Time reversal operator
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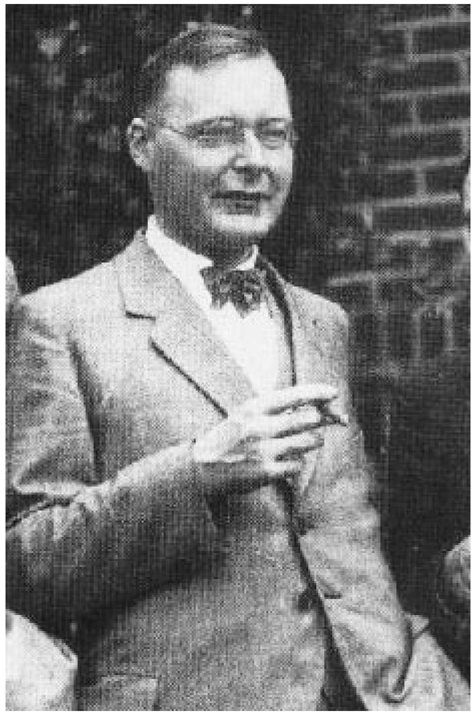
If a movie film is run backwards, all movement reversed can be seen: a falling stone will be replaced by a stone projected upwards. This is true because Newton's equation of motion in a uniform gravitational field is unchanged when the time t is replaced by $-t$. However, in the Schrödinger picture of quantum mechanics, the simple time inversion operator $t \rightarrow -t$ also changes the sign of the energy, because the energy operator is given by $i\hbar(\partial / \partial t)$. Thus in quantum mechanics, the time inversion operation has a much more drastic effect than simply reversing the motion. Since the idea of reversing the motion is perfectly sensible in classical mechanics, i.e., one which reverses directions of motion but does not change the sign of the energy. Here we construct such an operation, called time-reversal and denoted by $\hat{\Theta}$. It will turn out that $\hat{\Theta}$ is a very unusual operator, being non-linear.

$$\hat{\Theta} = \hat{U}\hat{K} \qquad (\hat{U} \text{ and } \hat{K} \text{ decomposition})$$

where $\hat{\Theta}$ is an anti-unitary operator, $\hat{U}$ is the unitary operator, and $\hat{K}$ is the complex conjugate operator.

H.A. Kramers
Hendrik Anthony "Hans" Kramers (2 February 1894 – 24 April 1952) was a Dutch physicist who worked with Niels Bohr to understand how electromagnetic waves interact with matter.



https://en.wikipedia.org/wiki/Hans_Kramers

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1. Classical mechanics

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:

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

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.

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 $\boldsymbol{F} = m\boldsymbol{a}$ 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.

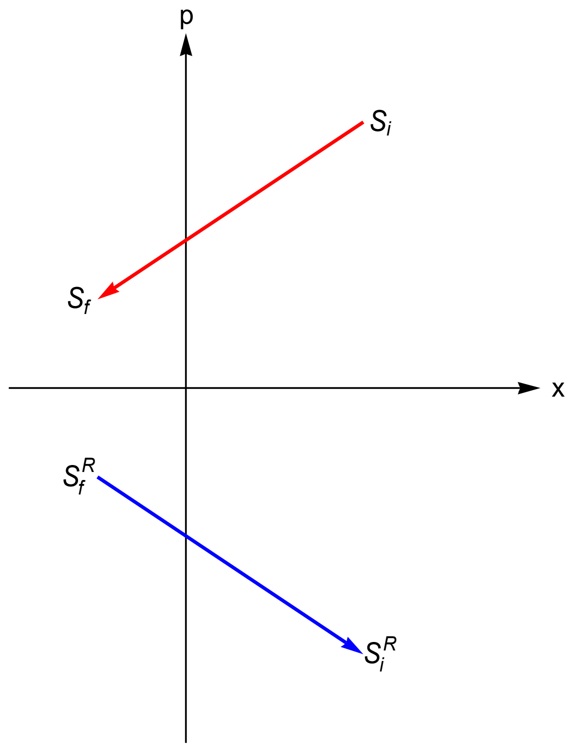


Fig. The mapping $S \rightarrow S_R$ in the phase space (x, p) for a reversible system.

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.

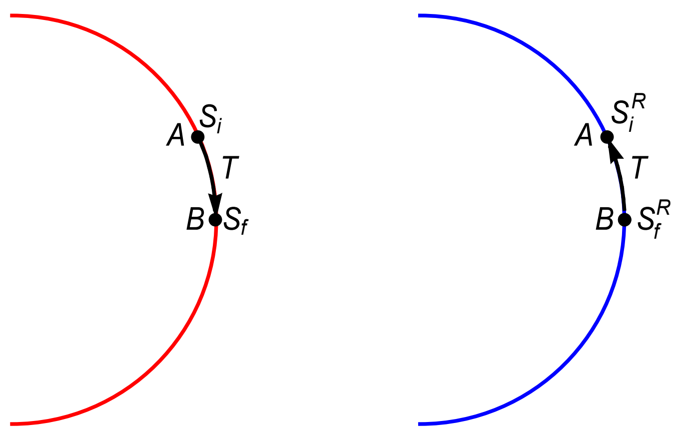


Fig. Classical trajectory of a particle undergoing the circular motion.

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.

$$\{u,v\} = \sum_i \left(\frac{\partial u}{\partial q_i}\frac{\partial v}{\partial p_i} - \frac{\partial u}{\partial p_i}\frac{\partial v}{\partial q_i}\right)$$

((**Proof**))

$$\begin{aligned}\frac{dQ}{dt} &= \sum_i \left(\frac{\partial Q}{\partial q_i}\dot{q}_i + \frac{\partial Q}{\partial p_i}\dot{p}_i\right)\\ &= \sum_i \left(\frac{\partial Q}{\partial q_i}\frac{\partial H}{\partial p_i} - \frac{\partial Q}{\partial p_i}\frac{\partial H}{\partial q_i}\right)\\ &= \{Q,H\}\end{aligned}$$

After an infinitesimal time *dt*, Q changes into Q',

$$Q' = Q + \{Q,H\}dt$$

Time-reversal invariance requires Q'^R to be changed into Q^R after time *dt*.

$$\begin{aligned}Q^R &= Q'^R + \{Q'^R, H\}dt\\ &= Q^R + \{Q,H\}^R dt + \{Q'^R, H\}dt\\ &= Q^R + \{Q,H\}^R dt + \{Q^R + \{Q,H\}^R dt, H\}dt\\ &= Q^R + \{Q,H\}^R dt + \{Q^R, H\}dt + O(dt)^2\end{aligned}$$

Then we have

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

((**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

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

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

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

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

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

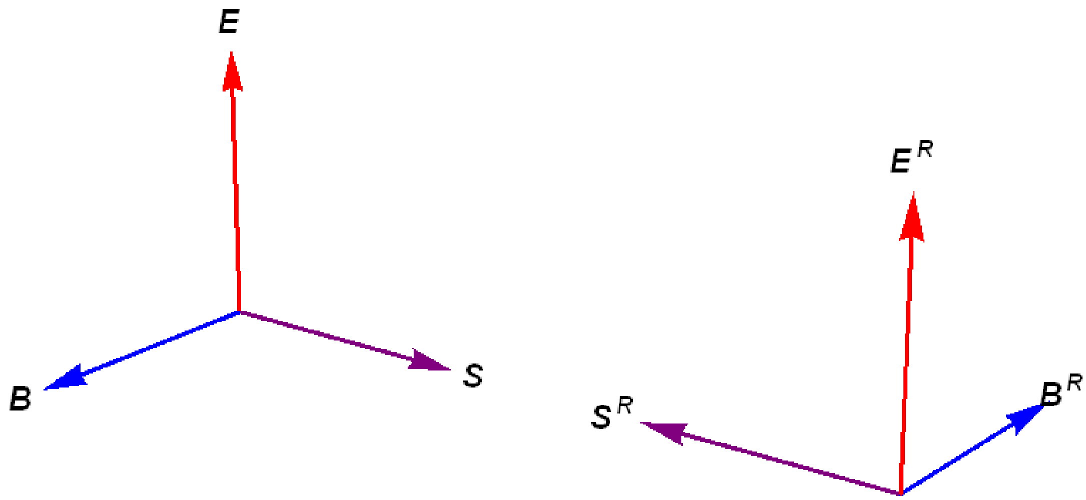
(iv) The poynting vector *S*

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

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

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

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

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

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

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

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

$$\psi^R(\boldsymbol{r},t) = \psi^*(\boldsymbol{r},-t)$$

$$\psi^R(\boldsymbol{r},t) = \langle r|\hat{\Theta}|\psi(-t)\rangle = \Theta\,\psi(\boldsymbol{r},-t) = \langle \boldsymbol{r}|\psi(-t)\rangle^*$$

where $\hat{\Theta}$ is the time reversal operator and Θ is the same operator in the $|\boldsymbol{r}\rangle$ representation.

If we consider a stationary state,

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

and

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

Then we have

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

or

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

When $t = 0$, we have

$$\psi^R(\boldsymbol{r},0) = \Theta\psi(\boldsymbol{r},0) = \psi^*(\boldsymbol{r},0)$$

((**Example-1**)) **Plane wave**

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

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

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

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

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

((**Example-2**)) $\hat{\Theta}i\hat{\Theta}^{-1} = -i\hat{1}$

Using the formula

$$\psi^R(\boldsymbol{r},0) = \Theta\psi(\boldsymbol{r},0) = \psi^*(\boldsymbol{r},0),$$

with the change of $\psi(\boldsymbol{r},0) \to i\psi(\boldsymbol{r},0)$, we get

$$\Theta[i\psi(\boldsymbol{r},0)] = [i\psi(\boldsymbol{r},0)]^* = -i\psi^*(\boldsymbol{r},0) = -i\Theta\psi(\boldsymbol{r},0),$$

For arbitrary wavefunction $\psi(\boldsymbol{r},0)$, we have

$$\Theta i = -i\Theta$$

or

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

In the operator in the quantum mechanics, this can be rewritten as

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

6. Quantum mechanical expression: analogy from classical mechanics

Time reversal is really just reversal of motion. Under time reversal

$$\langle \hat{x} \rangle' = \langle \hat{x} \rangle, \qquad \langle \hat{p} \rangle' = -\langle \hat{p} \rangle$$

and we also switch initial and final states. Imagine taking a movie of some process and then playing the movie backwards. Does the motion in the backward played movie obey the laws of physics? If yes, then the process is invariant under time reversal. If not, then it is non-invariant under time reversal.

In particular, setting t = 0,

$$\left|\psi^R(0)\right\rangle = \hat{\Theta}\left|\psi(0)\right\rangle, \qquad \text{or} \qquad \left|\psi^R\right\rangle = \hat{\Theta}\left|\psi\right\rangle$$

we see that $\hat{\Theta}$ maps the initial conditions of the original motion into the initial conditions of the time-reversed motion.

(a)

We start with the definition

$$\left|\psi^R(t=0)\right\rangle = \hat{\Theta}\left|\psi(t=0)\right\rangle$$

The analogy from the classical mechanics shows that

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

In quantum mechanics, this can be rewritten as

$$\langle \psi^R(t=0)|\hat{\boldsymbol{r}}|\psi^R(t=0)\rangle = \langle \psi(t=0)|\hat{\boldsymbol{r}}|\psi(t=0)\rangle$$

or

$$\langle \psi(t=0)|\hat{\boldsymbol{r}}|\psi^R(t=0)\rangle = \langle \psi(t=0)|\hat{\Theta}^+\hat{\boldsymbol{r}}\hat{\Theta}|\psi(t=0)\rangle = \langle \psi(t=0)|\hat{\boldsymbol{r}}|\psi(t=0)\rangle$$

where

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

Then we have

$$\hat{\Theta}^+\hat{\boldsymbol{r}}\hat{\Theta} = \hat{\boldsymbol{r}}, \qquad \hat{\Theta}\hat{\boldsymbol{r}}\hat{\Theta}^{-1} = \hat{\boldsymbol{r}}, \qquad \hat{\Theta}\hat{\boldsymbol{r}} = \hat{\boldsymbol{r}}\hat{\Theta}$$

We also get the similar expression for $\hat{\boldsymbol{p}}$,

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

from the analogy of classical mechanics, $\boldsymbol{p}^R = -\boldsymbol{p}$

(b)
Since

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

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

$\hat{\Theta}|\boldsymbol{r}'\rangle$ is the eigenket of $\hat{\boldsymbol{r}}$ with the eigenvalue $\boldsymbol{r}'$, leading to the expression

$$\hat{\Theta}|\boldsymbol{r}'\rangle = |\boldsymbol{r}'\rangle,$$

$\hat{\Theta}|\boldsymbol{p}'\rangle$ is the eigenket of $\hat{\boldsymbol{p}}$ with the eigenvalue $\boldsymbol{p}'$, leading to the expression

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

7. Wigner's time reversal transformation

We start with Schrödinger equation given by

$$i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = \hat{H}|\psi(t)\rangle \qquad (1)$$

where $\hat{H}$ is the Hamiltonian given by

$$\hat{H} = \frac{1}{2m}\hat{\boldsymbol{p}}^2 + V(\hat{\boldsymbol{r}})$$

where

$$[H, \hat{\Theta}] = 0, \qquad \text{or} \qquad \hat{\Theta}\hat{H}\hat{\Theta}^{-1} = \hat{H}$$

since

$$\hat{\Theta}\hat{\boldsymbol{p}}\hat{\Theta}^{-1} = -\hat{\boldsymbol{p}}, \qquad \hat{\Theta}\hat{\boldsymbol{r}}\hat{\Theta}^{-1} = \hat{\boldsymbol{r}}$$

The application of the operator $\hat{\Theta}$ to both sides of the Schrödinger equation gives

$$\hat{\Theta}i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = \hat{\Theta}\hat{H}|\psi(t)\rangle$$

or

$$\hbar\hat{\Theta}i\hat{\Theta}^{-1}\hat{\Theta}\frac{\partial}{\partial t}|\psi(t)\rangle = \hat{H}\hat{\Theta}|\psi(t)\rangle$$

or

$$-i\hbar\frac{\partial}{\partial t}\hat{\Theta}|\psi(t)\rangle = \hat{H}\hat{\Theta}|\psi(t)\rangle \tag{2}$$

If we change *t* into –*t* in Eq.(2),

$$i\hbar\frac{\partial}{\partial t}\Theta|\psi(-t)\rangle = \hat{H}\Theta|\psi(-t)\rangle \tag{3}$$

which satisfies the original Schrödinger equation. On the time-reversal $t \rightarrow t' = -t$, the state vector changes into a new state defined by

$$|\psi^R(t)\rangle = \hat{\Theta}|\psi(-t)\rangle$$

or

$$\langle \boldsymbol{r} | \psi^R(t) \rangle = \langle \boldsymbol{r} | \hat{\Theta} | \psi(-t) \rangle$$
$$= \Theta \langle \boldsymbol{r} | \psi(-t) \rangle$$
$$= \langle \boldsymbol{r} | \psi(-t) \rangle^*$$

or

$$\langle \boldsymbol{r} | \psi^R(t) \rangle = \langle \boldsymbol{r} | \psi(-t) \rangle^*$$

Here we note that

$$|\psi(-t)\rangle = \int d\boldsymbol{r}' |\boldsymbol{r}'\rangle \langle \boldsymbol{r}' | \psi(-t) \rangle$$

$$\hat{\Theta} |\psi(-t)\rangle = \int d\boldsymbol{r}' \langle \boldsymbol{r}' | \psi(-t) \rangle^* \hat{\Theta} |\boldsymbol{r}'\rangle$$
$$= \int d\boldsymbol{r}' |\boldsymbol{r}'\rangle \langle \boldsymbol{r}' | \psi(-t) \rangle^*$$

$$\langle \boldsymbol{r} | \hat{\Theta} | \psi(-t) \rangle = \int d\boldsymbol{r}' \langle \boldsymbol{r}' | \psi(-t) \rangle^* \hat{\Theta} |\boldsymbol{r}'\rangle$$
$$= \langle \boldsymbol{r} | \psi(-t) \rangle^*$$

8. The wave function at $t = 0$

At $t = 0$, we have the relation

$$\langle \boldsymbol{r} | \hat{\Theta} | \psi \rangle = \langle \boldsymbol{r} | \psi \rangle^*$$

Here we note that

$$|\psi\rangle = \int d\boldsymbol{r}' |\boldsymbol{r}'\rangle \langle \boldsymbol{r}' | \psi \rangle$$

$$\hat{\Theta} |\psi\rangle = \int d\boldsymbol{r}' \langle \boldsymbol{r}' | \psi \rangle^* \hat{\Theta} |\boldsymbol{r}'\rangle = \int d\boldsymbol{r}' |\boldsymbol{r}'\rangle \langle \boldsymbol{r}' | \psi \rangle^*$$

$$\langle \boldsymbol{r} | \hat{\Theta} | \psi \rangle = \int d\boldsymbol{r}' \langle \boldsymbol{r} | \boldsymbol{r}' \rangle \langle \boldsymbol{r}' | \psi \rangle^* = \langle \boldsymbol{r} | \psi \rangle^*$$

since

$$\hat{\Theta}(c|\boldsymbol{r}'\rangle) = c^* \hat{\Theta} |\boldsymbol{r}'\rangle = c^* |\boldsymbol{r}'\rangle$$

and

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

where $\hat{\Theta}$ is the anti-unitary operator,

$$\hat{\Theta} = \hat{U}\hat{K}, \qquad \hat{\Theta}(c|\boldsymbol{r}'\rangle) = \hat{U}\hat{K}(c|\boldsymbol{r}'\rangle) = c^*\hat{U}\hat{K}(|\boldsymbol{r}'\rangle) = c^*\hat{\Theta}|\boldsymbol{r}'\rangle$$

$$\hat{K}c\hat{K}^{-1} = c^*\hat{1},$$

where c is a complex number. $\hat{K}$ (the complex conjugate operator) is an operator which takes any complex number into its conjugate complex.

$$\hat{K}^{-1} = \hat{K}.$$

$\hat{\Theta} = \hat{U}\hat{K}$: $\hat{U}$ and $\hat{K}$ decomposition.

((**Note**)) $\langle \boldsymbol{p}|\hat{\Theta}|\psi\rangle = \langle -\boldsymbol{p}|\psi\rangle^*$

We also note that

$$|\psi\rangle = \int d\boldsymbol{p}'|\boldsymbol{p}'\rangle\langle \boldsymbol{p}'|\psi\rangle$$

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

$$\langle \boldsymbol{p}|\hat{\Theta}|\psi\rangle = \int d\boldsymbol{p}'\langle \boldsymbol{p}|\boldsymbol{p}'\rangle\langle -\boldsymbol{p}'|\psi\rangle^* = \langle -\boldsymbol{p}|\psi\rangle^*$$

since

$$\hat{\Theta}(c|\boldsymbol{p}'\rangle) = c^*\hat{\Theta}|\boldsymbol{p}'\rangle = c^*|-\boldsymbol{p}'\rangle$$

and

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

9. Property of the state vector under the time

$$\psi(\boldsymbol{r},t) = \langle \boldsymbol{r}|\exp(-\frac{i}{\hbar}\hat{H}t)|\psi(0)\rangle$$

$$\psi^R(r,t) = \psi^*(\boldsymbol{r},-t) = \langle \boldsymbol{r}|\exp(\frac{i}{\hbar}\hat{H}t)|\psi(0)\rangle^* = \langle\psi(0)|\exp(-\frac{i}{\hbar}\hat{H}t)|\boldsymbol{r}\rangle$$

We show that

$$\langle\tilde{\phi}(0)|\tilde{\psi}(0)\rangle = \langle\psi(0)|\phi(0)\rangle$$

$$|\tilde{\phi}(0)\rangle = |\phi^R\rangle, \qquad |\hat{\psi}(0)\rangle = |\psi^R\rangle$$

((**Proof**))

$$|\tilde{\psi}(0)\rangle = \Theta|\psi(0)\rangle = \Theta\sum_n |n\rangle\langle n|\psi(0)\rangle = \sum_n \hat{U}|n\rangle\langle n|\psi(0)\rangle^* = \sum_n \hat{U}|n\rangle\langle\psi(0)|n\rangle$$

$$|\tilde{\phi}(0)\rangle = \Theta|\phi(0)\rangle = \Theta\sum_m |m\rangle\langle m|\phi(0)\rangle = \sum_m \hat{U}|m\rangle\langle m|\phi(0)\rangle^* = \sum_n \hat{U}|m\rangle\langle\phi(0)|m\rangle$$

$$\langle\tilde{\phi}(0)| = \sum_n \langle\phi|m\rangle^*\langle m|\hat{U}^+$$

$$\begin{aligned}
\langle\tilde{\phi}(0)|\tilde{\psi}(0)\rangle &= \sum_{m,n}\langle\phi(0)|m\rangle^*\langle m|\hat{U}^+\hat{U}|n\rangle\langle\psi|n(0)\rangle \\
&= \sum_{m,n}\langle\phi(0)|m\rangle^*\delta_{m,n}\langle\psi(0)|n\rangle \\
&= \sum_n \langle\phi(0)|n\rangle^*\langle\psi(0)|n\rangle \\
&= \sum_n \langle\psi(0)|n\rangle\langle n|\phi(0)\rangle \\
&= \langle\psi(0)|\phi(0)\rangle
\end{aligned}$$

where

$$\hat{\Theta} = \hat{U}\hat{K}, \qquad \hat{\Theta}^{-1} = \hat{K}\hat{U}^+.$$

10. Note (Sakurai and Napolitano)

We mentioned earlier that it is best to avoid an anti-unitary operator acting on bras from the right. Nevertheless, we may use

$$\langle\beta|\hat{\Theta}|\alpha\rangle$$

which is to be understood always as

$$\left(\langle\beta|\right)\left(\hat{\Theta}|\alpha\rangle\right)$$

and never as

$$\left(\langle\beta|\hat{\Theta}\right)\left(|\alpha\rangle\right)$$

11. Time reversed state vector $|\psi^R(t)\rangle$

We apply the time reversal operator to the time-evolution operator $\hat{U}_T = \exp(-\frac{i}{\hbar}\hat{H}t)$.

$$|\psi(t)\rangle = \hat{U}_T(t)|\psi(0)\rangle = \exp(-\frac{i}{\hbar}\hat{H}t)|\psi(0)\rangle$$

where $\hat{U}_T(t) = \exp(-\frac{i}{\hbar}\hat{H}t)$ is the time evolution operator. The time reversed state vector is given by

$$\begin{aligned}
|\psi^R(t)\rangle &= \hat{\Theta}|\psi(-t)\rangle \\
&= \hat{\Theta}\hat{U}(-t)|\psi(0)\rangle \\
&= \hat{\Theta}\exp(\frac{i}{\hbar}\hat{H}t)\hat{\Theta}^{-1}\hat{\Theta}|\psi(0)\rangle \\
&= \exp(\hat{\Theta}\frac{i}{\hbar}\hat{H}t\hat{\Theta}^{-1})\hat{\Theta}|\psi(0)\rangle \\
&= \exp[\frac{t}{\hbar}\hat{\Theta}i\hat{H}\hat{\Theta}^{-1}]\hat{\Theta}|\psi(0)\rangle \\
&= \exp[\frac{t}{\hbar}\hat{\Theta}i\hat{\Theta}^{-1}\hat{\Theta}\hat{H}\hat{\Theta}^{-1}]\hat{\Theta}|\psi(0)\rangle \\
&= \exp(-\frac{i}{\hbar}\hat{H}t)\hat{\Theta}|\psi(0)\rangle \\
&= \hat{U}(t)\hat{\Theta}|\psi(0)\rangle
\end{aligned}$$

where

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

Then we have

$$|\psi^R(t)\rangle = \hat{\Theta}|\psi(-t)\rangle = \exp(-\frac{i}{\hbar}\hat{H}t)\hat{\Theta}|\psi(0)\rangle = \hat{U}(t)\hat{\Theta}|\psi(0)\rangle$$

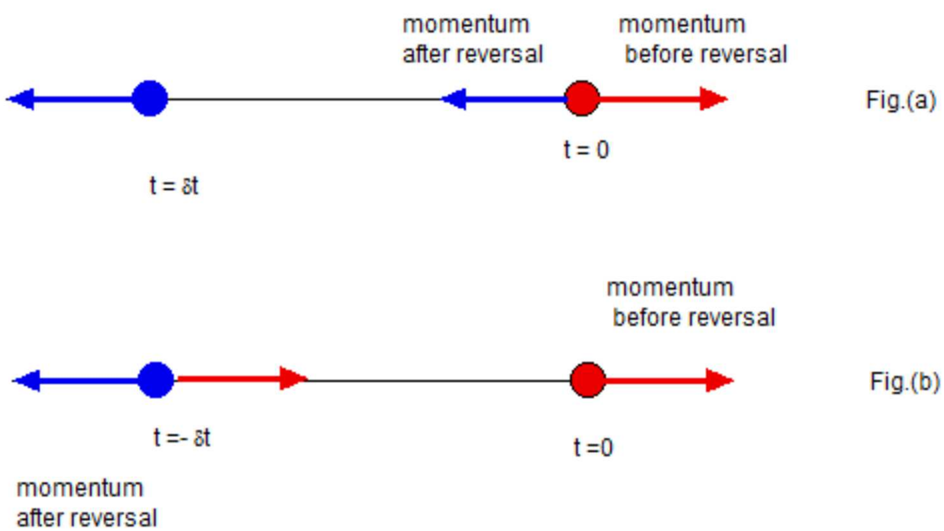
We note that

$$\begin{aligned}
\hat{\Theta}|\psi(-t)\rangle &= \hat{\Theta}\int d\boldsymbol{r}'|\boldsymbol{r}'\rangle\langle\boldsymbol{r}'|\psi(-t)\rangle \\
&= \int d\boldsymbol{r}'\Theta|\boldsymbol{r}'\rangle\langle\boldsymbol{r}'|\psi(-t)\rangle^* \\
&= \int d\boldsymbol{r}'|\boldsymbol{r}'\rangle\langle\boldsymbol{r}'|\psi(-t)\rangle^*
\end{aligned}$$

and

$$\langle\boldsymbol{r}|\hat{\Theta}|\psi(-t)\rangle = \langle\boldsymbol{r}|\psi(-t)\rangle^*$$

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



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

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

or

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

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

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

Using the property

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

we get

$$\begin{aligned}\hat{\Theta}i\hat{H} &= \hat{\Theta}i\hat{\Theta}^{-1}\hat{\Theta}\hat{H} \\ &= -i\hat{\Theta}H\end{aligned}$$

Then we have

$$\hat{H}\hat{\Theta} = \hat{\Theta}\hat{H} , \qquad \text{or} \qquad [\hat{H},\hat{\Theta}] = 0$$

((**Example**))

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

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

Thus $\hat{\Theta}|n\rangle$ is also the eigenket of $\hat{H}$ with the eigenvalue E_n (degenerate state)

13. Orbital angular momentum operator

We now consider the time-reversal for the spherical harmonics given by

$$\langle \boldsymbol{n}|l,m\rangle = Y_l^m(\theta,\phi) ,$$

Using the formula

$$\langle \boldsymbol{r}|\hat{\Theta}|\psi\rangle = \langle \boldsymbol{r}|\psi\rangle^* ,$$

we get the relation

$$\langle \boldsymbol{n}|\Theta|l,m\rangle = \langle \boldsymbol{n}|l,m\rangle^* = Y_l^m(\theta,\phi)^* = (-1)^m Y_l^{-m}(\theta,\phi),$$

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

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

This means that

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

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

and

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

We also have

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

or

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

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

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

14. Angular momentum $\hat{\boldsymbol{J}}$ and rotation oiperator $\hat{R}$

$\hat{\boldsymbol{L}}$ 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.

The operator $\hat{\Theta}$ anti-commutes with the component of the total angular momentum $\hat{\boldsymbol{J}}$ as

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

Consequently it commutes with the rotation operator $\hat{R} = \exp[-\frac{i}{\hbar}\varphi(\hat{\boldsymbol{J}}\cdot\boldsymbol{n})]$

$$\hat{\Theta}\hat{R}\hat{\Theta}^{-1} = \hat{R}, \qquad \text{or} \qquad \hat{R}\hat{\Theta} = \hat{\Theta}\hat{R}$$

since

$$\begin{aligned}
\hat{\Theta}\hat{R}\hat{\Theta}^{-1} &= \hat{\Theta}\exp[-\frac{i}{\hbar}\varphi(\hat{\boldsymbol{J}}\cdot\boldsymbol{n})]\hat{\Theta}^{-1} \\
&= \exp[-\frac{1}{\hbar}\varphi\hat{\Theta}i(\hat{\boldsymbol{J}}\cdot\boldsymbol{n})\hat{\Theta}^{-1}] \\
&= \exp[-\frac{1}{\hbar}\varphi(\hat{\Theta}i\hat{\Theta}^{-1})\hat{\Theta}(\hat{\boldsymbol{J}}\cdot\boldsymbol{n})\hat{\Theta}^{-1}] \\
&= \exp[-\frac{1}{\hbar}\varphi(-i)(-\hat{\boldsymbol{J}}\cdot\boldsymbol{n})\hat{\Theta}^{-1}] \\
&= \exp[-\frac{i}{\hbar}\varphi(\hat{\boldsymbol{J}}\cdot\boldsymbol{n})]
\end{aligned}$$

15. 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 (-***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 ($\boldsymbol{r}$).

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

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

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

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

and

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

17. Commutation relation $[\hat{J}_x, \hat{J}_y] = i\hbar\hat{J}_z$

$$\begin{aligned}\hat{\Theta}[\hat{J}_x, \hat{J}_y]\hat{\Theta}^{-1} &= \hat{\Theta}\hat{J}_x\hat{\Theta}^{-1}\hat{\Theta}\hat{J}_y\hat{\Theta}^{-1} - \hat{\Theta}\hat{J}_y\hat{\Theta}^{-1}\hat{\Theta}\hat{J}_x\hat{\Theta}^{-1} \\ &= (-\hat{J}_x)(-\hat{J}_y) - (-\hat{J}_y)(-\hat{J}_x) \\ &= [\hat{J}_x, \hat{J}_y] \\ &= i\hbar\hat{J}_z\end{aligned}$$

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

So we should expect that $\hat{J}$ transforms just as *i* does, which changes sign under the time reversal

18. Even and odd under the time reversal

$$\langle\tilde{\alpha}|\hat{\Theta}\hat{A}\hat{\Theta}^{-1}|\tilde{\alpha}\rangle = \langle\alpha|\hat{A}|\alpha\rangle \qquad (\hat{A} \text{ is Hermite operator})$$

When

$$\hat{\Theta}\hat{A}\hat{\Theta}^{-1} = \pm\hat{A} \quad \text{[plus (+); even and minus (-): odd)]}$$

we get

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

which means that

$$\langle\hat{A}\rangle' = \pm\langle\hat{A}\rangle$$

The expectation value taken with respect to the time-reversed state.

((**Note**))

$\hat{\Theta}\hat{A}\hat{\Theta}^{-1} = \hat{A}$: the observable $\hat{A}$ is even under the time reversal symmetry.

$\hat{\Theta}\hat{A}\hat{\Theta}^{-1} = -\hat{A}$: the observable $\hat{A}$ is odd under the time reversal symmetry.

(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

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

since

$$\begin{aligned}
\hat{\Theta}\hat{T}_x(a)\hat{\Theta}^{-1} &= \hat{\Theta}\exp(-\frac{i}{\hbar}\hat{p}a)\hat{\Theta}^{-1} \\
&= \exp[-\frac{1}{\hbar}a\hat{\Theta}i\hat{p}\hat{\Theta}^{-1}] \\
&= \exp[-\frac{1}{\hbar}a(\hat{\Theta}i\hat{\Theta}^{-1})(\hat{\Theta}\hat{p}\hat{\Theta}^{-1})] \\
&= \exp[-\frac{i}{\hbar}\hat{p}a] \\
&= \hat{T}_x(a)
\end{aligned}$$

From the above, we have

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

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

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

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

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

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

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

since

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

19. 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,

$$\langle\tilde{\beta}|\tilde{\alpha}\rangle = \langle\beta|\alpha\rangle^* = \langle\alpha|\beta\rangle \qquad \text{(fundamental property)}$$

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)

20. Property of $\hat{\Theta}$ (I)

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

Suppose that $|\beta\rangle = \hat{B}|\mu\rangle$. Then we have

$$|\tilde{\beta}\rangle = \hat{\Theta}|\beta\rangle = \hat{\Theta}\hat{B}|\mu\rangle = \hat{\Theta}\hat{B}\hat{\Theta}^{-1}\hat{\Theta}|\mu\rangle = \hat{\Theta}\hat{B}\hat{\Theta}^{-1}|\tilde{\mu}\rangle$$

The scalar product

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

21. Property of $\hat{\Theta}$ (II)

The time-reversal operator is expressed by

$$\hat{\Theta} = \hat{U}\hat{K} \qquad (\hat{U} \text{ and } \hat{K} \text{ decomposition})$$

where $\hat{U}$ is the unitary operator and $\hat{K}$ is the complex-conjugate operator that forms the complex conjugate of any coefficient that multiplies a ket.

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

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

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

22. The density operator and the expectation

One can then show that expectation operators must satisfy the identity

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

((**Proof**))

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

or

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

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

or

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

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

$$\langle\alpha|\hat{A}|\beta\rangle = \langle\tilde{\beta}|\hat{\Theta}\hat{A}\hat{\Theta}^{-1}|\tilde{\alpha}\rangle$$ ($\hat{A}$: Hermitian operator)

When we take the comple conjugate of Eq.(1), we get

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

or

$$\langle\beta|\hat{A}|\alpha\rangle=\langle\hat{\alpha}|(\hat{\Theta}\hat{A}\hat{\Theta}^{-1})^{+}|\beta\rangle \tag{2}$$

((Average of the operator $\hat{A}$ over the density operator $\hat{\rho}$))

If we look at the average of a Hermitian operator $\hat{A}$ over the density operator $\hat{\rho}$

$$\langle A\rangle=Tr[\hat{\rho}\hat{A}]=\sum_{n}\langle n|\hat{\rho}\hat{A}|n\rangle=\sum_{\tilde{n}}\langle\hat{n}|(\hat{\Theta}\hat{\rho}\hat{A}\hat{\Theta}^{-1})^{+}|\tilde{n}\rangle$$

Since the ket $|\tilde{n}\rangle$ is also complete,

$$\langle A\rangle=Tr(\hat{\Theta}\hat{\rho}\hat{A}\hat{\Theta}^{-1})^{+}=Tr(\hat{\Theta}\hat{\rho}\hat{\Theta}^{-1}\hat{\Theta}\hat{A}\hat{\Theta}^{-1})^{+}$$

If the density operator is invariant under the time reversal,

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

then we have

$$\langle A\rangle=Tr(\hat{\rho}\hat{\Theta}\hat{A}\hat{\Theta}^{-1})^{+}=Tr[(\hat{\Theta}\hat{A}\hat{\Theta}^{-1})^{+}\hat{\rho}^{+}]$$

Since the density operator is Hermitian operator ($\hat{\rho}^{+}=\hat{\rho}$),

$$\langle A\rangle=Tr[\hat{\rho}(\hat{\Theta}\hat{A}\hat{\Theta}^{-1})^{+}]=\langle(\hat{\Theta}\hat{A}\hat{\Theta}^{-1})^{+}\rangle.$$

23. Property of $\hat{\Theta}$ (IV)

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

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

where $\hat{A}$ is the Hermitian operator. Suppose that $\hat{\Theta}\hat{A}\hat{\Theta}^{-1}=\pm\hat{A}$

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

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.

21. Property of $\hat{\Theta}$ (V)

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

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

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

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

$$\hat{\Theta}[\hat{x}, \hat{p}]\hat{\Theta}^{-1} = -[\hat{x}, \hat{p}]$$

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

How about the commutation relation of the angular momentum?

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

$[\hat{L}_x, \hat{L}_y]$ is not Hermitian. using the formula $\langle\alpha|\hat{A}^+|\beta\rangle = \langle\tilde{\beta}|\hat{\Theta}\hat{A}\hat{\Theta}^{-1}|\tilde{\alpha}\rangle$

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

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

or

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

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

since

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

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. $\frac{\hat{\boldsymbol{p}}^2}{2m}$ 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

22. Property of $\hat{K}$ (I): $\hat{K}^2 = 1, \hat{K}^+\hat{K} = 1, \hat{K}^+ = \hat{K} = \hat{K}^{-1}$

We start from the following equation

$$\hat{K}|\psi\rangle = \hat{K}\sum_{\alpha'}|\alpha'\rangle\langle\alpha'|\psi\rangle = \sum_{\alpha'}|\alpha'\rangle\langle\alpha'|\psi\rangle^*$$

where

$$\sum_{\alpha'}|\alpha'\rangle\langle\alpha'| = \hat{1} \qquad \text{(closure relation)}$$

Then we get

$$\hat{K}^2|\psi\rangle = \hat{K}\hat{K}|\psi\rangle = \hat{K}\sum_{\alpha'}|\alpha'\rangle\langle\alpha'|\psi\rangle^* = \sum_{\alpha'}|\alpha'\rangle\langle\alpha'|\psi\rangle = |\psi\rangle$$

leading to the relation

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

We also have the relation

$$
\begin{aligned}
\langle\psi|\hat{K}^{+}\hat{K}|\psi\rangle &= (\sum_{\alpha'}\langle\alpha'|\psi\rangle\langle\alpha'|)(\sum_{\alpha''}|\alpha''\rangle\langle\alpha''|\psi\rangle^{*}) \\
&= \sum_{\alpha',\alpha''}\langle\psi|\alpha''\rangle\langle\alpha'|\psi\rangle\langle\alpha'|\alpha''\rangle \\
&= \sum_{\alpha'}\langle\psi|\alpha'\rangle\langle\alpha'|\psi\rangle \\
&= \langle\psi|\psi\rangle
\end{aligned}
.
$$

leading to the relation

$$\hat{K}^{+}\hat{K} = \hat{1},$$

since

$$\hat{K}|\psi\rangle = \hat{K}(\sum_{\alpha''}|\alpha''\rangle\langle\alpha''|\psi\rangle) = \sum_{\alpha''}|\alpha''\rangle\langle\alpha''|\psi\rangle^{*}$$

$$\langle\psi|\hat{K}^{+} = \sum_{\alpha''}\langle\alpha''|\langle\alpha''|\psi\rangle$$

In conclusion, we have

$$\hat{K}^{2} = 1, \qquad \hat{K}^{+}\hat{K} = 1, \qquad \hat{K}^{+} = \hat{K}^{-1} = \hat{K}.$$

23. Property of $\hat{K}$ (II): $\hat{K}c\hat{K} = c^{*}$

Here we use the formula

$$\hat{K}^{2} = \hat{1}.$$

For arbitrary state vector $|\psi\rangle$, we have

$$\hat{K}^{2}(c^{*}|\psi\rangle) = c^{*}|\psi\rangle$$

or

$$
\begin{aligned}
\hat{K}^{2}c^{*}|\psi\rangle &= \hat{K}\hat{K}c^{*}|\psi\rangle \\
&= \hat{K}cK|\psi\rangle
\end{aligned}
$$

Then we get the relation

$$\hat{K}c\hat{K} = c^*, \qquad \text{or} \qquad \hat{K}c\hat{K}^{-1} = c^*$$

24. Property of $\hat{K}$ (III): $\hat{K}\hat{A}\hat{K} = \hat{A}^*$

Suppose that $\hat{A}$ is an arbitrary operator. Then we get

$$\begin{aligned}
\hat{K}\hat{A}\hat{K}|\psi\rangle &= \hat{K}\hat{A}\hat{K}\sum_n |n\rangle\langle n|\psi\rangle \\
&= \hat{K}\sum_n \hat{A}|n\rangle\langle n|\psi\rangle^* \\
&= \hat{K}\sum_{n,m} |m\rangle\langle m|\hat{A}|n\rangle\langle n|\psi\rangle^* \\
&= \sum_{n,m} |m\rangle\langle m|\hat{A}|n\rangle^*\langle n|\psi\rangle
\end{aligned}$$

where $\langle n|m\rangle = \delta_{n,m}$. We note that

$$\hat{A}^+ = \left(\hat{A}^*\right)^T$$

or

$$\hat{A}^* = \left(\hat{A}^+\right)^T,$$

So we have

$$\langle n|\hat{A}^*|m\rangle = \langle n|\left(\hat{A}^+\right)^T|m\rangle = \langle m|\hat{A}^+|n\rangle$$

Then we get

$$\begin{aligned}
\hat{K}\hat{A}\hat{K}|\psi\rangle &= \sum_{n,m} |m\rangle\langle n|\hat{A}^+|m\rangle\langle n|\psi\rangle \\
&= \sum_{n,m} |m\rangle\langle m|\hat{A}^*|n\rangle\langle n|\psi\rangle \\
&= \hat{A}^*|\psi\rangle
\end{aligned}$$

or

$$\hat{K}\hat{A}\hat{K} = \hat{A}^*$$

where we use the closure relation.

25. Note on the property of $\hat{K}$

$$\hat{K}|\psi\rangle = \hat{K}\sum_n |n\rangle\langle n|\psi\rangle = \sum_n \hat{K}|n\rangle\langle n|\psi\rangle^*$$

We choose a basis that $\hat{K}|n\rangle = |n\rangle$. Then we get

$$\hat{K}|\psi\rangle = \sum_n |n\rangle\langle n|\psi\rangle^* .$$

Note that this definition is basis-dependent. But our definition of the time reversal operator is also basis-dependent, so the dependency actually cancels and there is no problem. In general, we can always write an anti-unitary operator in to the product of a unitary operator with $\hat{K}$;

26 Schrödinger equation for the time-reversed state (using operator)

We start with the Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}|\psi\rangle = \hat{H}|\psi\rangle$$

When $t \to t' = -t$, $\qquad |\psi\rangle \to |\psi^R\rangle$

$$i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = \hat{H}|\psi(t)\rangle, \qquad i\hbar\frac{\partial}{\partial t'}|\psi^R\rangle = \hat{H}|\psi^R\rangle$$

$$\hat{\Theta}i\hbar\hat{\Theta}^{-1}\hat{\Theta}\frac{\partial}{\partial t}\hat{\Theta}^{-1}\hat{\Theta}|\psi(t)\rangle = \hat{\Theta}\hat{H}\hat{\Theta}^{-1}\hat{\Theta}|\psi(t)\rangle$$

We use

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

$$\hat{U}(\hat{K}i\hbar\hat{K}^{-1})\hat{U}^{-1}\hat{U}\hat{K}\frac{\partial}{\partial t}\hat{K}^{-1}\hat{U}^{-1}\hat{U}\hat{K}|\psi(t)\rangle = \hat{\Theta}\hat{H}\hat{\Theta}^{-1}\hat{\Theta}|\psi(t)\rangle$$

Using the relations

$$\hat{K} i\hbar \hat{K}^{-1} = -i\hbar,$$

we get

$$-i\hbar \hat{U}\hat{U}^{-1}\hat{U}\hat{K}\frac{\partial}{\partial t}\hat{K}^{-1}\hat{U}^{-1}\hat{\Theta}|\psi(t)\rangle = \hat{\Theta}\hat{H}\hat{\Theta}^{-1}\hat{\Theta}|\psi(t)\rangle$$

or

$$-i\hbar \hat{U}\hat{K}\frac{\partial}{\partial t}\hat{K}^{-1}\hat{U}^{-1}\hat{\Theta}|\psi(t)\rangle = \hat{\Theta}\hat{H}\hat{\Theta}^{-1}\hat{\Theta}|\psi(t)\rangle$$

or

$$-i\hbar \frac{\partial}{\partial t}\hat{\Theta}|\psi(t)\rangle = \hat{\Theta}\hat{H}\hat{\Theta}^{-1}\hat{\Theta}|\psi(t)\rangle$$

$$i\hbar \frac{\partial}{\partial t'}\hat{\Theta}|\psi(-t')\rangle = \hat{\Theta}\hat{H}\hat{\Theta}^{-1}\hat{\Theta}|\psi(-t')\rangle$$

Using the relation

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

we have

$$i\hbar \frac{\partial}{\partial t'}\hat{\Theta}|\psi(-t')\rangle = \hat{H}\hat{\Theta}|\psi(-t')\rangle$$

Switching $t' \to t$

$$i\hbar \frac{\partial}{\partial t'}\hat{\Theta}|\psi(-t)\rangle = \hat{H}\hat{\Theta}|\psi(-t)\rangle$$

This means that the time-reversed state is defined by

$$|\psi^R(t)\rangle = \hat{\Theta}|\psi(-t)\rangle.$$

When t = 0,

$$\left|\psi^R\right\rangle = \hat{\Theta}\left|\psi(0)\right\rangle$$

27. Spin-less particle (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 $\left|\phi_n\right\rangle$ is nondegenerate. Then the corresponding energy eigenfunction is real (or more generally, a real function times a phase factor independent of ***r***).

((**Proof**))

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

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

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

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

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

We have

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

We note that

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

Then we have

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

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

28. Spin-less particle (II): Quenching of orbital angular momentum

Theorem: **quenching of orbital angular momentum**

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

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

((**Proof-1**))

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

since

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

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,

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

or

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

Therefore we have

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

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.

29. Real-space wave function at *t* = 0 of the time-reversal state

Real-space wave function of the time reverse state is obtained as follows.

$$\left|\tilde{\boldsymbol{r}}\right\rangle = \Theta\left|\boldsymbol{r}\right\rangle = \left|\boldsymbol{r}\right\rangle$$

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

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

from the definition. Since $\left\langle\hat{\boldsymbol{r}}\right| = \left\langle\boldsymbol{r}\right|$, we have

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

In summary, the real-space wave function of the time reversed state:

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

((Example))

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

30. Momentum-space wave function at *t* = 0 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.

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

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

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

Since

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

we have

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

When $\boldsymbol{k} \to -\boldsymbol{k}$, we have the momentum-space wave function of the time reversed state as

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

31. Degeneracy of Bloch states: $E(\boldsymbol{k}) = E(-\boldsymbol{k})$

We would expect the relation $E(\boldsymbol{k}) = E(-\boldsymbol{k})$ for the energy dispersion relation, to hold only when the direct (and hence the reciprocal) lattice admits of a center of inversion. A rather surprising result is that

$$E(\boldsymbol{k}) = E(-\boldsymbol{k})$$

always, whether or not the crystal is centro-symmetric.

We start with a Bloch eigenfunction (one-dimensional case), which is defined as

$$\psi_k(x) = e^{ikx} u_k(x)$$

and

$$H\psi_k(x) = E_k \psi_k(x)$$

where $u_{\boldsymbol{k}}(x)$ satisfies the periodic boundary condition.

$$u_k(x+a) = u_k(x)$$

$\psi_{\boldsymbol{k}}(x)$ is the energy eigenfunction of the Hamiltonian H with the energy.

$$\begin{aligned} T_x(a)\psi_k(x) &= T_x(a)[e^{ikx}u_k(x)] \\ &= e^{ik(x+a)}u_k(x+a) \\ &= e^{ika}e^{ikx}u_k(x) \\ &= e^{ika}\psi_k(x) \end{aligned}$$

where $T_x(a)$ is the translation operator. We now consider the time-reversed state at $t = 0$, which is defined as

$$\psi^R(x) = \psi_k^*(x) = e^{-ikx}u_k^*(x)$$

We note that

$$H^*\psi_k^*(x) = E_k^*\psi_k^*(x)$$

Both the Hamiltonian H and the energy eigenvlalue E_k are real. Thus we have

$$H\psi_k^*(x) = E_k\psi_k^*(x)$$

So it follows that $\psi_k(x)$ and $\psi_k^*(x)$ are wave functions with degenerate energy eigenvalue. Since

$$\begin{aligned} T_x(a)\psi_k^*(x) &= T_x(a)[e^{-ikx}u_k^*(x)] \\ &= e^{-ik(x+a)}u_k^*(x+a) \\ &= e^{-ika}e^{-ikx}u_k^*(x) \\ &= e^{-ika}\psi_k^*(x) \end{aligned}$$

The wave function $\psi_k^*(x)$ belongs to an eigenvalue with $-k$.

$$\psi_k^*(x) = \psi_{-k}(x).$$

while $\psi_k(x)$ belongs to an eigenvalue with k. Thus $\psi_k(x)$ and $\psi_k^*(x)$ are degenerate energy eigenstate with different k. The change of $k \rightarrow -k$ in the relation given by $H\psi_k(x) = E_k\psi_k(x)$ leads to

$$H\psi_{-k}(x) = E_{-k}\psi_{-k}(x), \qquad \text{or} \qquad H\psi_k^*(x) = E_{-k}\psi_k^*(x)$$

Then we have

$$E_{-\boldsymbol{k}} = E_{\boldsymbol{k}}.$$

So we can say that the property of $E_{-\boldsymbol{k}} = E_{\boldsymbol{k}}$ *can be derived from the time reversal property.*

((The relation, $E_{k+G} = E_k$**))**

This relation can be derived directly from the Bloch theorem.

From the Bloch theorem

$$\psi_k(x) = e^{ikx}u_k(x),$$

we get the relation

$$\psi_k(x+a) = e^{ika}\psi_k(x).$$

since

$$\psi_k(x+a) = e^{ik(x+a)}u_k(x+a) = e^{ika}e^{ikx}u_k(x) = e^{1ka}\psi_k(x)$$

We know that the reciprocal lattice G is defined by

$$G = \frac{2\pi}{a}n, \text{ } (n\text{: integer}).$$

When k is replaced by $k + G$,

$$\psi_{k+G}(x+a) = e^{i(k+G)a}\psi_{k+G}(x) = e^{ika}\psi_{k+G}(x),$$

since $e^{iGa} = e^{i2\pi n} = 1$. This implies that $\psi_{k+G}(x)$ is the same as $\psi_k(x)$.

$$\psi_{k+G}(x) = \psi_k(x).$$

or the energy eigenvalue of $\psi_{k+G}(x)$ is the same as that of $\psi_k(x)$,

$$E_{k+G} = E_k.$$

32. Wave function at $t = 0$ for the free particle; Symmetry of the energy dispersion with $E_{\boldsymbol{k}} = E_{-\boldsymbol{k}}$

We assume that

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

The energy eigenvalue problem

$$\hat{H}|\boldsymbol{k}\rangle = E_{\boldsymbol{k}}|\boldsymbol{k}\rangle$$

$$\hat{\Theta}\hat{H}|\boldsymbol{k}\rangle = \hat{\Theta}E_{\boldsymbol{k}}|\boldsymbol{k}\rangle$$

Then we have

$$\hat{\Theta}\hat{H}\hat{\Theta}^{-1}\hat{\Theta}|\boldsymbol{k}\rangle = \hat{\Theta}E_{\boldsymbol{k}}|\boldsymbol{k}\rangle$$

or

$$\hat{H}\hat{\Theta}|\boldsymbol{k}\rangle = E_{\boldsymbol{k}}\hat{\Theta}|\boldsymbol{k}\rangle$$

since $\hat{\Theta}\hat{H}\hat{\Theta}^{-1} = \hat{H}$. Here we note that

$$\hat{\Theta}|\boldsymbol{k}\rangle = |-\boldsymbol{k}\rangle$$

Then we have

$$\hat{H}|-\boldsymbol{k}\rangle = E_{\boldsymbol{k}}|-\boldsymbol{k}\rangle$$

When $\boldsymbol{k}$ is changed into $-\boldsymbol{k}$, we get

$$\hat{H}|\boldsymbol{k}\rangle = E_{-\boldsymbol{k}}|\boldsymbol{k}\rangle$$

leading to the property

$$E_{-\boldsymbol{k}} = E_{\boldsymbol{k}}.$$

33. Time reversal operator for spin 1/2 system (I)

We show that the time reversal operator for the spin 1/2 system is given by

$$\hat{\Theta} = -i\hat{\sigma}_y\hat{K}$$

((**Proof**))

$$\hat{\Theta}\hat{\sigma}_x\hat{\Theta}^{-1} = \hat{U}\hat{K}\hat{\sigma}_x\hat{K}^{-1}\hat{U}^+ = \hat{U}\hat{\sigma}_x{}^*\hat{U}^+ = \hat{U}\hat{\sigma}_x\hat{U}^+ = -\hat{\sigma}_x$$

$$\hat{\Theta}\hat{\sigma}_y\hat{\Theta}^{-1} = \hat{U}\hat{K}\hat{\sigma}_y\hat{K}^{-1}\hat{U}^+ = \hat{U}\hat{\sigma}_y{}^*\hat{U}^+ = -\hat{U}\hat{\sigma}_y\hat{U}^+ = -\hat{\sigma}_y$$

$$\hat{\Theta}\hat{\sigma}_z\hat{\Theta}^{-1} = \hat{U}\hat{K}\hat{\sigma}_z\hat{K}^{-1}\hat{U}^+ = \hat{U}\hat{\sigma}_z{}^*\hat{U}^+ = \hat{U}\hat{\sigma}_z\hat{U}^+ = \hat{\sigma}_z$$

or

$$\hat{U}\hat{\sigma}_x\hat{U}^+ = -\hat{\sigma}_x$$

$$\hat{U}\hat{\sigma}_y\hat{U}^+ = \hat{\sigma}_y$$

$$\hat{U}\hat{\sigma}_z\hat{U}^+ = \hat{\sigma}_z$$

We assume that the unitary operator is expressed by

$$\hat{U} = a\sigma_x + \beta\sigma_y + \gamma\sigma_z + \delta\hat{1}$$

where a, b, g, and d are complex numbers. Using the Mathematica, we find that

$$\hat{U} = \beta\sigma_y = -i\sigma_y$$

$$\hat{\Theta} = -i\sigma_y\hat{K}$$

Note that

$$\hat{\Theta}^2 = (-i\hat{\sigma}_y\hat{K})(-i\hat{\sigma}_y\hat{K}) = i\hat{\sigma}_y(\hat{K}i\hat{\sigma}_y\hat{K}) = i\hat{\sigma}_y(-i\hat{\sigma}_y{}^*) = \hat{\sigma}_y\hat{\sigma}_y{}^* = -\hat{1}$$

34. The time reversal operator for spin 1/2 system (II)

We show that $\hat{\Theta}$ for the spin 1/2 system is given by

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

We start with the relations

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

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

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

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

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

where η is a phase factor (a complex number of modulus unity). Similarly, we have

$$\hat{\Theta}\left|-z\right\rangle = \eta\left|+z\right\rangle.$$

In general, for the rotation operator $\hat{R} = \exp(-\frac{i}{\hbar}\hat{S}_z\phi)\exp(-\frac{i}{\hbar}\hat{S}_y\theta)$,

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

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

We note that

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

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

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

and

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

Thus we have

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

and

$$\begin{aligned}\hat{\Theta}\left|+\boldsymbol{n}\right\rangle &= \hat{\Theta}\hat{R}\left|+z\right\rangle \\ &= \hat{R}\hat{\Theta}\left|+z\right\rangle \\ &= \eta\hat{R}\left|-z\right\rangle \\ &= \eta\left|-\boldsymbol{n}\right\rangle\end{aligned}$$

Here we note that

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

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

where

$$\begin{aligned}\hat{R}_y(\theta) &= \exp(-\frac{1}{\hbar}\hat{S}_y\theta) \\ &= \exp(-i\hat{\sigma}_y\frac{\theta}{2}) \\ &= \cos\frac{\theta}{2}\hat{1} - i\hat{\sigma}_y\sin\frac{\theta}{2} \\ &= \begin{pmatrix}\cos\frac{\theta}{2} & -\sin\frac{\theta}{2} \\ \sin\frac{\theta}{2} & \cos\frac{\theta}{2}\end{pmatrix}\end{aligned}$$

Then

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

or

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

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

Therefore we have

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

with

$$\begin{aligned}\exp(-\frac{i}{\hbar}\hat{S}_y\pi) &= \exp(-\frac{i}{\hbar}\frac{\hbar}{2}\hat{\sigma}_y\pi) \\ &= \exp(-\frac{i}{2}\hat{\sigma}_y\pi) \\ &= -i\hat{\sigma}_y\end{aligned}$$

and

$$\exp(-i\hat{\sigma}_y\frac{\theta}{2}) = \begin{pmatrix} \cos\frac{\theta}{2} & -\sin\frac{\theta}{2} \\ \sin\frac{\theta}{2} & \cos\frac{\theta}{2} \end{pmatrix} = \hat{1}\cos\frac{\theta}{2} - i\sin\frac{\theta}{2}\hat{\sigma}_y$$

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

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

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

since

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

Let us apply $\hat{\Theta}$ to $\left|\psi\right\rangle$, again

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

or

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

This is an extraordinary result.

((**Note**))

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

We show that

$$\begin{aligned}\hat{\Theta}\hat{\sigma}_x\hat{\Theta}^{-1} &= -\hat{\sigma}_x, \\ \hat{\Theta}\hat{\sigma}_y\hat{\Theta}^{-1} &= -\hat{\sigma}_y \\ \hat{\Theta}\hat{\sigma}_z\hat{\Theta}^{-1} &= -\hat{\sigma}_z\end{aligned}$$

(a)

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

or

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

or

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

(b)

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

or

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

or

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

(c)

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

or

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

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).

35. 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

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

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

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 $|\psi\rangle$ ($|C|=1$), where C is a phase factor. When the replacement of $|\psi\rangle \rightarrow \hat{\Theta}|\psi\rangle$ is made in the above equation, we get

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

Then we have

$$C = C^*$$

So C is real.

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

36. Kramers' Degeneracy (I)

For $\hat{\Theta}^2 = -\hat{1}$, $|\psi\rangle$ and its time reversed state $\hat{\Theta}|\psi\rangle$) are orthogonal to each other.

((**Proof**))

We use the formula

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

where

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

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

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

Since $\hat{\Theta}^2|\psi\rangle = C|\psi\rangle$ with $C = \pm 1$

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

Then we have

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

and from definition

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

since $\langle \tilde{\beta} | = \langle \alpha |$. In the case C = -1,

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

showing that for such systems, time-reversed states ($|\psi\rangle$ and $|\alpha\rangle = \hat{\Theta}|\psi\rangle$) are orthogonal.

((Kramers' theorem))

As a corollary, if C = -1 and the Hamiltonian is invariant under time reversal, the energy eigenstates may be classified in degenerate time reversed pairs (Kramers doublet or Kramers degeneracy)

((**Proof**))

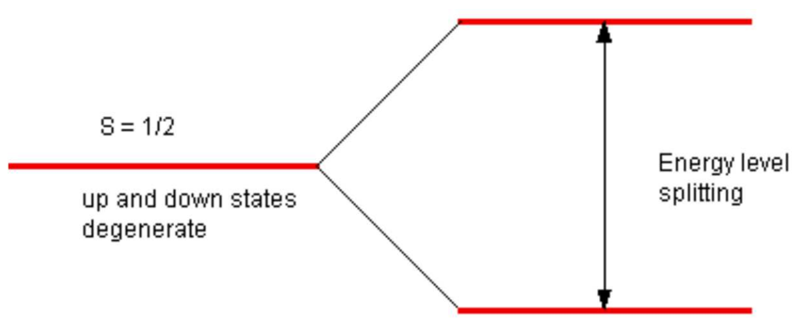
Since $\hat{H}$ is invariant under time reversal,

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

Let $|\phi_n\rangle$ and $|\tilde{\phi}_n\rangle = \hat{\Theta}|\phi_n\rangle$ 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 (degenerate states).



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 $\eta = 1$.

$$\begin{aligned}
\left|\Phi\right\rangle = & u_1\left|+z\right\rangle_1\left|+z\right\rangle_2\left|+z\right\rangle_3\left|+z\right\rangle_4....\left|+z\right\rangle_{N-1}\left|+z\right\rangle_N \\
& + u_2\left|+z\right\rangle_1\left|+z\right\rangle_2\left|+z\right\rangle_3\left|+z\right\rangle_4.....\left|+z\right\rangle_{N-1}\left|-z\right\rangle_N \\
& + u_3\left|+z\right\rangle_1\left|+z\right\rangle_2\left|+z\right\rangle_3\left|+z\right\rangle_4....\left|z\right\rangle_{N-1}\left|-z\right\rangle_N + \\
& \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \\
& + u_{N-1}\left|+z\right\rangle_1\left|-z\right\rangle_2\left|-z\right\rangle_3\left|-z\right\rangle_4....\left|-z\right\rangle_{N-1}\left|-z\right\rangle_N \\
& + u_N\left|-z\right\rangle_1\left|-z\right\rangle_2\left|-z\right\rangle_3\left|-z\right\rangle_4....\left|-z\right\rangle_{N-1}\left|-z\right\rangle_N
\end{aligned}$$

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

and

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

$$\left\langle\Phi\middle|\widetilde{\Phi}\right\rangle = u_1^* u_{2^N}{}^*[1+(-1)^N]$$

When N is odd, $\left\langle\Phi\middle|\widetilde{\Phi}\right\rangle = 0$.

37. Kramers degeneracy (II)

We use this formula

$$\left\langle\phi\middle|\psi\right\rangle = \left\langle\widetilde{\psi}\middle|\widetilde{\phi}\right\rangle$$

Suppose that

$$\left|\phi\right\rangle = \hat{\Theta}\left|\psi\right\rangle = \left|\widetilde{\psi}\right\rangle, \qquad \left|\widetilde{\phi}\right\rangle = \hat{\Theta}^2\left|\psi\right\rangle$$

Then we get

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

For $\hat{\Theta}^2 = -\hat{1}$, we get

$$\langle\tilde{\psi}|\psi\rangle = -\langle\tilde{\psi}|\psi\rangle = 0$$

Thus, for odd system, the time reversal converts a state $|\psi\rangle$ into an independent state. This is the basis for the Kramers' degeneracy.

All energy levels of s system containing an odd number of electrons must be at least doubly degenerate regardless of how low the symmetry is, provided that there are no magnetic fields present to remove the time-reversal symmetry. This theorem follows from the fact that, if

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

then $\hat{\Theta}|\psi\rangle$ is orthogonal to $|\psi\rangle$.

38. Physical explanation of the Kramers theorem (III)

Under the time reversal procedure, the spin state changes from $|\pm z\rangle$ to $|\mp z\rangle$.

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

The spin Hamiltonian is invariant under the time reversal.

$$\hat{H}\hat{\Theta} = \hat{\Theta}\hat{H}, \quad \text{or} \quad \hat{\Theta}\hat{H}\hat{\Theta}^{-1} = \hat{H}$$

Then the energy of the reversed spin state is the same as that of the original spin state before the time reversal. Since

$$\hat{S}_z|+z\rangle = \frac{\hbar}{2}|+z\rangle, \qquad \hat{S}_z|-z\rangle = \frac{\hbar}{2}|-z\rangle.$$

Since $\langle +z|-z\rangle = 0$, $|+z\rangle$ and $\hat{\Theta}|+z\rangle = \eta|-z\rangle$ are different states with the same energy eigenvalue. In other words, these two states are degenerate states with the same energy eigenvalue, forming the Kramers doublet. We note that the magnetic moment $\hat{\mu}$ is given by

$$\hat{\mu}_z = -\frac{2\mu_B}{\hbar}\hat{S}_z .$$

So the magnetic moments are different for the two states $\left|+z\right\rangle$ and $\hat{\Theta}\left|+z\right\rangle$.

$$\hat{\mu}_z\left|\pm z\right\rangle = -\frac{2\mu_B}{\hbar}\hat{S}_z\left|\pm z\right\rangle = \mp\mu_B\left|\pm z\right\rangle$$

39. Example of the Kramers theorem for spin systems

In the absence of an external magnetic field, there exists at least one doublet state (with double-degeneracy) among the energy levels of spin of odd number of electrons in the crystal field. This doublet is called the Kramers doublet. This theorem in general holds for any spin systems. Here we explain this theorem for the spin Hamiltonina given by

$$\hat{H} = D\hat{S}_z^{\ 2}$$

with spin S = 1, 1/2, 1, 3/2, and 2. When an external magnetic field is applied, the Kramers doublet is split.

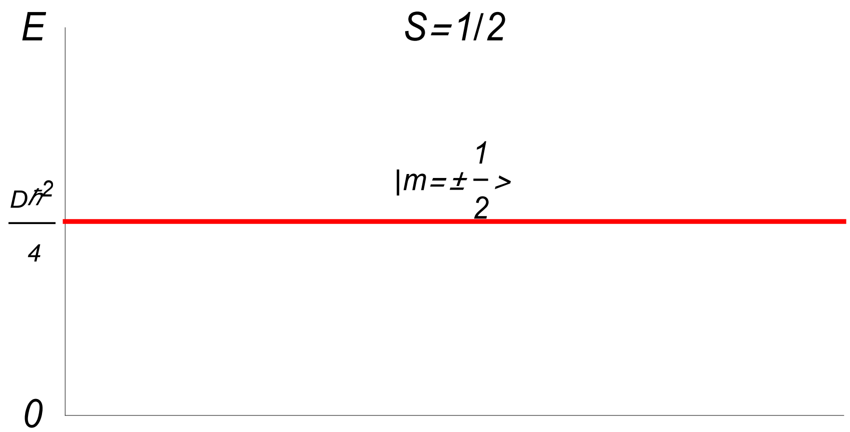
We consider the spin-orbit coupling

$$\hat{H}_{so} = \lambda_{so}\hat{\boldsymbol{L}}\cdot\hat{\boldsymbol{S}}$$

Because both angular momenta are odd, the Hamiltonian is even and symmetric under time-reversal. When there is no spin-orbit coupling, we know that the hydrogen atom has 2s + 1 = 2 degeneracy, but with spin-orbit coupling there is still 2-fold degeneracy because of the Kramer's degeneracy.

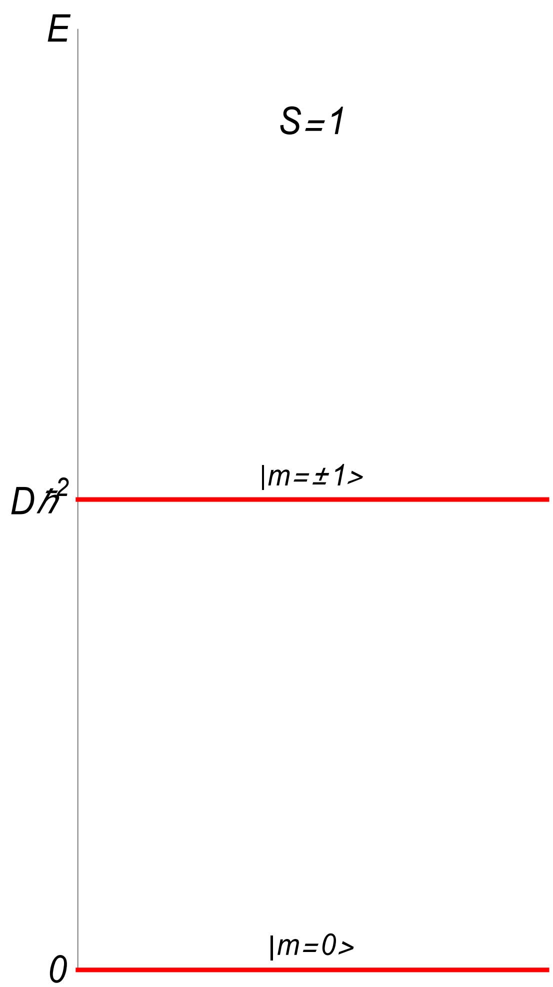
(a) Spin 1/2

There is one doublet (Kramers doublet) with $\left|S = 1/2, m = \pm 1/2\right\rangle$ (having an energy level $\frac{D\hbar^2}{4}$).



(b) Spin $S = 1$.

The energy level (energy 0) for the state $|S=1, m=0)\rangle$ is singlet (the ground state). The energy level (energy $D\hbar^2$) for the state $|S=1, m=\pm1\rangle$ is doublet.



Suppose that the spin Hamiltonian is given by

$$\hat{H} = D\hat{S}_z^{\ 2} + E(\hat{S}_x^{\ 2} - \hat{S}_y^{\ 2}) \qquad \text{with } S = 1.$$

We note that $[\hat{H}, \hat{\Theta}] = 0$

The Hamiltonian is given by

$$\hat{H} = \hbar^2 \begin{pmatrix} D & 0 & E \\ 0 & 0 & 0 \\ E & 0 & D \end{pmatrix}$$

$$\hat{H}|1,1\rangle = \hbar^2 [A|1,1\rangle + B|1,-1\rangle] \tag{1}$$

$\hat{H}|1,0\rangle = 0$ ($|1,0\rangle$ is the eigenstate of $\hat{H}$ with the eigenvalue 0)

$$\hat{H}|1,-1\rangle = \hbar^2 [B|1,1\rangle + A|1,-1\rangle] \tag{2}$$

In the subspace of {$|1,1\rangle$ and $|1,-1\rangle$}, the Hamiltonian can be written as

$$\begin{aligned}
\hat{H}_{sub} &= \hbar^2 \begin{pmatrix} D & E \\ E & D \end{pmatrix} \\
&= D\hbar^2 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + E\hbar^2 \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \\
&= \hbar^2 (D\hat{1} + E\hat{\sigma}_x)
\end{aligned}$$

$$\hat{H}_{sub}|\pm x\rangle = \hbar^2 (D\hat{1} + E\hat{\sigma}_x)|\pm x\rangle = \hbar^2 (D \pm E)|\pm x\rangle$$

with

$|+x\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}$ (eigenvalue: $(D+E)\hbar^2$)

$|-x\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}$ (eigenvalue: $(D-E)\hbar^2$)

In summary we have three states

$|\phi_1\rangle = |1,0\rangle$ (energy eigenvalue, 0)

$|\phi_2\rangle = \frac{1}{\sqrt{2}}[|1,1\rangle + |1,-1\rangle]$ (energy eigenvalue: $(D+E)\hbar^2$)

$|\phi_3\rangle = \frac{1}{\sqrt{2}}[|1,1\rangle - |1,-1\rangle]$ (energy eigenvalue: $(D-E)\hbar^2$)

The time reversal states:

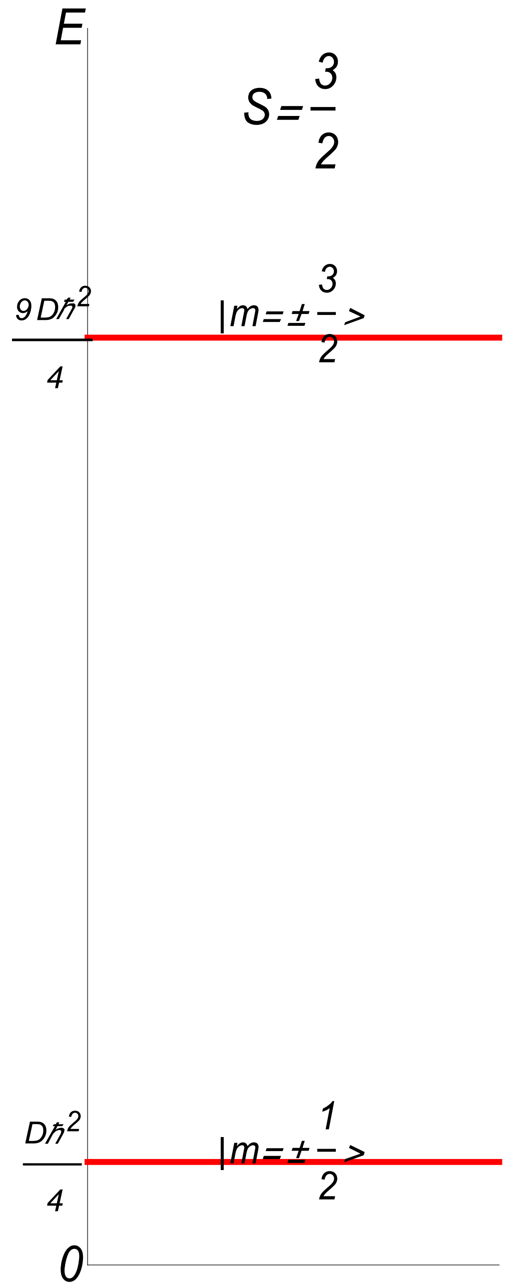
$$\hat{\Theta}|\phi_1\rangle = \hat{\Theta}|1,0\rangle = |1,0\rangle$$

$$\hat{\Theta}|\phi_2\rangle = \frac{1}{\sqrt{2}}\hat{\Theta}[|1,1\rangle + |1,-1\rangle] = \frac{1}{\sqrt{2}}[(-1)|1,-1\rangle + (-1)^{-1}|1,1\rangle] = -|\phi_2\rangle$$

$$\hat{\Theta}|\phi_3\rangle = \frac{1}{\sqrt{2}}\hat{\Theta}[|1,1\rangle - |1,-1\rangle] = \frac{1}{\sqrt{2}}[(-1)|1,-1\rangle - (-1)^{-1}|1,1\rangle] = |\phi_3\rangle$$

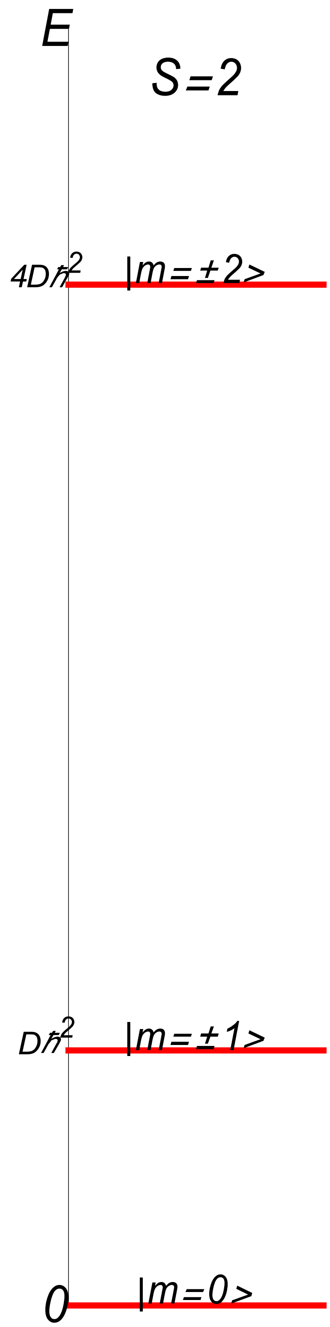
(c) Spin *S* = 3/2

The energy level (energy $D\hbar^2/4$) for the state $\left|S=\frac{3}{2}, m=\pm\frac{3}{2})\right\rangle$ is Kramers doublet (the ground state). The energy level (energy $\frac{9D\hbar^2}{4}$) for the state $\left|S=\frac{3}{2}, m=\pm\frac{1}{2})\right\rangle$ is Kramers doublet.



(d) Spin 2

There are two energy levels. The energy level (energy $4D\hbar^2$) for the state $\left|S=2, m=\pm 2)\right\rangle$ is doublet, and the energy level (energy $D\hbar^2$) for the state $\left|S=2, m=\pm 1)\right\rangle$ is also doublet. The energy level (energy 0) for the state $\left|S=2, m=0)\right\rangle$ is singlet.



40. $\hat{\Theta}^2 = \pm \hat{1}$

Suppose that

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

Using the definition of $\hat{\Theta}$ $(= \hat{U}\hat{K})$, we have

$$\hat{\Theta}^2 = \hat{U}\hat{K}\hat{U}\hat{K} = \hat{U}\hat{U}^*$$

We note that

$$\hat{U}^{-1} = \hat{U}^+ = (\hat{U}^T)^* = (\hat{U}^*)^T$$

or

$$\hat{U}^* = \hat{U}^{-1^T} = \hat{U}^{T^{-1}}$$

Then we get

$$\hat{\Theta}^2 = \hat{U}\hat{U}^* = \hat{U}\hat{U}^{T^{-1}} = \eta\hat{1}$$

From this we have

$$\hat{U} = \eta\hat{U}^T, \qquad \text{or} \qquad \hat{U}^T = \hat{U}\eta.$$

Then we get

$$\hat{U} = \eta\hat{U}^T = \eta\hat{U}\eta = \eta^2\hat{U}$$

leading to

$$\eta^2 = 1, \qquad \text{or} \qquad \eta = \pm 1$$

We may also write

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

The sign of $\hat{\Theta}^2$ is determined by the properties of $\hat{U}$, which in turn are governed by the nature of the complete set of kinematic variables required by the definition of a given physical system. Therefore these are two classes of quantum mechanical systems, even systems and odd systems.

41. $\hat{U} = \eta(-i\hat{\sigma}_y)$ for spin 1/2 system

We consider the expression of the unitary operator $\hat{U}$ for the spin 1/2 system. We start with the relation

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

with

$$\begin{aligned}
\hat{\Theta}\hat{\boldsymbol{\sigma}}\hat{\Theta}^{-1} &= \hat{U}K\hat{\boldsymbol{\sigma}}(\hat{U}K)^{-1} \\
&= \hat{U}K\hat{\boldsymbol{\sigma}}K^{-1}\hat{U}^{-1} \\
&= \hat{U}K\hat{\boldsymbol{\sigma}}K^{-1}\hat{U}^{+} \\
&= \hat{U}\hat{\boldsymbol{\sigma}}^{*}\hat{U}^{+}
\end{aligned}$$

Then we have

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

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

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

where

$$\hat{\sigma}_x = \hat{\sigma}_x{}^{*} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \hat{\sigma}_y = -\hat{\sigma}_y{}^{*} = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \hat{\sigma}_z = \hat{\sigma}_z{}^{*} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

Hence we find that the unitary operator $\hat{U}$ anti-commutes with $\hat{\sigma}_x$;

$$\{\hat{U}, \hat{\sigma}_x\} = \hat{U}\hat{\sigma}_x + \hat{\sigma}_x\hat{U} = 0$$

It also anti-commutes with $\hat{\sigma}_z$;

$$\{\hat{U}, \hat{\sigma}_z\} = \hat{U}\hat{\sigma}_z + \hat{\sigma}_z\hat{U} = 0 .$$

In contrast, $\hat{U}$ commutes with $\hat{\sigma}_y$;

$$[\hat{U}, \hat{\sigma}_y] = \hat{U}\hat{\sigma}_y - \hat{\sigma}_y\hat{U} = 0.$$

These commutation relations suggest that $\hat{U}$ is a function of $\hat{\sigma}_y$. We assume that

$$\hat{U} = \eta(-i\hat{\sigma}_y),$$

where η is a phase factor with $|\eta| = 1$. Since

$$\hat{U}^+ = \eta^*(i\hat{\sigma}_y{}^+) = \eta^* i\hat{\sigma}_y$$

so we have

$$\hat{U}\hat{U}^+ = \eta(-i\hat{\sigma}_y)\eta^* i\hat{\sigma}_y = |\eta|^2 \hat{\sigma}_y{}^2 = \hat{1}$$

((**Note**)) The commutation relations

$$\hat{\sigma}_x\hat{\sigma}_y = -\hat{\sigma}_y\hat{\sigma}_x = i\hat{\sigma}_z,$$
$$\hat{\sigma}_y\hat{\sigma}_z = -\hat{\sigma}_z\hat{\sigma}_y = i\hat{\sigma}_x,$$
$$\hat{\sigma}_z\hat{\sigma}_x = -\hat{\sigma}_x\hat{\sigma}_z = i\hat{\sigma}_y$$

---

42. Spin 1/2 system

$$\hat{\Theta} = \hat{U}\hat{K} = \eta(-\hat{\sigma}_y)\hat{K}$$

where $\hat{U}$ is the unitary operator, and $\hat{K}^2 = \hat{1}$.

$$\hat{U} = \eta(-i\hat{\sigma}_y) = \eta\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$$

$$\hat{U}^+\hat{U} = |\eta|^2\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \hat{1}$$

$$\hat{\Theta}^2 = \hat{U}\hat{K}\hat{U}\hat{K} = \hat{U}\hat{U}^* = |\eta|^2\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} = -\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = -\hat{1}$$

We assume that

$$\hat{U} = e^{i\phi}\hat{\sigma}_y = e^{i\phi}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \hat{K}^2 = 1$$

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

$$\hat{\Theta}^2 = \hat{U}\hat{K}\hat{U}\hat{K} = \hat{U}\hat{U}^* = e^{i\phi}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} e^{-i\phi}\begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix} = -\hat{1}$$

((Note))

$$\hat{\Theta} = (-i)\hat{\sigma}_y\hat{K}$$

$$\hat{\Theta}^{-1} = [(-i)\hat{\sigma}_y\hat{K}]^{-1} = \hat{K}^{-1}\hat{\sigma}_y{}^{-1}(-i)^{-1} = \hat{K}\hat{\sigma}_y{}^{+}i = \hat{K}\hat{\sigma}_y i$$

$$\hat{\Theta}\hat{\Theta}^{-1} = (-i)\hat{\sigma}_y\hat{K}\hat{K}\hat{\sigma}_y i = (-i)\hat{\sigma}_y\hat{K}^2\hat{\sigma}_y i = (-i)\hat{\sigma}_y{}^2 i = \hat{1}$$

$$\hat{\Theta}^{-1}\hat{\Theta} = \hat{K}\hat{\sigma}_y i(-i)\hat{\sigma}_y\hat{K} = \hat{K}\hat{\sigma}_y{}^2\hat{K} = \hat{K}^2 = \hat{1}$$

$$\hat{\Theta}^2 = (-i)\hat{\sigma}_y\hat{K}(-i)\hat{\sigma}_y\hat{K} = (-i)\hat{\sigma}_y(-i)^*\hat{\sigma}_y{}^* = \hat{\sigma}_y\hat{\sigma}_y{}^* = -\hat{\sigma}_y{}^2 = -\hat{1}$$

since

$$\hat{\sigma}_y{}^* = -\hat{\sigma}_y$$

---

43. *N* spin (1/2) particles system ($N \geq 2$)

For simplicity we choose $\eta = 1$. The time-reversal operator for the *N* spin (1/2) particles system can be expressed by

$$\hat{\Theta} = (-i)^N \hat{\sigma}_{1y} \otimes \hat{\sigma}_{2y} \otimes \hat{\sigma}_{3y} \otimes \cdots \otimes \hat{\sigma}_{Ny}\hat{K}$$

using the Kronecker product.

(a) For the 2-electrons system

$$\hat{\Theta} = (-i)\hat{\sigma}_{1y} \otimes (-i)\hat{\sigma}_{2y}\hat{K} = -\begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \\ 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix} K$$

$$\hat{\Theta}^2 = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \\ 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix} K \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \\ 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix} K$$

$$= \hat{1}$$

(Identity matrix with 4 x 4)

(b) For the 3-electrons system

$$\hat{\Theta} = (-i)\hat{\sigma}_{1y} \otimes (-i)\hat{\sigma}_{2y} \otimes (-i)\hat{\sigma}_{3y}\hat{K} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} K$$

$$\hat{\Theta}^2 = (-i)\hat{\sigma}_{1y} \otimes (-i)\hat{\sigma}_{2y} \otimes (-i)\hat{\sigma}_{3y}\hat{K}(-i)\hat{\sigma}_{1y} \otimes (-i)\hat{\sigma}_{2y} \otimes (-i)\hat{\sigma}_{3y}\hat{K}$$

$$= \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} K \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} K$$

$$= -\hat{1}$$

(Identity matrix with 8 x 8)

((**Note**))

$$(\hat{A}\otimes\hat{B})(|\psi_1\rangle\otimes|\psi_2\rangle)=\hat{A}|\psi_1\rangle\otimes\hat{B}|\psi_2\rangle .$$

44. Property of $\hat{\Theta}^2$

Two successive applications of the time reversal operator, i.e., two reversals of motion, leave the physical situation unchanged.

$$\hat{\Theta}^2|\psi\rangle = c|\psi\rangle \tag{1}$$

with $|c|=1$ (c is a complex number). The change in $|\psi\rangle\rightarrow\Theta|\psi\rangle$ of Eq.(1) leads to

$$\begin{aligned}\hat{\Theta}^2(\hat{\Theta}|\psi\rangle) &= \hat{\Theta}(\hat{\Theta}^2|\psi\rangle)\\ &= \hat{\Theta}(c|\psi\rangle\\ &= c^*\hat{\Theta}|\psi\rangle\end{aligned} \tag{2}$$

From Eqs.(1) and (2). we get

$$\begin{aligned}\hat{\Theta}^2(|\psi\rangle+\hat{\Theta}|\psi\rangle) &= \hat{\Theta}^2|\psi\rangle+\hat{\Theta}^3|\psi\rangle)\rangle\\ &= c|\psi\rangle+c^*\Theta|\psi\rangle)\rangle\end{aligned} \tag{3}$$

Equation (1) must hold for any state vector,

$$\hat{\Theta}^2(|\psi\rangle+\Theta|\psi\rangle)\rangle = c'(|\psi\rangle+\Theta|\psi\rangle)\rangle$$

for some *c'*, Then we have

$$\hat{\Theta}^2|\psi\rangle+\hat{\Theta}^3|\psi\rangle)\rangle = c'(|\psi\rangle+\Theta|\psi\rangle) = c'|\psi\rangle+c'\Theta|\psi\rangle \tag{4}$$

Comparing Eq.(3) with Eq.(4), we get

$$c=c', \qquad c'=c^*,$$

$$c^* = c$$

which means that c is real and

$$c = \pm 1.$$

$$\hat{\Theta}^2 |\psi\rangle = (\pm 1)|\psi\rangle$$

45. $\hat{\Theta}^2 = \pm 1$

We start with the definition of the time reversal operator

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

Then we have

$$\hat{\Theta}^2 = \hat{U}\hat{K}\hat{U}\hat{K} = \hat{U}\hat{U}^* = c$$

This can be rewritten as

$$\hat{U}^* = c\hat{U}^+ = c(\hat{U}^*)^T = c(c\hat{U}^+)^T = c^2\hat{U}^*$$

where we use the relation $\hat{U}^* = c\hat{U}^+$ twice. So we get

$$c^2 = 1$$

Note that c is real. This can be shown as follows.

$$(\hat{U}\hat{U}^*)^* = c^*, \qquad \text{or} \qquad \hat{U}^*\hat{U} = c^*$$

Since $\hat{U}^* = c\hat{U}^+$, we get

$$\hat{U}^*\hat{U} = c\hat{U}^+\hat{U} = c,$$

or $c = c^*$ (c is real)

So that we have

$$c = \pm 1$$

46. The matrix expression of the unitary operator $\hat{U}$

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

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

$$\hat{\Theta}(\hat{J}_x + i\hat{J}_y)\hat{\Theta}^{-1} = -(\hat{J}_x - i\hat{J}_y), \qquad \hat{\Theta}\hat{J}_+\hat{\Theta}^{-1} = -\hat{J}_-$$

$$\hat{\Theta}(\hat{J}_x - i\hat{J}_y)\hat{\Theta}^{-1} = -(\hat{J}_x + i\hat{J}_y), \qquad \hat{\Theta}\hat{J}_-\hat{\Theta}^{-1} = -\hat{J}_+$$

Note that

$$\hat{\Theta}\hat{J}_\pm\hat{\Theta}^{-1} = \hat{U}\hat{K}\hat{J}_\pm\hat{K}^{-1}\hat{U}^{-1} = \hat{U}\hat{J}_\pm{}^*\hat{U}^{-1} = \hat{U}\hat{J}_\pm\hat{U}^{-1} = -\hat{J}_\mp$$

$$\hat{\Theta}\hat{J}_z\hat{\Theta}^{-1} = \hat{U}\hat{K}\hat{J}_z\hat{K}^{-1}\hat{U}^{-1} = \hat{U}\hat{J}_z{}^*\hat{U}^{-1} = \hat{U}\hat{J}_z\hat{U}^{-1} = -\hat{J}_z$$

where the matrix elements of $\hat{J}_\pm$ and are real;

$$\hat{J}_\pm{}^* = \hat{J}_\pm, \qquad \hat{J}_z{}^* = \hat{J}_z$$

So we have

$$\hat{U}\hat{J}_\pm + \hat{J}_\mp\hat{U} = 0, \qquad \hat{U}\hat{J}_z + \hat{J}_z\hat{U} = 0$$

From these relations, we get the commutation relation

$$\hat{U}\hat{\boldsymbol{J}}^2 = \hat{\boldsymbol{J}}^2\hat{U}$$

with

$$\hat{\boldsymbol{J}}^2 = \hat{J}_z{}^2 + \frac{1}{2}(\hat{J}_+\hat{J}_- + \hat{J}_-\hat{J}_+)$$

Note that

$$\begin{aligned}\hat{U}\hat{\boldsymbol{J}}^2\hat{U}^{-1} &= \hat{U}[\hat{J}_z{}^2 + \frac{1}{2}(\hat{J}_+\hat{J}_- + \hat{J}_-\hat{J}_+)]\hat{U}^{-1} \\ &= \hat{U}\hat{J}_z\hat{U}^{-1}\hat{U}\hat{J}_z\hat{U}^{-1} + \frac{1}{2}(\hat{U}\hat{J}_+\hat{U}^{-1}\hat{U}\hat{J}_-\hat{U}^{-1} + \hat{U}\hat{J}_-\hat{U}^{-1}\hat{U}\hat{J}_+\hat{U}^{-1}) \\ &= \hat{J}_z{}^2 + \frac{1}{2}(\hat{J}_+\hat{J}_- + \hat{J}_-\hat{J}_+) \\ &= \hat{\boldsymbol{J}}^2\end{aligned}$$

Following the procedure introduced by **Sachs**, we determine the matrix element of $\hat{U}$.

(a) $\hat{U}\hat{J}_z + \hat{J}_z\hat{U} = 0$

$$\langle j,m|\hat{U}\hat{J}_z + \hat{J}_z\hat{U}|j,m'\rangle = \hbar(m+m')\langle j,m|\hat{U}|j,m'\rangle = 0$$

leading to

$$\langle j,m|\hat{U}|j,m'\rangle \neq 0 \qquad \text{only if } m+m'=0,$$

(b) $\hat{U}\hat{J}_+ + \hat{J}_-\hat{U} = 0$

$$\begin{aligned}\langle j,m|\hat{U}\hat{J}_+ + \hat{J}_-\hat{U}|j,m'\rangle &= \sum_{m''}[\langle j,m|\hat{U}|j,m''\rangle\langle j,m''|\hat{J}_+|j,m'\rangle + \langle j,m|\hat{J}_-|j,m''\rangle\langle j,m''|\hat{U}|j,m'\rangle] \\ &= \langle j,m|\hat{U}|j,m'+1\rangle\langle j,m'+1|\hat{J}_+|j,m'\rangle + \langle j,m|\hat{J}_-|j,m+1\rangle\langle j,m+1|\hat{U}|j,m'\rangle \\ &= 0\end{aligned}$$

For $m'+1=-m$, we have

$$\langle j,m|\hat{U}|j,-m\rangle\langle j,-m|\hat{J}_+|j,-m-1\rangle + \langle j,m|\hat{J}_-|j,m+1\rangle\langle j,m+1|\hat{U}|j,-m-1\rangle = 0$$

or

$$\frac{\langle j,m+1|\hat{U}|j,-m-1\rangle}{\langle j,m|\hat{U}|j,-m\rangle} = -\frac{\langle j,-m|\hat{J}_+|j,-m-1\rangle}{\langle j,m|\hat{J}_-|j,m+1\rangle} = -1 \qquad (1)$$

since

$$\hat{J}_+|j,m\rangle = \sqrt{(j-m)(j+m+1)}|j,m+1\rangle$$

$$\hat{J}_-|j,m\rangle = \sqrt{(j+m)(j-m+1)}|j,m-1\rangle$$

$$\hat{J}_+|j,-m-1\rangle = \sqrt{(j+m+1)(j-m)}|j,-m\rangle$$

$$\hat{J}_-|j,m+1\rangle = \sqrt{(j+m+1)(j-m)}|j,m\rangle$$

leading to

$$\frac{\langle j,-m|\hat{J}_+|j,-m-1\rangle}{\langle j,m|\hat{J}_-|j,m+1\rangle} = 1 .$$

From Eq.(1), we get

$$\frac{\langle j,m'|\hat{U}|j,-m'\rangle}{\langle j,m|\hat{U}|j,-m\rangle} = (-1)^{m-m'} = i^{2(m-m')}$$

Since $m-m'$ is an integer, we have the relation; $(-1)^{m'-m} = (-1)^{m-m'}$. The change of $m' \rightarrow -m'$ and $m \rightarrow -m$

$$\frac{\langle j,-m'|\hat{U}|j,m'\rangle}{\langle j,-m|\hat{U}|j,m\rangle} = (-1)^{m'-m} = i^{2(m'-m)}$$

$$\langle j,-m|\hat{U}|j,m\rangle = i^{2m}$$

Therefore, we have

$$\begin{aligned}\hat{\Theta}|j,m\rangle &= \hat{U}\hat{K}|j,m\rangle \\ &= \sum_{m'}|j,m'\rangle\langle j,m'|\hat{U}|j,m\rangle \\ &= |j,-m\rangle\langle j,-m|\hat{U}|j,m\rangle \\ &= i^{2m}|j,-m\rangle\end{aligned}$$

or

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

where m is either an integer or a half-integer. We note that

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

Thus we have

$$\hat{\Theta}^2|j,m\rangle = i^{-4m}\hat{\Theta}|j,m\rangle$$

47. The expression of *U* for *j* = 1

Here we show that for j =1, $\hat{\Theta}$ is given by

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

where $\hat{U} = \begin{pmatrix} 0 & 0 & 1 \\ 0 & -1 & 0 \\ 1 & 0 & 0 \end{pmatrix}$

((**Proof**))

$$\hat{U}\hat{J}_x + \hat{J}_x\hat{U} = 0, \qquad \hat{U}\hat{J}_y - \hat{J}_y\hat{U} = 0, \qquad \hat{U}\hat{J}_z + \hat{J}_z\hat{U} = 0$$

where

$$\hat{J}_x = \frac{\hbar}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \qquad \hat{J}_y = \frac{\hbar}{\sqrt{2}}\begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}, \qquad \hat{J}_x = \hbar\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

We assume that the unitary operator is given by

$$\hat{U} = \begin{pmatrix} U_{11} & U_{12} & U_{13} \\ U_{21} & U_{22} & U_{23} \\ U_{31} & U_{32} & U_{33} \end{pmatrix}$$

We note that

$$\hat{U}\hat{J}_z + \hat{J}_z\hat{U} = \hbar\begin{pmatrix} 2U_{11} & U_{12} & 0 \\ U_{21} & 0 & -U_{23} \\ 0 & -U_{32} & -2U_{33} \end{pmatrix} = 0$$

leading to $U_{11} = U_{12} = U_{21} = U_{23} = U_{32} = U_{33} = 0$

$$\hat{U}\hat{J}_x + \hat{J}_x\hat{U} = \hbar\begin{pmatrix} 0 & \frac{U_{13}+U_{22}}{\sqrt{2}} & 0 \\ \frac{U_{22}+U_{31}}{\sqrt{2}} & 0 & \frac{U_{13}+U_{22}}{\sqrt{2}} \\ 0 & \frac{U_{22}+U_{31}}{\sqrt{2}} & 0 \end{pmatrix} = 0$$

leading to $U_{13} = U_{31} = -U_{22}$ .From the condition of $\hat{U}^{+}\hat{U} = \hat{1}$, we have

$$\hat{U} = \begin{pmatrix} 0 & 0 & -1 \\ 0 & 1 & 0 \\ -1 & 0 & 0 \end{pmatrix}$$

This form of $\hat{U}$ satisfies the relation $\hat{U}\hat{J}_y - \hat{J}_y\hat{U} = 0$. We note that

$$\hat{\Theta}|1,1\rangle = \hat{U}\hat{K}|1,1\rangle = \begin{pmatrix} 0 & 0 & -1 \\ 0 & 1 & 0 \\ -1 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = -\begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} = -|1,-1\rangle$$

$$\hat{\Theta}|1,0\rangle = \hat{U}\hat{K}|1,0\rangle = \begin{pmatrix} 0 & 0 & -1 \\ 0 & 1 & 0 \\ -1 & 0 & 0 \end{pmatrix}\begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} = |1,0\rangle$$

$$\hat{\Theta}|1,-1\rangle = \hat{U}\hat{K}|1,-1\rangle = \begin{pmatrix} 0 & 0 & -1 \\ 0 & 1 & 0 \\ -1 & 0 & 0 \end{pmatrix}\begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} = -\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = -|1,1\rangle$$

$$\hat{\Theta}^2 = \hat{U}\hat{K}\hat{U}\hat{K} = \hat{U}\hat{U}^* = \hat{1}$$

48. Evaluation of $\hat{\Theta}$ and $\hat{\Theta}^2$ for electrons with spin 1/2

(a) One particle with spin 1/2

$j = 1/2$ with $m = \pm 1/2$

$m = 1/2 \qquad i^{-4m} = i^{-2} = \dfrac{1}{i^2} = -1$

$m = -1/2 \qquad i^{-4m} = i^2 = -1$

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

(b) Two particles with spin 1/2

$$D_{1/2} \times D_{1/2} = D_1 + D_0$$

$j = 1$

$m = 1 \qquad i^{-4m} = i^{-4} = \dfrac{1}{i^4} = 1$

$m = 0 \qquad i^{-4m} = -1$

$m = -1 \qquad i^{-4m} = i^4 = 1$

$j = 0$

$m = 0 \qquad i^{-4m} = 1$

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

(c) Three particles with spin 1/2

$$D_{1/2} \times D_{1/2} \times D_{1/2} = (D_1 + D_0) \times D_{1/2} = D_{3/2} + 2D_{1/2}$$

$j = 3/2$

$m = 3/2 \qquad i^{-4m} = i^{-6} = \dfrac{1}{i^6} = -1$

$m = 1/2 \qquad i^{-4m} = i^{-2} = -1$

$m = -1/2 \qquad i^{-4m} = i^2 = -1$

$m = -3/2 \qquad i^{-4m} = i^6 = -1$

$j = 1/2$

$m = 1/2 \qquad i^{-4m} = i^{-2} = \frac{1}{i^2} = -1$

$m = -1/2 \qquad i^{-4m} = i^2 = -1$

$$\hat{\Theta}^2 \left| j, m \right\rangle = -\left| j, -m \right\rangle$$

49. Rotation operator as a unitary operator

The unitary operator is given by $\hat{U} = \exp(-\frac{i}{\hbar}\hat{S}_y \pi)$ which is the rotation operator for spin S (=1/2, 1, 3/2, …).

(a) Spin 1/2

$$\hat{U} = \exp(-\frac{i}{\hbar}\hat{S}_y \pi) = -i\hat{\sigma}_y = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix},$$

$$\hat{\Theta}^2 = \hat{U}\hat{K}\hat{U}\hat{K} = \hat{U}\hat{U}^* = \hat{U}^2 = -\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

where we use the formula

$$\exp(-\frac{i}{\hbar}\hat{S}_y \theta) = \exp(-\frac{i}{2}\hat{\sigma}_y \theta) = \cos\frac{\theta}{2} - i\sin\frac{\theta}{2}\hat{\sigma}_y$$

(b) Spin 1

$$\hat{U} = \exp(-\frac{i}{\hbar}\hat{S}_y \pi) = \begin{pmatrix} 0 & 0 & 1 \\ 0 & -1 & 0 \\ 1 & 0 & 0 \end{pmatrix},$$

$$\hat{\Theta}^2 = \hat{U}\hat{K}\hat{U}\hat{K} = \hat{U}\hat{U}^* = \hat{U}^2 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

(c) Spin 3/2

$$\hat{U} = \exp(-\frac{i}{\hbar}\hat{S}_y \pi) = \begin{pmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \\ 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix},$$

$$\hat{\Theta}^2 = \hat{U}\hat{K}\hat{U}\hat{K} = \hat{U}\hat{U}^* = \hat{U}^2 = -\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

or

$$\hat{\Theta}^2 = (-1)^{2j}\hat{1} = (-1)^3\hat{1} = -\hat{1}$$

(d) Spin 2 $(j = 2)$

$$\hat{U} = \exp(-\frac{i}{\hbar}\hat{S}_y \pi) = \begin{pmatrix} 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \end{pmatrix},$$

$$\hat{\Theta}^2 = \hat{U}\hat{K}\hat{U}\hat{K} = \hat{U}\hat{U}^* = \hat{U}^2 = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

or

$$\hat{\Theta}^2 = (-1)^{2j}\hat{1} = (-1)^4\hat{1} = \hat{1}$$

(e) Spin 5/2 $(j = 5/2)$

$$\hat{U} = \exp(-\frac{i}{\hbar}\hat{S}_y\pi) = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \end{pmatrix},$$

$$\hat{\Theta}^2 = \hat{U}\hat{K}\hat{U}\hat{K} = \hat{U}\hat{U}^* = \hat{U}^2 = -\begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

or

$$\hat{\Theta}^2 = (-1)^{2j}\hat{1} = (-1)^5\hat{1} = -\hat{1}$$

Many particle systems

We consider the time reversal operator $\hat{\Theta}$ for N spins (spin 1/2).

$$\hat{\Theta} = (\hat{\sigma}_y^1\hat{\sigma}_y^2.....\hat{\sigma}_y^{N-1}\hat{\sigma}_y^N)\hat{K}$$

We note that

$$\begin{aligned} \hat{\Theta}^2 &= (\hat{\sigma}_y^1\hat{\sigma}_y^2.....\hat{\sigma}_y^{N-1}\hat{\sigma}_y^N)\hat{K}(\hat{\sigma}_y^1\hat{\sigma}_y^2.....\hat{\sigma}_y^{N-1}\hat{\sigma}_y^N)\hat{K} \\ &= (\hat{\sigma}_y^1\hat{\sigma}_y^2.....\hat{\sigma}_y^{N-1}\hat{\sigma}_y^N)\hat{K}\hat{\sigma}_y^1\hat{K}^{-1}\hat{K}\hat{\sigma}_y^2\hat{K}^{-1}....\hat{K}\hat{\sigma}_y^{N-1}\hat{K}^{-1}\hat{K}\hat{\sigma}_y^N\hat{K}^{-1})\hat{K}^2 \end{aligned}$$

Using the relation,

$$\hat{K}\hat{\sigma}_y^1\hat{K}^{-1} = (\hat{\sigma}_y^1)^* = -\hat{\sigma}_y^1, \qquad \hat{K}^2 = \hat{1}$$

we have

$$\begin{aligned}\hat{\Theta}^2 &= (\hat{\sigma}_y^1\hat{\sigma}_y^2.....\hat{\sigma}_y^{N-1}\hat{\sigma}_y^N)\hat{K}(\hat{\sigma}_y^1\hat{\sigma}_y^2.....\hat{\sigma}_y^{N-1}\hat{\sigma}_y^N)\hat{K} \\ &= (-1)^N(\hat{\sigma}_y^1)^2(\hat{\sigma}_y^2)^2....(\hat{\sigma}_y^N)^2 \\ &= (-1)^N\end{aligned}$$

For N = even $\quad \hat{\Theta}^2 = 1$

For N = odd $\quad \hat{\Theta}^2 = -1$

(a) $N = 2$

$$D_{1/2} \times D_{1/2} = D_1 + D_0$$

leading to the total spin with S = 1 and 0 (integer)

(b) N=3

$$D_{1/2} \times D_{1/2} \times D_{1/2} = D_{1/2} \times (D_1 + D_0) = D_{3/2} + 2D_{1/2}$$

leading to the total spin with S = 3/2 and 1/2 (integer)

50. Rotation operator for many spin systems

(a)

$$\hat{A}_1 = -i\hat{\sigma}_y = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$$

$$\hat{R}_y(\theta) = \exp(-\frac{i}{2}\hat{A}_1\theta) = \cos\frac{\theta}{2}\hat{1} - i\hat{\sigma}_y\sin\frac{\theta}{2}$$

When $\theta = \pi$,

$$\hat{\Theta} = \hat{R}_y(\theta = \pi) = \cos\frac{\pi}{2}\hat{1} - i\hat{\sigma}_y\sin\frac{\pi}{2} = -i\hat{\sigma}_y == \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$$

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

(b)

$$\hat{A}_2 = \hat{\sigma}_y \otimes \hat{1} + \hat{1} \otimes \hat{\sigma}_y$$
$$= \begin{pmatrix} 0 & -i & -i & 0 \\ i & 0 & 0 & -i \\ i & 0 & 0 & -i \\ 0 & i & i & 0 \end{pmatrix}$$

$$\hat{\Theta} = \hat{R}_y(\pi) = \exp(-\frac{i}{2}\hat{A}_2\pi) = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \\ 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}$$

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

(c)

$$\hat{A}_3 = \hat{\sigma}_y \otimes \hat{1} \otimes \hat{1} + \hat{1} \otimes \hat{\sigma}_y \otimes \hat{1} + \hat{1} \otimes \hat{1} \otimes \hat{\sigma}_y$$
$$= \begin{pmatrix} 0 & -i & -i & 0 & -i & 0 & 0 & 0 \\ i & 0 & 0 & -i & 0 & -i & 0 & 0 \\ i & 0 & 0 & -i & 0 & 0 & -i & 0 \\ 0 & i & i & 0 & 0 & 0 & 0 & -i \\ i & 0 & 0 & 0 & 0 & -i & -i & 0 \\ 0 & i & 0 & 0 & i & 0 & 0 & -i \\ 0 & 0 & i & 0 & i & 0 & 0 & -i \\ 0 & 0 & 0 & i & 0 & i & i & 0 \end{pmatrix}$$

$$\hat{\Theta} = \hat{R}_y(\pi) = \exp(-\frac{i}{2}\hat{A}_3\pi) = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

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

51. Mathematica for the case of $j = 3/2$

Matrices j = 3/2

```
Clear["Global`*"]; j = 3/2; exp_* := exp /. {Complex[re_, im_] :> Complex[re, -im]};
Jx[j_, n_, m_] := ℏ/2 Sqrt[(j - m) (j + m + 1)] KroneckerDelta[n, m + 1] +
  ℏ/2 Sqrt[(j + m) (j - m + 1)] KroneckerDelta[n, m - 1];
Jy[j_, n_, m_] := -ℏ/2 i Sqrt[(j - m) (j + m + 1)] KroneckerDelta[n, m + 1] +
  ℏ/2 i Sqrt[(j + m) (j - m + 1)] KroneckerDelta[n, m - 1]; Jz[j_, n_, m_] := ℏ m KroneckerDelta[n, m];
Jx = Table[Jx[j, n, m], {n, j, -j, -1}, {m, j, -j, -1}];
Jy = Table[Jy[j, n, m], {n, j, -j, -1}, {m, j, -j, -1}];
Jz = Table[Jz[j, n, m], {n, j, -j, -1}, {m, j, -j, -1}];

Jx // MatrixForm
```

$$\begin{pmatrix} 0 & \frac{\sqrt{3}\hbar}{2} & 0 & 0 \\ \frac{\sqrt{3}\hbar}{2} & 0 & \hbar & 0 \\ 0 & \hbar & 0 & \frac{\sqrt{3}\hbar}{2} \\ 0 & 0 & \frac{\sqrt{3}\hbar}{2} & 0 \end{pmatrix}$$

```
Jy // MatrixForm
```

$$\begin{pmatrix} 0 & -\frac{1}{2} i\sqrt{3}\hbar & 0 & 0 \\ \frac{1}{2} i\sqrt{3}\hbar & 0 & -i\hbar & 0 \\ 0 & i\hbar & 0 & -\frac{1}{2} i\sqrt{3}\hbar \\ 0 & 0 & \frac{1}{2} i\sqrt{3}\hbar & 0 \end{pmatrix}$$

```
Jz // MatrixForm
```

$$\begin{pmatrix} \frac{3\hbar}{2} & 0 & 0 & 0 \\ 0 & \frac{\hbar}{2} & 0 & 0 \\ 0 & 0 & -\frac{\hbar}{2} & 0 \\ 0 & 0 & 0 & -\frac{3\hbar}{2} \end{pmatrix}$$

```
h1 = MatrixExp[-ⅈ Jy/ℏ θ] // Simplify;

h11 = h1 /. {θ → π}; h11 // MatrixForm
```

$$\begin{pmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \\ 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}$$

```
h11.h11 // MatrixForm
```

$$\begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$$

52. Spherical tensor under the time reversal

Suppose that the operator $\hat{A}$ is either even or odd.

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

So we see that we have

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

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

In an eigenstate of the angular momentum ($|\alpha, j, m\rangle$, we have

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

with

$$\left|\psi\right\rangle = \left|\alpha, j, m\right\rangle$$

$$\left|\tilde{\psi}\right\rangle = \hat{\Theta}\left|\alpha, j, m\right\rangle = i^m \left|\alpha, j, -m\right\rangle, \qquad \left\langle\tilde{\psi}\right| = \left(i^*\right)^m \left\langle\alpha, j, -m\right|$$

Then we have

$$\begin{aligned}\left\langle\alpha, j, m\right|\hat{A}\left|\alpha, j, m\right\rangle &= \pm i^m \left(i^*\right)^m \left\langle\alpha, j, -m\right|\hat{A}\left|\alpha, j, -m\right\rangle \\ &= \pm\left(\left|i\right|^2\right)^m \left\langle\alpha, j, -m\right|\hat{A}\left|\alpha, j, -m\right\rangle \\ &= \pm\left\langle\alpha, j, -m\right|\hat{A}\left|\alpha, j, -m\right\rangle\end{aligned}$$

Let $\hat{A}$ be a component of a spherical tensor

$$\hat{A} = \hat{T}_{q=0}^{(k)}$$

which is Hermitian operator. $\hat{T}_{q\neq 0}^{(k)}$ is not Hermitian operator.

((**Note**))

For example, the spherical components of $\hat{\boldsymbol{r}}$ are given by

$$T_1^{(1)} = -\frac{1}{\sqrt{2}}(\hat{x} + i\hat{y}), \qquad T_0^{(1)} = \hat{z}, \qquad T_{-1}^{(1)} = \frac{1}{\sqrt{2}}(\hat{x} - i\hat{y})$$

$$T_1^{(1)+} = -\frac{1}{\sqrt{2}}(\hat{x} - i\hat{y}), \qquad T_0^{(1)+} = \hat{z}, \qquad T_{-1}^{(1)+} = \frac{1}{\sqrt{2}}(\hat{x} + i\hat{y})$$

where

$$\begin{aligned}\hat{\Theta} T_1^{(1)} \hat{\Theta}^{-1} &= -\frac{1}{\sqrt{2}}\hat{\Theta}(\hat{x} + i\hat{y}) \\ &= -\frac{1}{\sqrt{2}}[\hat{\Theta}\hat{x} + \Theta(i\hat{y})] \\ &= -\frac{1}{\sqrt{2}}(\hat{x} - i\hat{y}) \\ &= -T_{-1}^{(1)}\end{aligned}$$

$$\hat{\Theta}T_0^{(1)}\hat{\Theta}^{-1} = \hat{\Theta}\hat{z} = \hat{z}$$

$$\begin{aligned}\hat{\Theta}T_{-1}^{(1)}\hat{\Theta}^{-1} &= \frac{1}{\sqrt{2}}\hat{\Theta}(\hat{x} - i\hat{y}) \\ &= \frac{1}{\sqrt{2}}[\hat{\Theta}\hat{x} - \Theta(i\hat{y})] \\ &= \frac{1}{\sqrt{2}}(\hat{x} + i\hat{y}) \\ &= -T_1^{(1)}\end{aligned}$$

We define $T_{q=0}^{(k)}$ to be even (sign: +) or odd (sign: -) under the time reversal

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

Then we have

$$\langle \alpha, j, m|T_{q=0}^{(k)}|\alpha, j, m\rangle = \pm\langle \alpha, j, -m|T_{q=0}^{(k)}|\alpha, j, -m\rangle \qquad (1)$$

The state $|\alpha, j, -m\rangle$ is obtained by rotation

$$\hat{R}_y(\theta = \pi)|\alpha, j, m\rangle = e^{i\varphi}|\alpha, j, -m\rangle$$

We also know the formula given by

$$\hat{R}_y^{+}(\theta)\hat{T}_q^{(k)}\hat{R}_y(\theta) = \sum_{q'=-k}^{k}\langle k, q|\hat{R}_y(\theta)|k, q'\rangle^* \hat{T}_{q'}^{(k)}$$

So we get

$$\begin{aligned}\hat{R}_y^{+}(\pi)\hat{T}_{q=0}^{(k)}\hat{R}_y(\pi) &= \sum_{q'=-k}^{k}\langle k, q=0|\hat{R}_y(\pi)|k, q'\rangle^* \hat{T}_{q'}^{(k)} \\ &= \langle k, 0|\hat{R}_y(\pi)|k, 0\rangle^* \hat{T}_0^{(k)} + \sum_{q'\neq 0}\langle k, q=0|\hat{R}_y(\pi)|k, q'\rangle^* \hat{T}_{q'}^{(k)} \\ &= (-1)^k \hat{T}_0^k + \sum_{q'\neq 0}\langle k, q=0|\hat{R}_y(\pi)|k, q'\rangle^* \hat{T}_{q'}^k\end{aligned}$$

where

$$\langle k,0|\hat{R}_y(\pi)|k,0\rangle = P_k(\cos\pi) = (-1)^k$$

We note that

$$\langle \alpha, j,m|\hat{T}_q^k|\alpha, j,m\rangle = 0 \qquad \text{for } q \neq 0 \qquad \text{(from the } m\text{-selection rule)}$$

So we get

$$\langle \alpha, j,m|\hat{R}_y^+(\pi)\hat{T}_{q=0}^{(k)}\hat{R}_y(\pi)|\alpha, j,m\rangle = (-1)^k \langle \alpha, j,m|\hat{T}_0^k|\alpha, j,m\rangle$$

or

$$\begin{aligned}\langle \alpha, j,m|\hat{T}_0^k|\alpha, j,m\rangle &= (-1)^k \langle \alpha, j,m|\hat{R}_y^+(\pi)\hat{T}_{q=0}^{(k)}\hat{R}_y(\pi)|\alpha, j,m\rangle \\ &= (-1)^k \langle \alpha, j,-m|\hat{T}_{q=0}^{(k)}|\alpha, j,-m\rangle\end{aligned}$$

or

$$\langle \alpha, j,-m|\hat{T}_{q=0}^{(k)}|\alpha, j,-m\rangle = (-1)^k \langle \alpha, j,m|\hat{T}_0^k|\alpha, j,m\rangle \qquad (2)$$

since

$$\hat{R}_y(\theta=\pi)|\alpha, j,m\rangle = e^{i\varphi}|\alpha, j,-m\rangle, \qquad \langle \alpha, j,m|\hat{R}_y^+(\theta=\pi) = e^{-i\varphi}|\alpha, j,-m\rangle$$

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

$$\langle \alpha, j,m|T_{q=0}^{(k)}|\alpha, j,m\rangle = \pm(-1)^k \langle \alpha, j,m|T_{q=0}^{(k)}|\alpha, j,m\rangle$$

((**Note**)) **Wigner-Eckart theorem.**

$$\langle \alpha'; j',m'|\hat{T}_q^{(k)}|\alpha; j,m\rangle = \langle j,k;m,q\,|\,j,k;j',m'\rangle\langle \alpha' j'\|\hat{T}^{(k)}\|\alpha j\rangle$$

with the selection rule,

$$m' = m+q\,,\ \ j' = j+k, j+k-1, ..., |\,j-k\,|\,.$$

53. Electric dipole moment of neutron

In the accepted time-reversal invariant theory of the electromagnetic interaction. The electric dipole moment, the electric dipole moment ($\hat{D} = e\hat{\boldsymbol{r}}$) with a charge e is even under the time reversal. This is consistent with the fact that no electric dipole moment has been observed for any particle.

$$\langle \alpha, j, m | T_{q=0}^{(1)} | \alpha, j, m \rangle = -\langle \alpha, j, m | T_{q=0}^{(1)} | \alpha, j, m \rangle$$

with

$$T_{q=0}^{(1)} = e\hat{D}_z \qquad \text{(which is even under the time-reversal)}$$

Then we get

$$\langle \alpha, j, m | T_{q=0}^{(1)} | \alpha, j, m \rangle = \langle \alpha, j, m | e\hat{D}_z | \alpha, j, m \rangle = 0$$

which implies that no electric dipole moment.

At the present time very accurate measurements are being made on the neutron to see if even a very small electric dipole moment exists, Any such observation would indicate a breakdown of time-reversal symmetry in the theory. It would also indicate a breakdown of space inversion symmetry because accepted space inversion theory has the electric dipole moment as an odd parity operator. Thus if the particle has definite parity, the diagonal matrix elements of the dipole would also vanish for this reason.

((**Note**))

The neutron electric dipole moment (EDM) is a measure for the distribution of positive and negative charge inside the neutron. A finite electric dipole moment can only exist if the centers of the negative and positive charge distribution inside the particle do not coincide. So far, no neutron EDM has been found. The current best upper limit amounts to

$$|d_n| < 2.9 \times 10^{-26} \ e\cdot\text{cm}.$$

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APPENDIX Formula

$$\left|\psi^R\right\rangle = \hat{\Theta}\left|\psi\right\rangle$$

1. $\hat{\Theta} = \hat{U}\hat{K}$, $\hat{\Theta}^{-1} = \hat{K}\hat{U}^+$, ($\hat{U}$; unitary operator, $\hat{K}$; complex conjugate operator)
   $\hat{\Theta}^+ = \hat{K}^+\hat{U}^+ = \hat{K}\hat{U}^+$. $\hat{\Theta}^{-1} = \hat{\Theta}^+$. $\hat{\Theta}\hat{\Theta}^{-1} = \hat{U}\hat{K}^2\hat{U}^+ = \hat{1}$.
2. $\hat{K}^2 = 1$, $\hat{K}^+\hat{K} = 1$, $\hat{K}^+ = \hat{K}^{-1} = \hat{K}$.
3. $\hat{K}c\hat{K}^{-1} = c^*$ where c is a complex
4. $\hat{K}\hat{A}\hat{K}^{-1} = \hat{A}^*$ where $\hat{A}$ is any operator.
5. $\hat{\Theta} = \eta\exp(-\frac{i\pi}{\hbar}\hat{J}_y)\hat{K}$ for spin j
6. $\hat{\Theta} = \eta\exp(-\frac{i\pi}{2}\hat{\sigma}_y)\hat{K} = \eta(-i\hat{\sigma}_y)\hat{K}$ for spin 1/2
7. $\hat{\Theta}\left|l,m\right\rangle = (-1)^m\left|l,-m\right\rangle$ for orbital angular momentum
8. $\hat{\Theta}^2\left|j,m\right\rangle = i^{-4m}\hat{\Theta}\left|j,m\right\rangle$
9. $\hat{\Theta}\left|j,m\right\rangle = i^{2m}\left|j,-m\right\rangle$

10. $\hat{\Theta} = (-i)^N \hat{\sigma}_{1y} \otimes \hat{\sigma}_{2y} \otimes \hat{\sigma}_{3y} \otimes \cdots \otimes \hat{\sigma}_{Ny} \hat{K}$.

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

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

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

14. $\langle \tilde{\alpha} | \hat{\Theta} \hat{A} \hat{\Theta}^{-1} | \tilde{\alpha} \rangle = \langle \alpha | \hat{A} | \alpha \rangle$ ($\hat{A}$ is Hermite operator)

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

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

17. $\psi^R(\boldsymbol{r}, t) = \langle \boldsymbol{r} | \psi^R(t) \rangle = \langle \boldsymbol{r} | \psi(-t) \rangle^* = \psi^*(\boldsymbol{r}, -t)$

18. $\psi^R(\boldsymbol{r}, 0) = \Theta \psi(\boldsymbol{r}, 0) = \psi^*(\boldsymbol{r}, 0)$

19. $|\psi^R(t)\rangle = \hat{\Theta} |\psi(-t)\rangle$. $|\psi^R(0)\rangle = \hat{\Theta} |\psi(0)\rangle$

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

21 $\langle \boldsymbol{k} | \tilde{\phi}_n \rangle = \phi_n^*(-\boldsymbol{k}) = \langle -\boldsymbol{k} | \phi_n \rangle^*$

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

23. $\hat{\Theta} \hat{H} \hat{\Theta}^{-1} = \hat{H}$ ($\hat{H}$: Hamiltonian)

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

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

26. $\hat{\Theta} \hat{\boldsymbol{J}} \hat{\Theta}^{-1} = -\hat{\boldsymbol{J}}$ ($\hat{\boldsymbol{J}}$; angular momentum

27. $\hat{\Theta} \hat{R} \hat{\Theta}^{-1} = \hat{R}$ ($\hat{R}$, rotation operator)

28. $\hat{\Theta} \hat{T}_x(a) \hat{\Theta}^{-1} = \hat{T}_x(a)$ ($\hat{T}_x(a)$; translation operator)

29. $\hat{\Theta} \hat{\pi} \hat{\Theta}^{-1} = \hat{\pi}$ ($\hat{\pi}$; parity operator)

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

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

32. $\langle \alpha'; j', m' | \hat{T}_q^{(k)} | \alpha; j, m \rangle = \langle j, k; m, q | j, k; j', m' \rangle \langle \alpha' j' \| \hat{T}^{(k)} \| \alpha j \rangle$

33. $(\hat{A} \otimes \hat{B})(|\psi_1\rangle \otimes |\psi_2\rangle) = \hat{A} |\psi_1\rangle \otimes \hat{B} |\psi_2\rangle$