r}\rangle.$$

Thus the state $\hat{\Theta}|\boldsymbol{r}\rangle$ is the position eigenket of $\hat{\boldsymbol{r}}$ with the eigenvalue ($\boldsymbol{r}$).

$$\hat{\Theta}|\boldsymbol{r}\rangle = |\boldsymbol{r}\rangle.$$

We note that the relation $\hat{\Theta}i\hat{\Theta}^{-1} = -i$ can be derived directly from the commutation relation [P. Stehle, Quantum Mechanics (Holden-Day, Inc., 1966)] as follows.

$$\begin{aligned}
\hat{\Theta}i\hbar\hat{\Theta}^{-1} &= \hat{\Theta}[\hat{x},\hat{p}]\hat{\Theta}^{-1} \\
&= \hat{\Theta}\hat{x}\hat{\Theta}^{-1}\hat{\Theta}\hat{p}\hat{\Theta}^{-1} - \hat{\Theta}\hat{p}\hat{\Theta}^{-1}\hat{\Theta}\hat{x}\hat{\Theta}^{-1} \\
&= -\hat{x}\hat{p} + \hat{p}\hat{x} \\
&= -i\hbar\hat{1}
\end{aligned}$$

or

$$\hat{\Theta} i \hat{\Theta}^{-1} = -i\hat{1},$$

where

$$[\hat{x}, \hat{p}] = i\hbar\hat{1},$$

$$\hat{\Theta}\hat{x}\hat{\Theta}^{-1} = \hat{x}, \quad \hat{\Theta}\hat{p}\hat{\Theta}^{-1} = -\hat{p}.$$

8. Summary

Most operators of interest are either even or odd under the time reversal. $\hat{\Theta}\hat{A}\hat{\Theta}^{-1} = \pm\hat{A}$ (+: even, -: odd).

(1) $\hat{\Theta} i \hat{\Theta}^{-1} = -i\hat{1}$ (i is a pure imaginary, $\hat{1}$ is the identity operator).

(2) $\hat{\Theta}\hat{\boldsymbol{p}}\hat{\Theta}^{-1} = -\hat{\boldsymbol{p}}$: $\hat{\Theta}|\boldsymbol{p}\rangle = |-\boldsymbol{p}\rangle$.

(3) $\hat{\Theta}\hat{\boldsymbol{p}}^2\hat{\Theta}^{-1} = \hat{\boldsymbol{p}}^2$.

(4) $\hat{\Theta}\hat{\boldsymbol{r}}\hat{\Theta}^{-1} = \hat{\boldsymbol{r}}$: $\hat{\Theta}|\boldsymbol{r}\rangle = |\boldsymbol{r}\rangle$).

(5) $\hat{\Theta}V(\hat{\boldsymbol{r}})\hat{\Theta}^{-1} = V(\hat{\boldsymbol{r}})$: ($V(\hat{\boldsymbol{r}})$ is a potential).

(6) $\hat{\Theta}\hat{\boldsymbol{S}}\hat{\Theta}^{-1} = -\hat{\boldsymbol{S}}$ ($\hat{\boldsymbol{S}}$ is the spin angular momentum).

(7) $\hat{H}$, when $\hat{H} = \dfrac{\hat{p}^2}{2m} + V(\hat{x})$ and $V(\hat{x})$ is a potential energy.

$$\hat{\Theta}\hat{H}\hat{\Theta}^{-1} = \hat{H}.$$

The relation is independent of the form of $V(\hat{x})$.

(8) $\hat{T}_x(a)$; translation operator

$$\hat{\Theta}\hat{T}_x(a)\hat{\Theta}^{-1} = \hat{T}_x(a),$$

or

$$\hat{\Theta}\hat{T}_x(a) = \hat{T}_x(a)\hat{\Theta}.$$

$$\hat{\Theta}\hat{T}(a)|x\rangle = \hat{\Theta}|x+a\rangle = |x+a\rangle,$$

$$\hat{T}(a)\hat{\Theta}|x\rangle = \hat{T}(a)|x\rangle = |x+a\rangle$$

(9) $\hat{R}$: rotation operator

$$\hat{\Theta}\hat{R}\hat{\Theta}^{-1} = \hat{R} \quad \text{or} \quad \hat{\Theta}\hat{R} = \hat{R}\hat{\Theta}.$$

$$\hat{R}\hat{\Theta}|\boldsymbol{r}\rangle = \hat{R}|\boldsymbol{r}\rangle = |\Re\boldsymbol{r}\rangle, \quad \hat{\Theta}\hat{R}|\boldsymbol{r}\rangle = \hat{\Theta}|\Re\boldsymbol{r}\rangle = |\Re\boldsymbol{r}\rangle.$$

(10) $\hat{\Theta}\hat{\pi}\hat{\Theta}^{-1} = \hat{\pi}$, or $\hat{\Theta}\hat{\pi} = \hat{\pi}\hat{\Theta}$.

$$\hat{\pi}\hat{\Theta}|\boldsymbol{r}\rangle = \hat{\pi}|\boldsymbol{r}\rangle = |-\boldsymbol{r}\rangle, \quad \hat{\Theta}\hat{\pi}|\boldsymbol{r}\rangle = \hat{\Theta}|-\boldsymbol{r}\rangle = |-\boldsymbol{r}\rangle$$

9. Property of the time-reversal operator $\hat{\Theta}$

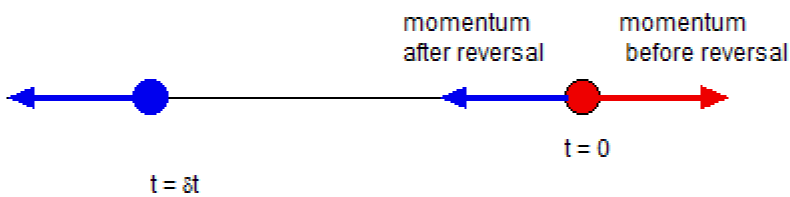


Fig.(a)

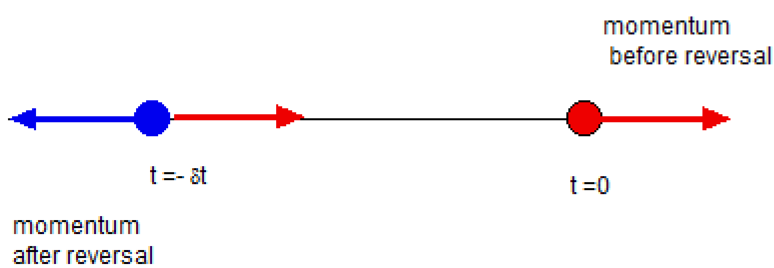


Fig.(b)

We consider a state represented by $|\psi(0)\rangle$ at t = 0. First, we apply $\hat{\Theta}$ to the state $|\psi(0)\rangle$, and then let the system evolve under the influence of the Hamiltonian $\hat{H}$.

$$(\hat{1} - \frac{i}{\hbar}\hat{H}\delta t)\hat{\Theta}|\psi(0)\rangle.$$

(see Fig.(a)). This state is the same as

$$\hat{\Theta}|\psi(-\delta t)\rangle = \hat{\Theta}[1 - \frac{i}{\hbar}\hat{H}(-\delta t)]|\psi(0)\rangle,$$

if the motion obeys the symmetry under time reversal (see Fig.(b)). In other words, we have

$$\hat{\Theta}(\hat{1} + \frac{i}{\hbar}\hat{H}\delta t)\left|\psi(0)\right\rangle = (1 - \frac{i}{\hbar}\hat{H}\delta t)\hat{\Theta}\left|\psi(0)\right\rangle,$$

or

$$\hat{\Theta}i\hat{H}\left|\psi(0)\right\rangle = -i\hat{H}\hat{\Theta}\left|\psi(0)\right\rangle.$$

Since $\left|\psi(0)\right\rangle$ is arbitrary state, we have

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

(i) If $\hat{\Theta}$ is anti-unitary, we have

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

or

$$\hat{\Theta}\hat{H}\hat{\Theta}^{-1} = \hat{H}.$$

Suppose that $\left|n\right\rangle$ is the eigenket of $\hat{H}$ with the eigenvalue E_n. Then we have

$$\hat{\Theta}\hat{H}\left|n\right\rangle = \hat{H}\hat{\Theta}\left|n\right\rangle = \hat{\Theta}E_n\left|n\right\rangle = E_n\hat{\Theta}\left|n\right\rangle.$$

Thus $\hat{\Theta}\left|n\right\rangle$ is the eigenket of $\hat{H}$ with the eigenvalue E_n.

(ii) If $\hat{\Theta}$ is unitary, we have

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

or

$$\hat{\Theta}\hat{H}\left|n\right\rangle = -\hat{H}\hat{\Theta}\left|n\right\rangle = -\hat{\Theta}E_n\left|n\right\rangle = (-E_n)\hat{\Theta}\left|n\right\rangle.$$

Thus $\hat{\Theta}\left|n\right\rangle$ *is the eigenket of* $\hat{H}$ *with the eigenvalue (*$-E_n$*). The change of sign of the energy is in conflict with our classical mechanics about the behavior of the energy if all the velocities are reversed. It is inconsistent with the energy conservation.*

10. Anti-unitary operator and anti-linear operator

$$|\psi\rangle \to |\tilde{\psi}\rangle = \hat{\Theta}|\psi\rangle .$$

The time reversal operator acts only to the right because it entails taking the complex conjugate. If one define the time-reversal operator in terms of bras and kets,

$$\langle\tilde{\beta}|\tilde{\alpha}\rangle = \langle\beta|\alpha\rangle^* = \langle\alpha|\beta\rangle ,$$

where

$$|\tilde{\alpha}\rangle = \hat{\Theta}|\alpha\rangle ,$$

and

$$|\tilde{\beta}\rangle = \hat{\Theta}|\beta\rangle ,$$

are the time-reversal states. The operator $\hat{\Theta}$ is said to be *anti-unitary* if

$$\langle\tilde{\beta}|\tilde{\alpha}\rangle == \langle\beta|\alpha\rangle^* = \langle\alpha|\beta\rangle ,$$

and

$$\hat{\Theta}(C_1|\alpha\rangle + C_2|\beta\rangle) = C^*{}_1\hat{\Theta}|\alpha\rangle + C_2{}^*\hat{\Theta}|\beta\rangle) .$$

(anti-linear operator)

((**Note**))

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

where $\hat{U}$ is the unitary operator.

$$\begin{aligned}|\tilde{\alpha}\rangle &= \hat{\Theta}|\alpha\rangle \\ &= \hat{U}\hat{K}|\alpha\rangle \\ &= \sum_{\alpha'}\hat{U}\hat{K}|\alpha'\rangle\langle\alpha'|\alpha\rangle \\ &= \sum_{\alpha'}\hat{U}|\alpha'\rangle\langle\alpha'|\alpha\rangle^*\end{aligned}$$

$$\left|\tilde{\beta}\right\rangle = \hat{\Theta}\beta$$
$$= \hat{U}\hat{K}\left|\beta\right\rangle$$
$$= \sum_{\alpha''}\hat{U}\hat{K}\left|\alpha''\right\rangle\left\langle\alpha''\right|\beta\rangle$$
$$= \sum_{\alpha'}\hat{U}\left|\alpha''\right\rangle\left\langle\alpha''\right|\beta\rangle^*$$

$$\left\langle\tilde{\beta}\middle|\tilde{\alpha}\right\rangle = \sum_{\alpha',\alpha''}\langle\alpha''|\beta\rangle\langle\alpha''|\hat{U}^+\hat{U}|\alpha'\rangle\langle\alpha'|\alpha\rangle^*$$
$$= \sum_{\alpha',\alpha''}\langle\alpha''|\beta\rangle\delta_{\alpha',\alpha''}\langle\alpha'|\alpha\rangle^*$$
$$= \sum_{\alpha'}\langle\alpha|\alpha'\rangle\langle\alpha'|\beta\rangle$$
$$= \langle\alpha|\beta\rangle$$
$$= \langle\beta|\alpha\rangle^*$$

One can then show that expectation operators must satisfy the identity

$$\left\langle\tilde{\beta}\middle|\hat{\Theta}\hat{A}\hat{\Theta}^{-1}\middle|\tilde{\alpha}\right\rangle = \langle\alpha|\hat{A}^+|\beta\rangle = \langle\beta|\hat{A}|\alpha\rangle^*.$$

((**Proof**))

$$|\gamma\rangle = \hat{A}|\alpha\rangle, \; |\tilde{\gamma}\rangle = \hat{\Theta}|\gamma\rangle = \hat{\Theta}\hat{A}|\alpha\rangle,$$

or

$$\langle\gamma| = \langle\alpha|\hat{A}^+,$$

$$\langle\alpha|\hat{A}^+|\beta\rangle = \langle\gamma|\beta\rangle$$
$$= \left\langle\tilde{\gamma}\middle|\tilde{\beta}\right\rangle^*$$
$$= \left\langle\tilde{\beta}\middle|\tilde{\gamma}\right\rangle$$
$$= \left\langle\tilde{\beta}\middle|\hat{\Theta}\hat{A}\middle|\alpha\right\rangle$$
$$= \left\langle\tilde{\beta}\middle|\hat{\Theta}\hat{A}\hat{\Theta}^{-1}\hat{\Theta}\middle|\alpha\right\rangle$$
$$= \left\langle\tilde{\beta}\middle|\hat{\Theta}\hat{A}\hat{\Theta}^{-1}\middle|\tilde{\alpha}\right\rangle$$

For the Hermitian operator $\hat{A}$,

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

Most operators of interest are either even or odd under the time reversal.

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

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

$$\begin{aligned}
\langle \alpha | \hat{A} | \beta \rangle &= \langle \tilde{\beta} | \hat{\Theta}\hat{A}\hat{\Theta}^{-1} | \tilde{\alpha} \rangle \\
&= \langle \tilde{\beta} | \pm \hat{A} | \tilde{\alpha} \rangle \\
&= \pm \langle \tilde{\beta} | \hat{A} | \tilde{\alpha} \rangle \\
&= \pm \langle \tilde{\alpha} | \hat{A} | \tilde{\beta} \rangle^{*}
\end{aligned}$$

If $|\alpha\rangle = |\beta\rangle$,

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

This is consistent with the result expected from the classical mechanics.

We can now see the invariance of the fundamental commutation relations under the time reversal

$$[\hat{x}, \hat{p}] = i\hbar \hat{1} .$$

Using

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

we have

$$\begin{aligned}
\langle \alpha | [\hat{x}, \hat{p}] | \beta \rangle &= \langle \tilde{\beta} | \hat{\Theta}[\hat{x}, \hat{p}]\hat{\Theta}^{-1} | \tilde{\alpha} \rangle \\
&= \langle \tilde{\beta} | \hat{\Theta}\hat{x}\hat{\Theta}^{-1}\hat{\Theta}\hat{p}\hat{\Theta}^{-1} - \hat{\Theta}\hat{p}\hat{\Theta}^{-1}\hat{\Theta}\hat{x}\hat{\Theta}^{-1} | \tilde{\alpha} \rangle \\
&= -\langle \tilde{\beta} | [\hat{x}, \hat{p}] | \tilde{\alpha} \rangle
\end{aligned}$$

or

$$\langle\alpha|i\hbar|\beta\rangle = -\langle\tilde{\beta}|i\hbar|\tilde{\alpha}\rangle = \langle\tilde{\beta}|\hat{\Theta}i\hbar\hat{\Theta}^{-1}|\tilde{\alpha}\rangle,$$

or

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

The operator $i\hbar\hat{1}$ *flips sign under the time-reversal operator.*

How about the commutation relation of the angular momentum?

$$[\hat{L}_x, \hat{L}_y] = i\hbar\hat{L}_z,$$

$$\begin{aligned}\langle\alpha|[\hat{L}_x, \hat{L}_y]|\beta\rangle &= \langle\tilde{\beta}|\hat{\Theta}[\hat{L}_x, \hat{L}_y]\hat{\Theta}^{-1}|\tilde{\alpha}\rangle \\ &= \langle\tilde{\beta}|\hat{\Theta}\hat{L}_x\hat{\Theta}^{-1}\hat{\Theta}\hat{L}_y\hat{\Theta}^{-1} - \hat{\Theta}\hat{L}_y\hat{\Theta}^{-1}\hat{\Theta}\hat{L}_x\hat{\Theta}^{-1}|\tilde{\alpha}\rangle \\ &= \langle\tilde{\beta}|[\hat{L}_x, \hat{L}_y]|\tilde{\alpha}\rangle\end{aligned}$$

$$\begin{aligned}\langle\alpha|i\hbar\hat{L}_z|\beta\rangle &= \langle\tilde{\beta}|i\hbar\hat{L}_z|\tilde{\alpha}\rangle \\ &= \langle\tilde{\beta}|\hat{\Theta}(i\hbar\hat{L}_z)\hat{\Theta}^{-1}|\tilde{\alpha}\rangle =\end{aligned}$$

or

$$\hat{\Theta}(i\hbar\hat{L}_z)\hat{\Theta}^{-1} = i\hbar\hat{L}_z$$

$$\hat{\Theta}[\hat{L}_x, \hat{L}_y]\hat{\Theta}^{-1} = [\hat{L}_x, \hat{L}_y]$$

Finally we now consider the raising and lowering operator for the simple harmonics. These operators are even under the time reversal.

$$\hat{\Theta}\hat{a}\hat{\Theta}^{-1} = \hat{a}, \quad \text{and} \quad \hat{\Theta}\hat{a}^{+}\hat{\Theta}^{-1} = \hat{a}^{+}$$

where

$$\hat{a} = \frac{\beta}{\sqrt{2}}\left(\hat{x} + \frac{i\hat{p}}{m\omega_0}\right)$$

$$\hat{a}^{+} = \frac{\beta}{\sqrt{2}}\left(\hat{x} - \frac{i\hat{p}}{m\omega_0}\right)$$

The Hamiltonian are usually invariant under the time reversal.

$$\hat{\Theta}\hat{H}\hat{\Theta}^{-1} = \hat{H} .$$

Here we list a few terms which might appear in a Hamiltonian and discuss whether they violate the time reversal or parity.

1. $\dfrac{\hat{\boldsymbol{p}}^2}{2m}$ is invariant under both

2. $\hat{\boldsymbol{p}} \cdot \hat{\boldsymbol{r}}$ is invariant under parity but not time reversal.

3. $\hat{\boldsymbol{L}} \cdot \hat{\boldsymbol{p}}$ is invariant under time reversal but not parity.

4. $\boldsymbol{S} \cdot \boldsymbol{B}$ and $\hat{\boldsymbol{p}} \cdot \hat{\boldsymbol{A}}$ is invariant under both

5. Quenching of the orbital angular momentum

11. Theorem-I

We state an important theorem on the reality of the energy eigenfunction of a spinless particle.

((**Theorem**))
Suppose that the Hamiltonian is invariant under time reversal and the energy eigenkets $|\phi_n\rangle$ is nondegenerate. Then the corresponding energy eigenfunction is real (or more generally, a real function times a phase factor independent of $\boldsymbol{r}$.

((**Proof**))

The Hamiltonian $\hat{H}$ is invariant under the time reversal.

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

$$\hat{H}\hat{\Theta}|\phi_n\rangle = \hat{\Theta}\hat{H}|\phi_n\rangle = E_n\Theta|\phi_n\rangle$$

Thus $|\tilde{\phi}_n\rangle = \hat{\Theta}|\phi_n\rangle$ and $|\phi_n\rangle$ have the same energy. The nondegeneracy assumption prompts us to conclude that $\hat{\Theta}|\phi_n\rangle$ and $|\phi_n\rangle$ must have the same state.

$$|\tilde{\phi}_n\rangle = \hat{\Theta}|\phi_n\rangle = |\phi_n\rangle$$

We have

$$\left|\widetilde{\boldsymbol{r}}\right\rangle = \Theta\left|\boldsymbol{r}\right\rangle = \left|\boldsymbol{r}\right\rangle, \qquad \left\langle\widetilde{\boldsymbol{r}}\middle|\widetilde{\phi}_n\right\rangle = \left\langle\boldsymbol{r}\middle|\phi_n\right\rangle^* = \phi_n^*(\boldsymbol{r})$$

We note that

$$\left\langle\widetilde{\boldsymbol{r}}\middle|\widetilde{\phi}_n\right\rangle = \left\langle\boldsymbol{r}\middle|\phi_n\right\rangle = \phi_n(\boldsymbol{r})$$

Then we have

$$\phi_n^*(\boldsymbol{r}) = \phi_n(\boldsymbol{r})$$

The wave function $\phi_n(\mathbf{r})$ is real.

12. Therem-II

Theorem: quenching of orbital angular momentum

When $\hat{H}$ is invariant under time reversal and $\left|\phi_n\right\rangle$ is nondegenerate, the orbital angular momentum is quenched;

$$\left\langle\phi_n\middle|\hat{\boldsymbol{L}}\middle|\phi_n\right\rangle = 0$$

((**Proof-1**))

$$\left\langle\phi_n\middle|\hat{\boldsymbol{L}}\middle|\phi_n\right\rangle = \left\langle\widetilde{\phi}_n\middle|\hat{\Theta}\hat{\boldsymbol{L}}\hat{\Theta}^{-1}\middle|\widetilde{\phi}_n\right\rangle = -\left\langle\widetilde{\phi}_n\middle|\hat{\boldsymbol{L}}\middle|\widetilde{\phi}_n\right\rangle = -\left\langle\phi_n\middle|\hat{\boldsymbol{L}}\middle|\phi_n\right\rangle$$

since

$$\left|\widetilde{\phi}_n\right\rangle = \hat{\Theta}\left|\phi_n\right\rangle = \left|\phi_n\right\rangle$$

Then we have

$$\left\langle\phi_n\middle|\hat{\boldsymbol{L}}\middle|\phi_n\right\rangle = 0$$

((**Proof-2**))

From the definition

$$\left\langle\phi_n\middle|\hat{\boldsymbol{L}}\middle|\phi_n\right\rangle^* = \left\langle\phi_n\middle|\hat{\boldsymbol{L}}^+\middle|\phi_n\right\rangle = \left\langle\phi_n\middle|\hat{\boldsymbol{L}}\middle|\phi_n\right\rangle$$

When $\left\langle\boldsymbol{r}\middle|\phi_n\right\rangle = \phi_n(\boldsymbol{r}) = \phi_n^*(\boldsymbol{r})$ is real,

$$\langle\phi_n|\hat{\boldsymbol{L}}|\phi_n\rangle^* = \int [\langle\phi_n|\boldsymbol{r}\rangle\frac{\hbar}{i}(\boldsymbol{r}\times\nabla)\langle\boldsymbol{r}|\phi_n\rangle]^* d\boldsymbol{r} = \int [\langle\phi_n|\boldsymbol{r}\rangle^* \frac{\hbar}{i}(\boldsymbol{r}\times\nabla)\langle\boldsymbol{r}|\phi_n\rangle^*]^* d\boldsymbol{r}$$

or

$$\langle\phi_n|\hat{\boldsymbol{L}}|\phi_n\rangle^* = \int \langle\phi_n|\boldsymbol{r}\rangle[-\frac{\hbar}{i}(\boldsymbol{r}\times\nabla)]\langle\boldsymbol{r}|\phi_n\rangle d\boldsymbol{r} = -\langle\phi_n|\hat{\boldsymbol{L}}|\phi_n\rangle$$

Therefore we have

$$\langle\phi_n|\hat{\boldsymbol{L}}|\phi_n\rangle = 0\,.$$

The expectation value of $\boldsymbol{L}$ for any non-degenerate state is zero. If the crystal field has sufficiently low symmetry to remove all the orbital degeneracy, then, to lowest order, the orbital angular momentum is zero and we say that the crystal field has completely quenched it. For this reason, the static susceptibility of iron-group is found experimentally to arise predominantly from the spin.

((Note)) Curie law
The Curie law indicates that the ground state in the absence of the magnetic field is degenerate.

((**Example**))
$Y_l^m(\theta,\phi)$ is complex because the states $|l,\pm m\rangle$ are degenerate. Wavefunction of a plane wave $\exp(\frac{i\boldsymbol{p}\cdot\boldsymbol{r}}{\hbar})$ for the state $|\boldsymbol{p}\rangle$ is complex. It is degenerate with $\exp(-\frac{i\boldsymbol{p}\cdot\boldsymbol{r}}{\hbar})$ for the state $|-\boldsymbol{p}\rangle$.

13. Momentum-space wave function of the time-reversal state

It is apparent that the momentum-space wave function of the time-reversed state is not just the complex conjugate of the original momentum-space wave function.

$$|\tilde{\boldsymbol{k}}\rangle = \Theta|\boldsymbol{k}\rangle = |-\boldsymbol{k}\rangle,$$

$$|\tilde{\phi}_n\rangle = \hat{\Theta}|\phi_n\rangle$$

$$\langle\tilde{\boldsymbol{k}}|\tilde{\phi}_n\rangle = \langle\boldsymbol{k}|\phi_n\rangle^* = \phi_n^*(\boldsymbol{k})$$

Since

$$\langle\tilde{\boldsymbol{k}}| = \langle-\boldsymbol{k}|$$

$$\langle-\boldsymbol{k}|\tilde{\phi}_n\rangle = \phi_n^*(\boldsymbol{k})$$

or

The momentum-space wave function of the time reversed state:

$$\langle \boldsymbol{k}|\tilde{\phi}_n\rangle = \phi_n^*(-\boldsymbol{k}) = \langle -\boldsymbol{k}|\phi_n\rangle^*$$

((Note))

Real-space wave function of the time reverse state

$$|\tilde{\boldsymbol{r}}\rangle = \Theta|\boldsymbol{r}\rangle$$
$$|\tilde{\phi}_n\rangle = \hat{\Theta}|\phi_n\rangle$$
$$\langle \tilde{\boldsymbol{r}}|\tilde{\phi}_n\rangle = \langle \boldsymbol{r}|\phi_n\rangle^* = \phi_n^*(\boldsymbol{r})$$

from the definition.

Since

$$\langle \tilde{\boldsymbol{r}}| = \langle \boldsymbol{r}|$$

$$\langle \boldsymbol{r}|\tilde{\phi}_n\rangle = \phi_n^*(\boldsymbol{r})$$

or

The momentum-space wave function of the time reversed state:

$$\langle \boldsymbol{r}|\tilde{\phi}_n\rangle = \phi_n^*(\boldsymbol{r})$$

14. The time reversal operator for spin 1/2 system

$$\hat{\Theta}\hat{S}_z\hat{\Theta}^{-1} = -\hat{S}_z$$

$$\hat{\Theta}\hat{S}_z = -\hat{S}_z\hat{\Theta}$$

$$\hat{S}_z\hat{\Theta}|+\rangle = -\hat{\Theta}\hat{S}_z|+\rangle = -\frac{\hbar}{2}\Theta|+\rangle$$

The time reverse state $\hat{\Theta}|+\rangle$ is the eigenket of $\hat{S}_z$ with an eigenvalue $-\frac{\hbar}{2}$. Then we have

$$\hat{\Theta}|+\rangle = \eta|-\rangle$$

where η is a phase factor (a complex number of modulus unity).

In general

$$\left|+\right\rangle_n = \hat{R}\left|+\right\rangle = \exp(-\frac{i}{\hbar}\hat{S}_z\phi)\exp(-\frac{i}{\hbar}\hat{S}_y\theta)\left|+\right\rangle$$

$$\hat{\Theta}\left|+\right\rangle_n = \hat{\Theta}\exp(-\frac{i}{\hbar}\hat{S}_z\phi)\hat{\Theta}^{-1}\hat{\Theta}\exp(-\frac{i}{\hbar}\hat{S}_y\theta)\hat{\Theta}^{-1}\hat{\Theta}\left|+\right\rangle$$

Since

$$\hat{\Theta}\exp(-\frac{i}{\hbar}\hat{S}_z\phi)\hat{\Theta}^{-1} = \exp(-\frac{i}{\hbar}\hat{S}_z\phi)$$

$$\hat{\Theta}\exp(-\frac{i}{\hbar}\hat{S}_y\theta)\hat{\Theta}^{-1} = \exp(-\frac{i}{\hbar}\hat{S}_y\theta)$$

since

$$\hat{\Theta}\hat{\boldsymbol{S}}\hat{\Theta}^{-1} = -\hat{\boldsymbol{S}}$$

and

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

Thus we have

$$\hat{\Theta}\hat{R}\hat{\Theta}^{-1} = \hat{R}$$

$$\begin{aligned}\hat{\Theta}\left|+\right\rangle_n &= \exp(-\frac{i}{\hbar}\hat{S}_z\phi)\exp(-\frac{i}{\hbar}\hat{S}_y\theta)\hat{\Theta}\left|+\right\rangle \\ &= \hat{R}\hat{\Theta}\left|+\right\rangle \\ &= \eta\hat{R}\left|-\right\rangle \\ &= \eta\left|-\right\rangle_n\end{aligned}$$

Here we note that

$$\left|-\right\rangle_n = \exp(-\frac{i}{\hbar}\hat{S}_z\phi)\exp(-\frac{i}{\hbar}\hat{S}_y\theta)\left|-\right\rangle$$

$$\left|-\right\rangle = \exp(-\frac{i}{\hbar}\hat{S}_y\pi)\left|+\right\rangle$$

Then

$$\begin{aligned}\hat{\Theta}\left|+\right\rangle_n &= \hat{R}\hat{\Theta}\left|+\right\rangle \\ &= \eta\left|-\right\rangle_n \\ &= \eta\exp(-\frac{i}{\hbar}\hat{S}_z\phi)\exp(-\frac{i}{\hbar}\hat{S}_y\theta)\left|-\right\rangle \\ &= \eta\exp(-\frac{i}{\hbar}\hat{S}_z\phi)\exp[-\frac{i}{\hbar}\hat{S}_y(\theta+\pi)]\left|+\right\rangle\end{aligned}$$

or

$$\exp(-\frac{i}{\hbar}\hat{S}_z\phi)\exp[-\frac{i}{\hbar}\hat{S}_y(\theta)]\hat{\Theta}\left|+\right\rangle = \eta\exp(-\frac{i}{\hbar}\hat{S}_z\phi)\exp[-\frac{i}{\hbar}\hat{S}_y(\theta+\pi)]\left|+\right\rangle$$

$$\hat{\Theta}\left|+\right\rangle = \eta\exp(-\frac{i}{\hbar}\hat{S}_y\pi)\left|+\right\rangle$$

Therefore we have

$$\hat{\Theta} = \eta\exp(-\frac{i}{\hbar}\hat{S}_y\pi)\hat{K} = -i\eta\hat{\sigma}_y\hat{K}$$

where $\hat{K}$ is an operator which takes the complex conjugate and $-i\hat{\sigma}_y$ is a unitary operator. We now calculate

$$\left|\psi\right\rangle = C_+\left|+\right\rangle + C_-\left|-\right\rangle$$

$$\begin{aligned}\hat{\Theta}\left|\psi\right\rangle &= -i\eta\hat{\sigma}_y\hat{K}(C_+\left|+\right\rangle + C_-\left|-\right\rangle) \\ &= -i\eta\hat{\sigma}_y(C_+^*\left|+\right\rangle + C_-^*\left|-\right\rangle) \\ &= -i\eta(C_+^*\hat{\sigma}_y\left|+\right\rangle + C_-^*\hat{\sigma}_y\left|-\right\rangle) \\ &= \eta(C_+^*\left|-\right\rangle - C_-^*\left|+\right\rangle)\end{aligned}$$

since

$$\hat{\sigma}_y\left|+\right\rangle = i\left|-\right\rangle, \quad \text{and} \qquad \hat{\sigma}_y\left|-\right\rangle = -i\left|+\right\rangle$$

Let us apply $\hat{\Theta}$ again

$$\begin{aligned}\hat{\Theta}^2|\psi\rangle &= \hat{\Theta}[\eta(C_+^*|-\rangle - C_-^*|+\rangle)] \\ &= -i\eta\hat{\sigma}_y\hat{K}[\eta(C_+^*|-\rangle - C_-^*|+\rangle)] \\ &= -i\eta\hat{\sigma}_y[\eta^*(C_+|-\rangle - C_-|+\rangle)] \\ &= -i[(C_+\hat{\sigma}_y|-\rangle - C_-\hat{\sigma}_y|+\rangle)] \\ &= -i[(C_+(-i)|+\rangle - C_-i|+\rangle)] = -(C_+|+\rangle + C_-|-\rangle) = -|\psi\rangle \\ &=\end{aligned}$$

or

$$\hat{\Theta}^2 = -\hat{1}$$

This is an extraordinary result.

((**Note**))

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

We show that

$$\hat{\Theta}\hat{\sigma}_x\hat{\Theta}^{-1} = -\hat{\sigma}_x,$$
$$\hat{\Theta}\hat{\sigma}_y\hat{\Theta}^{-1} = -\hat{\sigma}_y$$
$$\hat{\Theta}\hat{\sigma}_z\hat{\Theta}^{-1} = -\hat{\sigma}_z$$

(a)

$$\begin{aligned}\hat{\Theta}\hat{\sigma}_x\hat{\Theta}^{-1}|\psi\rangle &= -\hat{\Theta}\hat{\sigma}_x\hat{\Theta}(C_+|+\rangle + C_-|-\rangle) \\ &= -(-i\eta\hat{\sigma}_y\hat{K})\hat{\sigma}_x(-i\eta\hat{\sigma}_y\hat{K})(C_+|+\rangle + C_-|-\rangle)\end{aligned}$$

or

$$\hat{\Theta}\hat{\sigma}_x\hat{\Theta}^{-1}|\psi\rangle = -(-i\eta\hat{\sigma}_y K)\hat{\sigma}_x(-i\eta\hat{\sigma}_y)(C_+^*|+\rangle + C_-^*|-\rangle)$$

$$
\begin{aligned}
&= i\eta\hat{\sigma}_y K\hat{\sigma}_x(-i\eta)(iC_+^*|-\rangle - iC_-^*|+\rangle) \\
&= i\eta\hat{\sigma}_y K\hat{\sigma}_x(\eta)(C_+^*|-\rangle - C_-^*|+\rangle) \\
&= i\eta\hat{\sigma}_y K\eta(C_+^*\hat{\sigma}_x|-\rangle - C_-^*\hat{\sigma}_x|+\rangle) \\
&= i\eta\hat{\sigma}_y K\eta(C_+^*|+\rangle - C_-^*|-\rangle) \\
&= i\eta\hat{\sigma}_y\eta^*(C_+|+\rangle - C_-|-\rangle) \\
&= i|\eta|^2(C_+\hat{\sigma}_y|+\rangle - C_-\hat{\sigma}_y|-\rangle) \\
&= i(iC_+|-\rangle + iC_-|-\rangle) \\
&= -(C_+|-\rangle + C_-|+\rangle) \\
&= -\hat{\sigma}_x(C_+|+\rangle + C_-|-\rangle) \\
&= -\hat{\sigma}_x|\psi\rangle
\end{aligned}
$$

or

$$\hat{\Theta}\hat{\sigma}_x\hat{\Theta}^{-1} = -\hat{\sigma}_x$$

(b)

$$\hat{\Theta}\hat{\sigma}_y\hat{\Theta}^{-1}|\psi\rangle = -\hat{\Theta}\hat{\sigma}_y\hat{\Theta}(C_+|+\rangle + C_-|-\rangle) = -(-i\eta\hat{\sigma}_y K)\hat{\sigma}_y(-i\eta\hat{\sigma}_y K)(C_+|+\rangle + C_-|-\rangle)$$

or

$$
\begin{aligned}
\hat{\Theta}\hat{\sigma}_y\hat{\Theta}^{-1}|\psi\rangle &= -(-i\eta\hat{\sigma}_y K)\hat{\sigma}_y(-i\eta\hat{\sigma}_y)(C_+^*|+\rangle + C_-^*|-\rangle) \\
&= i\eta\hat{\sigma}_y K(-i\eta)\hat{\sigma}_y^{\,2}(C_+^*|+\rangle + C_-^*|-\rangle) \\
&= i\eta\hat{\sigma}_y K(-i\eta)(C_+^*|+\rangle + C_-^*|-\rangle) \\
&= i\eta\hat{\sigma}_y i\eta^*(C_+|+\rangle + C_-|-\rangle) \\
&= -|\eta|^2\hat{\sigma}_y(C_+|+\rangle + C_-|-\rangle) \\
&= -\hat{\sigma}_y(C_+|+\rangle + C_-|-\rangle) \\
&= -\hat{\sigma}_y|\psi\rangle
\end{aligned}
$$

or

$$\hat{\Theta}\hat{\sigma}_y\hat{\Theta}^{-1} = -\hat{\sigma}_y$$

(c)

$$\hat{\Theta}\hat{\sigma}_z\hat{\Theta}^{-1}|\psi\rangle = -\hat{\Theta}\hat{\sigma}_z\hat{\Theta}(C_+|+\rangle + C_-|-\rangle)$$
$$= -(-i\eta\hat{\sigma}_y K)\hat{\sigma}_z(-i\eta\hat{\sigma}_y K)(C_+|+\rangle + C_-|-\rangle)$$

or

$$\begin{aligned}
\hat{\Theta}\hat{\sigma}_z\hat{\Theta}^{-1}|\psi\rangle &= -(-i\eta\hat{\sigma}_y K)\hat{\sigma}_z(-i\eta\hat{\sigma}_y)(C_+^{\ *}|+\rangle + C_-^{\ *}|-\rangle) \\
&= i\eta\hat{\sigma}_y K\hat{\sigma}_z(-i\eta)(iC_+^{\ *}|-\rangle - iC_-^{\ *}|+\rangle) \\
&= i\eta\hat{\sigma}_y K\hat{\sigma}_z\eta(C_+^{\ *}|-\rangle - C_-^{\ *}|+\rangle) \\
&= i\eta\hat{\sigma}_y K\eta(C_+^{\ *}\hat{\sigma}_z|-\rangle - C_-^{\ *}\hat{\sigma}_z|+\rangle) \\
&= i\eta\hat{\sigma}_y K\eta(-C_+^{\ *}|-\rangle - C_-^{\ *}|+\rangle) \\
&= i\eta\hat{\sigma}_y\eta^*(-C_+|-\rangle - C_-|+\rangle) \\
&= -i|\eta|^2(C_+\hat{\sigma}_y|-\rangle + C_-\hat{\sigma}_y|+\rangle) \\
&= -i(-iC_+|+\rangle + iC_-|-\rangle) \\
&= -C_+|+\rangle + C_-|-\rangle) \\
&= -\hat{\sigma}_z(C_+|+\rangle + C_-|-\rangle) = -\hat{\sigma}_z|\psi\rangle
\end{aligned}$$

or

$$\hat{\Theta}\hat{\sigma}_z\hat{\Theta}^{-1} = -\hat{\sigma}_z$$

Finally we show that $|\psi\rangle$ and $|\tilde{\psi}\rangle = \hat{\Theta}|\psi\rangle$ are orthogonal.

$$|\psi\rangle = C_+|+\rangle + C_-|-\rangle = \begin{pmatrix} C_+ \\ C_- \end{pmatrix}$$

$$|\tilde{\psi}\rangle = \hat{\Theta}|\psi\rangle = \eta(C_+^{\ *}|-\rangle - C_-^{\ *}|+\rangle) = \begin{pmatrix} -\eta C_-^{\ *} \\ \eta C_+^{\ *} \end{pmatrix}$$

$$\langle\tilde{\psi}|\psi\rangle = \begin{pmatrix} -\eta^* C_- & \eta^* C_+ \end{pmatrix}\begin{pmatrix} C_+ \\ C_- \end{pmatrix} = 0$$

Suppose that $[\hat{H}, \hat{\Theta}] = \hat{0}$. In this case, $|\psi\rangle$ and $|\tilde{\psi}\rangle = \hat{\Theta}|\psi\rangle$ are the eigenkets of $\hat{H}$ with the same energy eigenvalue. Since $|\psi\rangle$ and $|\tilde{\psi}\rangle = \hat{\Theta}|\psi\rangle$ are orthogonal to each other, these two states are degenerate. (Kramers theorem).

In contrast, we may note that two successive application of $\hat{\Theta}$ to a spinless state,

$$\hat{\Theta}^2 = \hat{1}$$

((**Proof**))

$$\hat{\Theta}|l,m\rangle = (-1)^m |l,-m\rangle$$

$$\begin{aligned}\hat{\Theta}^2|l,m\rangle &= \hat{\Theta}(-1)^m |l,-m\rangle \\ &= (-1)^m \hat{\Theta}|l,-m\rangle \\ &= (-1)^{2m}|l,m\rangle \\ &= |l,m\rangle\end{aligned}.$$

15. Time reversal state: general case

More generally

$$\hat{\Theta}^2| j = half - \text{int}eger\rangle = -| j = half - \text{int}eger\rangle$$

$$\hat{\Theta}^2| j = \text{int}eger\rangle = | j = \text{int}eger\rangle$$

or

$$\hat{\Theta}^2| j,m\rangle = (-1)^{2j}| j,m\rangle$$

((**Proof**))

We first note that

$$\hat{\Theta} = \eta \exp(-\frac{i\pi}{\hbar}\hat{J}_y)\hat{K} \qquad \text{(generalization)}$$

We now consider a state

$$|\alpha\rangle = \sum_m | j,m\rangle\langle j,m|\alpha\rangle$$

$$\hat{\Theta}\hat{\Theta}|\alpha\rangle = \hat{\Theta}(\hat{\Theta}\sum_m |j,m\rangle\langle j,m|\alpha\rangle)$$
$$= \hat{\Theta}(\eta\sum_m \exp(-\frac{i\pi}{\hbar}\hat{J}_y)\hat{K}|j,m\rangle\langle j,m|\alpha\rangle)$$
$$= \hat{\Theta}(\eta\sum_m \exp(-\frac{i\pi}{\hbar}\hat{J}_y)|j,m\rangle\langle j,m|\alpha\rangle^*)$$
$$= \eta^*\hat{\Theta}(\sum_m \exp(-\frac{i\pi}{\hbar}\hat{J}_y)|j,m\rangle\langle j,m|\alpha\rangle^*)$$
$$= \eta^*(\sum_m \exp(-\frac{i\pi}{\hbar}\hat{J}_y)\hat{\Theta}|j,m\rangle\langle j,m|\alpha\rangle^*)$$
$$= \eta^*\sum_m \exp(-\frac{i\pi}{\hbar}\hat{J}_y)\eta\exp(-\frac{i\pi}{\hbar}\hat{J}_y)\hat{K}|j,m\rangle\langle j,m|\alpha\rangle^*$$
$$= \eta^*\sum_m \exp(-\frac{i\pi}{\hbar}\hat{J}_y)\eta\exp(-\frac{i\pi}{\hbar}\hat{J}_y)|j,m\rangle\langle j,m|\alpha\rangle$$
$$= |\eta|^2\sum_m \exp(-\frac{2i\pi}{\hbar}\hat{J}_y)|j,m\rangle\langle j,m|\alpha\rangle$$
$$= \sum_m \exp(-\frac{2i\pi}{\hbar}\hat{J}_y)|j,m\rangle\langle j,m|\alpha\rangle$$
$$= \sum_m (-1)^{2j}|j,m\rangle\langle j,m|\alpha\rangle$$
$$= (-1)^{2j}|\alpha\rangle$$

where

$$\exp(-\frac{2i\pi}{\hbar}\hat{J}_y)|j,m\rangle = \hat{R}_y(2\pi)|j,m\rangle = (-1)^{2j}|j,m\rangle \text{ (in general)}$$

Then we have

$$\hat{\Theta}^2|\alpha\rangle = (-1)^{2j}|\alpha\rangle$$

or

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

((**Note**))
Obviously, a double reversal of time, corresponding to the application of $\hat{\Theta}^2$ to all states, has no physical consequence.

$$\hat{\Theta}^2|\psi\rangle = C|\psi\rangle$$

for all $|\psi\rangle$ $(|C| = 1)$ C: phase factor

$$C(\hat{\Theta}|\psi\rangle) = \hat{\Theta}^2(\hat{\Theta}|\psi\rangle) = \hat{\Theta}^3|\psi\rangle = \hat{\Theta}\hat{\Theta}^2|\psi\rangle = \hat{\Theta}C|\psi\rangle = C^*\hat{\Theta}|\psi\rangle$$

Then we have

$$C = C^*$$

So C is real.

C = 1 or -1, depending on the nature of the system.

16. Kramer's theorem

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

where

$$|\alpha\rangle = \hat{\Theta}|\psi\rangle, \qquad |\tilde{\alpha}\rangle = \hat{\Theta}|\alpha\rangle = \hat{\Theta}(\hat{\Theta}|\psi\rangle) = \hat{\Theta}^2|\psi\rangle$$

$$|\beta\rangle = |\psi\rangle, \; |\tilde{\beta}\rangle = \hat{\Theta}|\psi\rangle = |\alpha\rangle$$

Since $\hat{\Theta}^2|\psi\rangle = C|\psi\rangle$

$$|\tilde{\alpha}\rangle = \hat{\Theta}^2|\psi\rangle = C|\psi\rangle$$

Then

$$\langle\tilde{\beta}|\tilde{\alpha}\rangle = \langle\alpha|C|\psi\rangle = \langle\alpha|\beta\rangle = \langle\alpha|\psi\rangle$$

In the case C = -1,

$$\langle\alpha|\psi\rangle = 0$$

showing that for such systems, time-reversed states are orthogonal.

((Kramer's theorem))

As a corollaly, if C = -1 and the Hamiltonian is invariant under time reversal, the energy eigenstates may be classified in degenerate time reversed pairs.

Kramer's degeneracy.

((**Proof**))

Since H is invariant under time reversal,

$$[\hat{H},\hat{\Theta}]=\hat{0}.$$

Let $|\phi_n\rangle$ and $\hat{\Theta}|\phi_n\rangle$ be the energy eigenket and its time-reversed states, respectively.

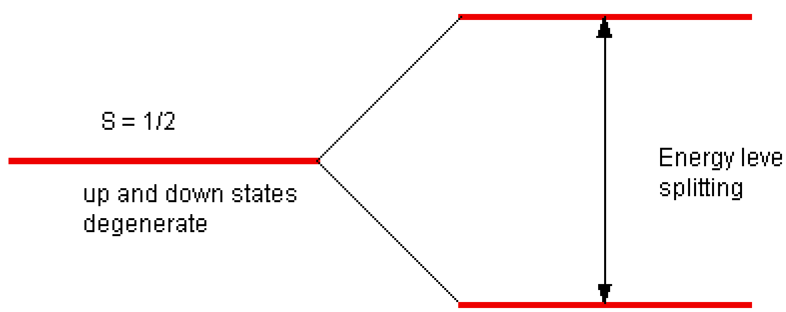
$$\hat{H}\hat{\Theta}|\phi_n\rangle=\hat{\Theta}\hat{H}|\phi_n\rangle=\hat{\Theta}E_n|\phi_n\rangle=E_n\hat{\Theta}|\phi_n\rangle$$

$\hat{\Theta}|\phi_n\rangle$ and $|\phi_n\rangle$ belong to the same energy eigenvalue.

When $\hat{\Theta}^2=-\hat{1}$ (half-integer), $\hat{\Theta}|\phi_n\rangle$ and $|\phi_n\rangle$ are orthogonal.

This means that $\hat{\Theta}|\phi_n\rangle$ and $|\phi_n\rangle$ (having the same energy) must correspond to distinct states.

Kramer's doublet



When the magnetic field $\boldsymbol{B}$ is applied, $\hat{H}$ may then contain terms like

$$\hat{\boldsymbol{S}}\cdot\boldsymbol{B}$$

$$\hat{\boldsymbol{P}}\cdot\hat{\boldsymbol{A}}+\hat{\boldsymbol{A}}\cdot\hat{\boldsymbol{P}}$$

$\hat{\boldsymbol{S}},\hat{\boldsymbol{P}}$ are added under time reversal, we have $[\hat{H},\hat{\Theta}]\neq\hat{0}$

((**Note**)) Suppose that there are N electrons. N is an even or an odd integer number.
We use $\eta=1$.

$$|\Phi\rangle = u_1|+\rangle_1|+\rangle_2|+\rangle_3|+\rangle_4....|+\rangle_{N-1}|+\rangle_N + u_2|+\rangle_1|+\rangle_2|+\rangle_3|+\rangle_4.....|+\rangle_{N-1}|-\rangle_N$$
$$+ u_3|+\rangle_1|+\rangle_2|+\rangle_3|+\rangle_4....|-\rangle_{N-1}|-\rangle_N + ... + u_{2^N}|-\rangle_1|-\rangle_2|-\rangle_3|-\rangle_4....|-\rangle_{N-1}|-\rangle_N$$

$$-i\hat{\sigma}_y\hat{K}|+\rangle = |-\rangle,$$

and

$$-i\hat{\sigma}_y\hat{K}|-\rangle = -|+\rangle$$

$$\langle\Phi|\tilde{\Phi}\rangle = u_1^*(-1)^N u_{2^N}{}^* + u_1^* u_{2^N}{}^*$$

When N is odd, $\langle\Phi|\tilde{\Phi}\rangle = 0$.

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