Chapter 6: SYMMETRY IN QUANTUM MECHANICS

Since the beginning of physics, symmetry considerations have provided us with an extremely powerful and useful tool in our effort in understanding nature. Gradually they become the backbone of our theoretical formulation of physical laws.

—— T.D. Lee, Particle Physics and an Introduction to Field Theory

For example,

1. Theory of relativity: physical laws are invariant in any reference systems.
2. Quantum field theory: gauge invariance. In 1954, C.N. Yang and Robert Mills extended the gauge theory of Abelian group for QED to non-Abelian group for QCD.
3. (Super)String theory: super-symmetry, or the one-to-one correspondence between boson and fermion. This is an extension to symmetry groups in QFT towards combining QFT and general relativity, i.e., a theory for everything —— Einstein’s dream.
4. The fundamental postulate of statistical mechanics: given an isolated system in equilibrium, it is found with equal probability in each of its accessible microstates.

6.1 Continuous Symmetry

Time evolution invariance (time-independent $H$), space translation invariance, rotational invariance, etc. Noether’s (first) theorem states that any differentiable (continuous) symmetry in a physical system corresponds to a conservation law.

A continuous symmetry can be described by an infinitesimal translational operator

$$\hat{\Omega}(\Delta \lambda)_{\Delta \lambda \to 0} = 1 - i \frac{\Delta \lambda}{\hbar} \hat{G}$$  \hspace{1cm} (6.1)

and the corresponding finite translational operator:

$$\Omega(\lambda) = \exp(-i \frac{G}{\hbar} \lambda), \text{ and } \hat{\Omega}(\lambda)|\Psi(0)\rangle = |\Psi(\lambda)\rangle.$$  \hspace{1cm} (6.2)

Time evolution: \hspace{0.5cm} $G \equiv i \hbar \frac{\partial}{\partial t} = H; \hspace{0.5cm} U(t) = \exp(-iHt / \hbar).$  \hspace{1cm} (6.3)

Space translation: \hspace{0.5cm} $G \equiv -i \hbar \nabla = \mathbf{p}; \hspace{0.5cm} T(r) = \exp(-i \mathbf{p} \cdot \mathbf{r} / \hbar).$  \hspace{1cm} (6.4)

Rotation: \hspace{0.5cm} $G \equiv -i \hbar \frac{\partial}{\partial \varphi} = \mathbf{J}; \hspace{0.5cm} D(\mathbf{n}, \varphi) = \exp[-i(\mathbf{J} \cdot \mathbf{n})\varphi / \hbar].$  \hspace{1cm} (6.5)

Translational invariance means that $\Omega^\dagger H \Omega = H \Rightarrow H \Omega = \Omega H \Rightarrow [G, H] = 0.$ \hspace{1cm} (6.6)
(1) Using **Ehrenfest’s theorem**, one obtain

\[ \frac{\hbar}{i} \frac{d}{dt} \langle G \rangle = \langle [G, H] \rangle = 0. \]  \hspace{1cm} (6.7)

(2) In the **Heisenberg picture**, the equation of motion becomes

\[ \frac{\hbar}{i} \frac{d}{dt} G_H = [G, H] = 0. \]  \hspace{1cm} (6.8)

(3) \( G \) and \( H \) have the same set of eigenstates.

Assume \( |n\rangle \) is an energy eigenstate (eigenket) with eigenvalues of \( E_n \), then

\[ H \left( \Omega |n\rangle \right) = \Omega H |n\rangle = E_n \left( \Omega |n\rangle \right), \]  \hspace{1cm} (6.9)

so the translated state \( \Omega(\lambda) |n(0)\rangle = |n(\lambda)\rangle \) is also an eigenstate of \( H \) with the same energy, i.e., states \( |n\rangle \) and \( |n(\lambda)\rangle \) are degenerate, and all the translated states are degenerate for an invariant translation \( \Omega \).

One example is the rotation invariance, \([D(R), H] = 0\), where a rotation \( R \) is represented by the rotation axis \( \mathbf{n} \) and the rotation angle \( \varphi \), and which implies that \([J, H] = 0\) and \([J^2, H] = 0\).

Then we can form the common eigenkets of \( H, J^2, \) and \( J_z \) denoted by \( |njm\rangle \), and all the rotated states

\[ D(R) |njm\rangle = \sum_{m'=-j}^{j} D^{(ij)}_{m,m'}(R) |njm'\rangle \]  \hspace{1cm} (6.10)

have the same energy. The above expression suggests that (1) if the original state has only \( J_z = mh \) component, then under rotation different \( m \)-values are mixed up. (2) An arbitrary rotated state, which is a linear combination of \((2j+1)\) states of \( |njm'\rangle \), has the same energy, then each of these \((2j+1)\) states are degenerate.

### 6.2 Time Reversion Invariance

We have discussed the continuous symmetry, which can be obtained by applying successively infinitesimal symmetry operations. But not all symmetry operations are continuous, instead, there are many important discrete symmetry operations, such as time reversion, space inversion, crystal lattice translation and rotation, etc. These discrete symmetry operations also lead to
conservation laws, except for time-reversal invariance. However, its consequences for quantum mechanics are indispensible.

Time-reversal means motion reversal. Let’s begin with classical physics. If a particle subject to a force field \( \mathbf{F}(\mathbf{r}) = -\nabla V(\mathbf{r}) \), then reversing time (or reversing the motion) causes the particle to go backward along the same trajectory as the forward motion.

Formally, it \( \mathbf{r}(t) \) is a solution to

\[
m \frac{d^2 \mathbf{r}(t)}{dt^2} = \mathbf{F}(\mathbf{r}) = -\nabla V(\mathbf{r}),
\]

then \( \mathbf{r}(-t) \) is also a possible solution. Time-reversal invariance requires no dissipation force, which depends on motion.

The non-relativistic quantum mechanics allows one to formulate the time reversal in a way close to classical mechanics, but the form of the result depends on the representation. Consider the time-independent Schrödinger equation,

\[
i\hbar \frac{d\psi(\mathbf{r}, t)}{dt} = \mathcal{H}\psi(\mathbf{r}, t),
\]

Under time reversal given by \( t \rightarrow -t \), the equation becomes

\[
i\hbar \frac{d\psi(\mathbf{r}, -t)}{dt} = \mathcal{H}\psi(\mathbf{r}, -t),
\]

The solution \( \psi(\mathbf{r}, -t) \) doesn’t satisfy the original Schrödinger equation (6.12). Take the complex conjugate of Eq. (6.13),

\[
i\hbar \frac{d\psi^*(\mathbf{r}, -t)}{dt} = \mathcal{H}^*\psi^*(\mathbf{r}, -t),
\]

therefore when \( t \rightarrow -t \), \( \psi(\mathbf{r}, t) \rightarrow \psi^T(\mathbf{r}, t) = \psi^*(\mathbf{r}, -t) \) and \( \mathcal{H} \rightarrow \mathcal{H}^T = \mathcal{H}^* \). The off-diagonal matrix element of \( \mathcal{H} \):

\[
\mathcal{H}_{12} = \langle \psi_1(t) | \mathcal{H} | \psi_2(t) \rangle.
\]

Then the time-reversed matrix element

\[
\mathcal{H}_{12}^T = \langle \psi_2(-t) | \mathcal{H}^T | \psi_1(-t) \rangle.
\]

The transformed Hamiltonian coincide with the original one if it is real, for example, the ordinary one particle Hamiltonian in a real potential,

\[
\mathcal{H} = -\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{r}),
\]
then the system is time-reversal invariant (TRI), and both $\psi(r, t)$ and $\psi^*(r, -t)$ are solutions to the same Schrödinger equation (6.12).

**Time-reversal operator** $\Theta$ defined as $|\psi^T\rangle \equiv \Theta |\psi\rangle$, which is an anti-unitary operator. Thus, we expect that $|p^T\rangle = \Theta |p\rangle = e^{i\phi} |p\rangle$. Let’s work out the explicit form of $\Theta$. Since quantum states are linear, i.e., $|\psi\rangle$ is a linear combination of other states, $|\psi\rangle = a|\alpha\rangle + b|\beta\rangle$, then

$$\Theta\left(a|\alpha\rangle + b|\beta\rangle\right) = a^*|\alpha^T\rangle + b^*|\beta^T\rangle,$$  \hspace{1cm} (6.18)

$\Theta$ is antilinear. So we can write $\Theta = UK$, where $U$ is an unitary operator, while the complex conjugate operator $K$ has the following property:

$$K\left(a|\alpha\rangle\right) = a^*K|\alpha\rangle.$$  \hspace{1cm} (6.19)

Expressing state $|\alpha\rangle$ in terms of a complete set of basis states,

$$|\alpha\rangle = \sum_{n}a_{n}\langle a_{n}|\alpha\rangle,$$  \hspace{1cm} (6.20)

we apply the time-reversal operator,

$$|\alpha^T\rangle = UK|\alpha\rangle = \sum_{n}\langle a_{n}|\alpha^*\rangle UK|a_{n}\rangle = \sum_{n}\langle \alpha|a_{n}\rangle U|a_{n}\rangle.$$  \hspace{1cm} (6.21)

Similarly, we have $|\beta\rangle = \sum_{n}a_{n}\langle a_{n}|\beta\rangle$, then

$$|\beta^T\rangle = \sum_{n}\langle \beta|a_{n}\rangle U|a_{n}\rangle,$$  \hspace{1cm} and $$\langle \beta^T| = \sum_{n}\langle a_{n}|\beta\rangle a_{n}|U^\dagger\rangle,$$  \hspace{1cm} (6.22)

Then taking the scalar product we find that

$$\langle \beta^T|alpha^T\rangle = \sum_{n}\sum_{m}\langle \alpha|a_{n}\rangle \langle a_{m}|\beta\rangle \langle a_{m}|U^\dagger U|a_{n}\rangle = \sum_{n}\langle \alpha|a_{n}\rangle \langle a_{n}|\beta\rangle = \langle \alpha|\beta\rangle,$$  \hspace{1cm} (6.23)

because $U^\dagger U = 1$, and $\langle a_{m}|a_{n}\rangle = \delta_{mn}$.

Using the coordinate representation, the time-reversed state

$$|\psi^T\rangle = \Theta |\psi\rangle = \int \psi(\mathbf{r}) K(r, \psi) d^3r = \int |\psi(\mathbf{r})\rangle \langle \mathbf{r}| d^3r.$$  \hspace{1cm} (6.24)

The time-reversed wave function

$$\psi^T(\mathbf{r}) = \langle \mathbf{r}|\psi^T\rangle = \langle \mathbf{r}|\psi^*\rangle = \int \langle \mathbf{r}|\mathbf{r}'\rangle \langle \psi|\psi'\rangle d^3r' = \langle \psi|\mathbf{r}\rangle = \langle \mathbf{r}|\psi\rangle^* = \psi^*(\mathbf{r}).$$  \hspace{1cm} (6.25)

Thus we reproduced our previous result of $t \rightarrow -t$, $\psi(\mathbf{r}, t) \rightarrow \psi^T(\mathbf{r}, -t) = \psi^*(\mathbf{r}, -t)$.  

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The consequence of time reversal

A. The time-reversed states: \( \Theta |r\rangle = |r\rangle \), while \( \Theta |p\rangle = |-p\rangle \). (up to a phase)

The time-dependent wave function:
\[
\Psi(t) = \sum_{j=1} e^{-iE_j t/\hbar} c_j \psi_j \rightarrow \Psi^T(t) = \sum_{j=1} e^{-iE_j t/\hbar} c_j^* \psi_j^* .
\] (6.26)

B. The time-reversed operator: \( \hat{A} \rightarrow \hat{A}^\dagger = \Theta^{-1} \hat{A} \Theta \)
\[
\Theta^{-1} \hat{r} \Theta = \hat{r}, \quad \Theta^{-1} \hat{p} \Theta = -\hat{p} .
\] (6.27)

The corresponding observables are even and odd under time reversal, respectively.

For a particle in a real potential, \( H = \frac{\hat{p}^2}{2m} + V(r) \),
\[
\Theta^{-1} H \Theta = H, \quad \text{or} \quad H \Theta = \Theta H .
\] (6.28)

It is time-reversal invariant (TRI). TRI is violated in nature. However, this violation was only observed as a small effect in specific process of decay of neutral K- and B-mesons.

The fundamental commutator \( [\hat{r}_i, \hat{p}_j] = i\hbar \delta_{ij} \) is preserved under time reversal:
\[
\Theta^{-1} [\hat{r}_i, \hat{p}_j] \Theta = [\hat{r}_i, -\hat{p}_j] = -i\hbar \delta_{ij} ,
\] (6.29)
while \( \Theta^{-1} i\hbar \delta_{ij} \Theta = -i\hbar \delta_{ij} \). Similarly, in order to preserve \( [\hat{J}_i, \hat{J}_j] = i\hbar \epsilon_{ijk} \hat{J}_k \), the angular momentum operator must be odd under time reversal:
\[
\Theta^{-1} \hat{J} \Theta = -\hat{J} .
\] (6.30)

Then the angular momentum state \( |l, m\rangle \rightarrow |l, -m\rangle \) under time reversal, which is consistent with
\[
Y_l^m(\theta, \phi) \rightarrow Y_l^{-m}(\theta, \phi) = (-1)^m Y_l^{-m}(\theta, \phi) .
\] (6.31)
where \( Y_l^m(\theta, \phi) \) is the wave function for state \( |l, m\rangle : Y_l^m(\theta, \phi) = \langle \theta, \phi | l, m \rangle \).

Then
\[
\Theta |l, m\rangle = (-1)^m |l, -m\rangle .
\] (6.32)

Time reversal for spin-half systems

A state with spin directed along a unit vector \( \mathbf{n} \) with polar angle \( \alpha \) and azimuthal angle \( \beta \) is given in terms of the spin-up state along the z-axis \( |+\rangle \equiv |z; +\rangle \) by
\[
|\mathbf{n}; +\rangle = e^{-iS_z \beta /\hbar} e^{-iS_x \alpha /\hbar} |+\rangle ,
\] (6.33)
\[
|\mathbf{n}; -\rangle = e^{-iS_z \beta /\hbar} e^{-iS_y (\alpha + \pi) /\hbar} |+\rangle .
\] (6.34)

Under the time reversion, based on Eq. (6.32) we expect that
\[ \Theta |\mathbf{n};+\rangle = \eta |\mathbf{n};-\rangle. \]  (6.35)

Comparing Eqs. (6.34) and (6.35),

\[ \Theta = \eta e^{-i\pi S_z/\hbar} K. \]  (6.36)

Note that

\[ e^{-i\pi S_z/\hbar} |+\rangle = + |-\rangle \quad \text{and} \quad e^{-i\pi S_z/\hbar} |-\rangle = - |+\rangle. \]  (6.37)

**Question: how to prove the above equations?**

Then for an arbitrary spin-half state \( |\chi\rangle = c_+ |+\rangle + c_- |-\rangle \),

\[ \Theta |\chi\rangle = \eta c_+ |-\rangle - \eta c_- |+\rangle \]  (6.38)

\[ \Theta^2 |\chi\rangle = \eta^2 (c_+ |+\rangle + c_- |-\rangle) = - |\chi\rangle. \]  (6.39)

Hence for spin-half states we have the most usual property,

\[ \Theta^2 = -1. \]  (6.40)

More generally,

\[ \Theta^2 = -1, \quad \text{for } j = \text{half-integer} \]  (6.41)

\[ \Theta^2 = +1, \quad \text{for } j = \text{integer} \]  (6.42)

The time-reversal operator becomes

\[ \Theta = \eta e^{-i\pi J_y/\hbar} K. \]  (6.43)

For an arbitrary state with a well-defined angular momentum quantum number \( j \) (e.g., a rotated eigenstate \( D(R) |jm\rangle \)), \( |\chi\rangle = \sum_m |jm\rangle \langle jm|\chi\rangle \), we have

\[ \Theta |\chi\rangle = \eta \sum_m e^{-i\pi J_y/\hbar} |jm\rangle \langle jm|\chi\rangle \]  (6.44)

\[ \Theta^2 |\chi\rangle = \eta^2 \eta \sum_m e^{-i2\pi J_y/\hbar} |jm\rangle \langle jm|\chi\rangle = \sum_m e^{-i2\pi J_y/\hbar} |jm\rangle \langle jm|\chi\rangle \]  (6.45)

Because (**Question: how to derive this?**) \n
\[ e^{-i2\pi J_y/\hbar} |jm\rangle = (-1)^{2j} |jm\rangle, \]  (6.46)

we obtain the final result:

\[ \Theta^2 |\chi\rangle = (-1)^{2j} |\chi\rangle. \]  (6.47)

**Question: But is the above result consistent with Eq. (6.32), \( \Theta |l,m\rangle = (-1)^m |l,-m\rangle \)?**

In general, one can take.

\[ \Theta |j,m\rangle = (-1)^m |j,-m\rangle = i^{2m} |j,-m\rangle. \]  (6.48)
6.3 Space Inversion and Parity

Another discrete symmetry if the Hamiltonian is important for the search and classification of stationary states. The space inversion (parity transformation) operator $\Pi$ changes the sign of spatial coordinates so that the localization state of a particle $|r\rangle$ transforms as

$$\Pi |r\rangle = |-r\rangle.$$  \hspace{1cm} (6.49)

It follows that

$$\Pi |p\rangle = |-p\rangle,$$  \hspace{1cm} (6.50)

$$\psi^{\prime}\langle r | \Pi | \psi \rangle = \langle -r | \psi \rangle = \psi(-r).$$  \hspace{1cm} (6.51)

Note: in one-dimension, $\psi(-x)$ is the mirror image of $\psi(x)$ about the origin.

From Eq. (6.49) one can derive $\Pi^2 |r\rangle = \Pi |-r\rangle = |r\rangle$, then

$$\Pi^2 = I.$$  \hspace{1cm} (6.52)

From this we obtain that

1) $\Pi = \Pi^{-1}$.

2) The eigenvalue of $\Pi$ are $\pm 1$.

3) $\Pi$ is Hermitian and unitary.

4) Then $\Pi^{-1} = \Pi^\dagger = \Pi$.

Parity ($\pi$): eigenvalue of the operator $\Pi$. If a state has a definite parity, then

$$\Pi |\psi\rangle = |\psi^{\prime}\rangle = \pi_{\psi} |\psi\rangle,$$  \hspace{1cm} (6.53)

where $\pi_{\psi}$ is either $+1$ or $-1$. $\psi(-r) = \langle -r | \psi \rangle = \langle r | \Pi | \psi \rangle = \langle r | \pi_{\psi} | \psi \rangle = \pm \langle -r | \psi \rangle = \pm \psi(r)$.

Space reversion of operators:

$$\Pi^{-1}r\Pi = -r,$$  \hspace{1cm} (6.54)

and

$$\Pi^{-1}\hat{p}\Pi = -\hat{p},$$  \hspace{1cm} (6.55)

Which can proved by considering the infinitesimal space transformation

$$\Pi T(dr) = T(-dr)\Pi,$$  \hspace{1cm} (6.56)

$$\Pi \left(I - \frac{\vec{\hat{p}} \cdot dr}{\hbar}\right) = \left(I + \frac{\vec{\hat{p}} \cdot dr}{\hbar}\right)\Pi.$$  \hspace{1cm} (6.57)

Then we obtain
\[ \Pi \mathbf{p} + \mathbf{p} \Pi = \{\Pi, \mathbf{p}\} = 0, \] or equivalently \( \Pi^{-1} \mathbf{p} \Pi = -\mathbf{p} \). \hfill (6.58)

**Angular momentum under space reversion:**

\[ \Pi^{-1} \mathbf{L} \Pi = \mathbf{L}, \quad \text{or} \quad [\Pi, \mathbf{L}] = 0, \] \hfill (6.59)

because the orbital angular momentum \( \hat{\mathbf{L}} = \mathbf{r} \times \mathbf{p} \).

Under rotations, vectors \( \mathbf{r}, \mathbf{p} \) and \( \mathbf{L} \) behave in the same way; however, under space reversion, parities of \( \mathbf{r} \) and \( \mathbf{p} \) are odd \((-1)\) while the parity of \( \mathbf{L} \) is even \((+1)\)! The former is called **polar vectors**, while the latter is called **axial vectors** or **pseudovector**.

Consider the scalar operators \( \mathbf{S} \cdot \mathbf{r}, \mathbf{S} \cdot \mathbf{L} \) and \( \mathbf{r} \cdot \mathbf{p} \), under rotations they behave in the same way like an ordinary scalar; however, under space reversion,

\[ \Pi^{-1} \mathbf{S} \cdot \mathbf{r} \Pi = -\mathbf{S} \cdot \mathbf{r}, \quad \text{while} \quad \Pi^{-1} \mathbf{S} \cdot \mathbf{L} \Pi = \mathbf{S} \cdot \mathbf{L} \quad \text{and} \quad \Pi^{-1} \mathbf{r} \cdot \mathbf{p} \Pi = \mathbf{r} \cdot \mathbf{p}. \] \hfill (6.60)

So the operator \( \mathbf{S} \cdot \mathbf{r} \) is a **pseudoscalar**.

Space reversion in 3D can be written as a matrix,

\[ R^\Pi = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \] \hfill (6.61)

and it commutes with an arbitrary 3D real-space rotation: \( R^\Pi R = RR^\Pi \), therefore,

\[ \Pi D(R) = D(R) \Pi. \] \hfill (6.62)

Since quantum rotation operator \( D(R) = e^{-i\frac{\mathbf{J} \cdot \mathbf{n}}{\hbar} \phi} \), and an infinitesimal rotation \( D(R) = I - i \frac{\mathbf{J} \cdot \mathbf{n}}{\hbar} d\phi \),

we obtain that

\[ \Pi^{-1} \mathbf{J} \Pi = \mathbf{J}, \quad \text{or} \quad [\Pi, \mathbf{J}] = 0. \] \hfill (6.63)

Not all wave functions are eigenstate of \( \Pi \), i.e., they might not have definite parities. An eigenstate of orbital angular momentum is expected to have a definite parity (Q: why?) The common eigenstate of \( \hat{\mathbf{L}}^2 \) and \( \hat{L}_z \) is denoted as \(|nlm\rangle\), then the wave function

\[ \langle \mathbf{r} | nlm \rangle = R_n(r) Y_l^m(\theta, \phi). \] \hfill (6.64)

Under the space reversion transformation \( \mathbf{r} \rightarrow -\mathbf{r}, \)

\[ \begin{align*}
\mathbf{r} & \rightarrow -\mathbf{r}, \\
\theta & \rightarrow \pi - \theta \quad \text{and} \quad (\cos \theta \rightarrow -\cos \theta) \\
\phi & \rightarrow \pi + \phi \quad \text{and} \quad [e^{im\phi} \rightarrow (-1)^m e^{im\phi}] 
\end{align*} \hfill (6.65)

Using the expression for spherical harmonics,
\[ Y_l^m(\theta, \phi) = (-1)^m \sqrt{\frac{(2l+1)(l-m)!}{4\pi(l+m)!}} P_l^m(\cos \theta) e^{im\phi}. \] (6.66)

For positive \( m \),
\[ P_l^{m+l}(\cos \theta) = \frac{(-1)^{m+l}}{2^l l!} \frac{(l+m)!}{(l-m)!} \sin^{-m+l}(\theta) \frac{d}{d(\cos \theta)} \frac{\sin^{2l} \theta}{\sin^{-m+l}(\theta)}. \] (6.67)

We can show that
\[ Y_l^m \rightarrow (-1)^l Y_l^{-m}, \] (6.68)
under space reversion as \( \theta \) and \( \phi \) change as in Eq. (6.65). Therefore, we find the parity for the eigenstate of \( \ket{nlm} \)
\[ \Pi \ket{nlm} = (-1)^l \ket{nlm}. \] (6.69)

An alternative way to prove the above expression is to work with \( m = 0 \) and using the ladder operator \( L_\pm \). Because \( \Pi \) and \( L_\pm \) (\( m = 0, 1, 2, \ldots, l \)) commute, \( L_\pm \ket{l,0} \) must all have the same parity as that of \( \ket{l,0} \), which is obviously equal to \((-1)^l\).

**Spontaneous symmetry breaking**

Consider the double-well potential as shown on the right. The two lowest eigenstates are denoted as the symmetric state \( \ket{S} \) and the anti-symmetric state \( \ket{A} \) with eigenenergies of \( E_S \) and \( E_A \). **Question**: which state has lower energy? Why?

We can form
\[ \ket{R} = \frac{1}{\sqrt{2}} \left( \ket{S} + \ket{A} \right), \] (6.70)
\[ \ket{L} = \frac{1}{\sqrt{2}} \left( \ket{S} - \ket{A} \right). \] (6.71)

Since \( \ket{S} \) and \( \ket{A} \) are not degenerate, \( \ket{R} \) and \( \ket{L} \) are not eigenstates of \( H \), so they are non-stationary. If at \( t = 0 \), \( \ket{\psi} = \ket{R} \), then
\[ |\psi(t)\rangle = \frac{1}{\sqrt{2}} \left( e^{-iE_S t/\hbar} |S\rangle + e^{-iE_A t/\hbar} |A\rangle \right) = e^{-i\Omega t} \left( \cos(\omega t) |R\rangle + \sin(\omega t) |L\rangle \right), \]  

(6.72)

where \( \Omega = (E_A + E_S) / 2\hbar \) and \( \omega = (E_A - E_S) / 2\hbar \), oscillating between \( |R\rangle \) are \( |L\rangle \). The system is \textit{NOT polarized} in average, though it is polarized instantaneously.

This behavior is a dynamical manifestation of quantum tunneling. Now if the barrier becomes infinitely high \( (V_0 \gg E_A, E_S) \), as shown on the right. Then \( |S\rangle \) and \( |A\rangle \) are \textit{degenerate} (\( \omega \) becomes very small, and the oscillation period becomes extremely long), which means that \( |R\rangle \) and \( |L\rangle \) also eigenstates of \( H \). Then both \( |R\rangle \) and \( |L\rangle \) are stationary states – once the system stays in either \( |R\rangle \) or \( |L\rangle \), it stays there forever, and it is \textbf{polarized}.

A symmetric potential might lead to asymmetric (no well-defined parity) ground-state due to degeneracy – the \textbf{spontaneous symmetry breaking}. It is crucial in nature, responsible for many fundamental mechanisms, such as the formation of magnets, superconductors, and Higgs mechanisms.

One example is the \textbf{optical isomerism}. Two forms of the same chemical compound, isomers, were found to rotate polarized light in two different directions – one to the left, the other to the right. Isomers are essentially identical chemical compounds. They have the same number and type of atoms and the same structure, almost. The difference in the two isomers of a compound is that one is the mirror image of the other, so that it is not superposable on its mirror image. They are called \textit{chiral} objects, and its \textit{chirality} is designated as left-handed or right-handed. Achiral objects are superposable to their mirror images, such as a right circular cone.

\[ \text{Fig. 12.2: Symmetric and antisymmetric states when the potential barrier is infinity.} \]

\[ \text{Fig. 6.3: The ammonia molecules.} \]

\[ \text{Fig. 6.4: Two generic amino acids.} \]
One example is the ammonia molecule, as seen above. They correspond to the \( |R\rangle \) and \( |L\rangle \) states, and the common eigenstates of parity and Hamiltonian (\( |S\rangle \) and \( |A\rangle \)) are the superpositions of them. The oscillation frequency \( f = \omega / 2\pi = 24,000 \) MHz, with wave length \( \lambda \approx 1 \) cm.

Other chiral organic molecules, such as amino acids and sugar, have very longer oscillation time, on the order of \( 10^4 – 10^6 \) years. In lab we always produce equal mixtures of R-type and L-type such organic molecules; but interestingly, living organisms were able to synthesize and use only one isomer and never the other.

**Violation of Parity Conservation**

In 1947 Cecil F. Powell photographed cloud chamber tracks of charged particles and identified the pi meson – the particle postulated twelve years earlier by the physicist Hideki Yukawa, as the intermediary for the nuclear force. Two years later, he identified the \( \tau \)-meson, which disintegrated into three pions, and the \( \theta \)-meson, which disintegrated into two pions.

Both particles have exactly the same mass and lifetime (within experimental error). However, since the pion has parity of -1, two pions would combine to produce a net parity of \((-1)(-1) = +1\), and three pions would combine to have total parity of \((-1)(-1)(-1) = -1\). Hence, if conservation of parity holds, the \( \theta \)-meson should have parity of +1, and the \( \tau \)-meson of -1. This is the \( \theta-\tau \) puzzle.

The conservation of parity was confirmed experimentally for the strong and electromagnetic interactions, and scientists naturally believed that it is also conserved for weak interactions those particles are involved. In 1956, T.D. Lee and C.N. Yang pointed out that there was no experimental evidence of parity conservation for weak interactions. They

![Gamma-positron decay](image)
argued that $\theta$- and $\tau$- mesons would be identical if parity is violated in weak interactions. A few months later, C.S. Wu et al. confirmed their idea.

They looked at the change of pseudoscalar $\langle S \rangle \cdot p$ under mirror reflection, which shall just change the sign if parity is conserved. Therefore, for the beta-decay process of $^{60}\text{Co} \rightarrow ^{60}\text{Ni} + e^- + \bar{\nu}_e$, if $^{60}\text{Co}$ is polarized, then number of up and down electrons emitted must be equal. Instead, they found perfect correlation with asymmetric beta-decay signals to the degree of nuclear polarization. Thus parity conservation in weak interaction is violated.

6.4 Barry’s phase, or geometric phase


The arbitrary phase of a quantum state, $\delta$ (phase factor $e^{i\delta}$), is obviously cannot be determined experimentally. Mathematically we set it to be some values for consistency. But Barry’s phase is uniquely defined by a contour integration.

For a time-dependent Schrödinger equation,

$$i\hbar \frac{\partial}{\partial t} \left| \psi_n(t) \right\rangle = H \left| \psi_n(t) \right\rangle = E_n \left| \psi_n(t) \right\rangle$$

(6.73)

The general solution is

$$\left| \psi_n(t) \right\rangle = e^{i\delta} e^{-iE_n t/\hbar} \left| \psi_n(0) \right\rangle$$

(6.74)

Then under adiabatic variation, i.e., Hamiltonian varies extremely slowly, we can write

$$i\hbar \frac{\partial}{\partial t} \left| \psi_n(t) \right\rangle = H(t) \left| \psi_n(t) \right\rangle = E_n(t) \left| \psi_n(t) \right\rangle$$

(6.75)

The general solution is

$$\left| \psi_n(t) \right\rangle = e^{i\gamma_n(t)} e^{-i\alpha_n(t)} \left| \phi_n(t) \right\rangle$$

(6.76)

Here the dynamical phase is

$$\alpha_n(t) = \frac{1}{\hbar} \int_0^t E(t') dt'$$

(6.77)

and the geometric (Berry’s) phase is

$$\gamma_n(t) = \int_0^t i \left\langle \phi_n(t') \left| \frac{\partial}{\partial t} \phi_n(t') \right\rangle \right| dt'$$

(6.78)

The variation in time is dictated by a parameter or a set of parameter, for example, position $r$. 

then using the chain rule, \( \frac{\partial \phi}{\partial t} = \frac{\partial \phi}{\partial r} \frac{\partial r}{\partial t} \), one obtains

\[
\gamma_n(t) = \int_t^{r_f} i \langle \phi_n(r) \rangle [\nabla_r \phi_n(r)] \cdot dr
\]  

(6.79)

In the case of the vector \( r \) traces a closed contour, i.e., \( r_i = r(0) = r(T) = r_f \), the contour integration determines uniquely the geometric phase

\[
\gamma_n(C) = i \oint_C \langle \phi_n(r) \rangle [\nabla_r \phi_n(r)] \cdot dr
\]  

(6.80)

Now the geometric phase \( \gamma_n(C) \) depends only on the contour integral, independent of arbitrary quantum phase. That is when \( |\phi_n(r, t)\rangle \rightarrow e^{i\delta(r)} |\phi_n(r, t)\rangle \), Eq. (6.80) is invariant.

**Berry’s phase for spin-1/2 system:** \( \gamma_{\pm}(C) = \mp \frac{1}{2} \Omega \), where \( \Omega \) is the solid angle subtended by the path through the vector \( r(t) \) travels. This is a significant result due to ultra-relativity.


6.5 Wigner-Eckart Theorem

Early this semester we studied the quantum radiation theory, i.e., the interaction of electromagnetic field with atoms. It is often necessary to evaluate matrix elements of vector and tensor operators with respect to angular-momentum eigenstates.

For example, within the electric dipole approximation, we need to evaluate
\[
\langle f | \mathbf{p} | i \rangle = \imath m \omega_f \langle f | \mathbf{r} | i \rangle. \tag{6.81}
\]

However, when the first-order electric dipole transition vanishes (forbidden), the second-order magnetic dipole and electric quadrupole approximations are responsible for the much weaker optical transitions. The corresponding tensor operators are
\[
\hat{M}^+ = \frac{1}{2}[(\mathbf{k} \cdot \mathbf{r})(\bar{\mathbf{\xi}} \cdot \bar{\mathbf{p}}) + (\bar{\mathbf{\xi}} \cdot \mathbf{r})(\mathbf{k} \cdot \bar{\mathbf{p}})], \quad \hat{M}^- = \frac{1}{2}[(\mathbf{k} \cdot \mathbf{r})(\bar{\mathbf{\xi}} \cdot \bar{\mathbf{p}}) - (\bar{\mathbf{\xi}} \cdot \mathbf{r})(\mathbf{k} \cdot \bar{\mathbf{p}})]. \tag{6.82}
\]

These are Cartesian tensor operators, defined as
\[
T_{ijk \ldots} = UVW_{ik \ldots}
\]
where \( U, \ V, \ W \ldots \) are vector operators. A rank \( k \) Cartesian operator \( T^{(k)} \) has \( 3^k \) components; under rotation \( R \) (a \( 3 \times 3 \) matrix) it transforms as the following,
\[
T_{ijk \ldots} \rightarrow \sum_i \sum_j \sum_{k'} R_{i,i'}R_{j,j'}R_{k,k'} \ldots T'_{i',j',k'} \tag{6.84}
\]

6.5.1 Irreducible spherical tensors

But the Cartesian tensor \( (k > 1) \) is reducible, i.e., it can be decomposed to a number of irreducible spherical tensors, which are denoted as \( T^{(k)}_q \). For example, the rank 2 tensor,
\[
UV_j = \frac{U \cdot V}{3} \delta_j + \frac{UV_j - UV_i}{2} + \left( \frac{UV_j + UV_i}{2} - \frac{U \cdot V}{3} \delta_j \right), \tag{6.85}
\]
is decomposed into a scalar, vector, and a rank 2 spherical tensor, corresponding to \( 3 \times 3 = 1 + 3 + 5 \).

A rank \( k \) spherical tensor operator \( T^{(k)}_q \) has \( 2k+1 \) \( (q \text{ runs from } -k \text{ to } k) \) components; under rotation, it transform as
\[
D^1(R)T^{(k)}_q D(R) = \sum_{q=-k}^k D^{k\gamma}_\delta T^{(k)}_\gamma \tag{6.86}
\]
Considering an infinitesimal rotation, one can verify that the above condition is equivalent to
\[
[J_z, T^{(k)}_q] = \hbar T^{(k)}_q; \quad [J_{\pm}, T^{(k)}_q] = \sqrt{(k \pm q)(k \pm q + 1)} \hbar T^{(k)}_q. \tag{6.87}
\]
Eq. (6.87) suggests a one-to-one correspondence between a spherical tensor $T_q^{(k)}$ and spherical harmonics $Y_{l}^{m}(\theta, \phi)$, when $k = l$ and $q = m$. Here $(\theta, \phi)$ defines a unit vector $\mathbf{n} = \left\{ \frac{x}{r}, \frac{y}{r}, \frac{z}{r} \right\}$ with $r = \sqrt{x^2 + y^2 + z^2}$. We can write down $Y_{l}^{m}(\theta, \phi)$ as

$$
Y_{l}^{m}(\theta, \phi) = \frac{\sqrt{2l+1}}{4\pi} \sin(\theta) e^{im\phi} = \frac{\sqrt{2l+1}}{4\pi} \frac{x + iy}{r},
$$

$$
Y_{l}^{0}(\theta, \phi) = \frac{\sqrt{2l+1}}{4\pi} \sin(\theta) = \frac{\sqrt{2l+1}}{4\pi} \frac{z}{r},
$$

$$
Y_{l}^{-m}(\theta, \phi) = \frac{\sqrt{2l+1}}{4\pi} \sin(\theta) e^{-im\phi} = \frac{\sqrt{2l+1}}{4\pi} \frac{x - iy}{r}. \tag{6.88}
$$

Similarly, we can define a rank 1 spherical tensor for an arbitrary vector $\mathbf{V}$ as the following:

$$
T^{(1)}_1 = -\frac{V_x + iV_y}{\sqrt{2}} \equiv V_{+1}, \quad T^{(1)}_0 = V_z \equiv V_0, \quad T^{(1)}_{-1} = -\frac{V_x - iV_y}{\sqrt{2}} \equiv V_{-1}, \tag{6.89}
$$

where $V_{\pm 1}$ and $V_0$ are alternative components of the vector $\mathbf{V}$.

Then a rank 2 Cartesian tensor operator $T^{(2)}_q$ for two vectors $\mathbf{U}$ and $\mathbf{V}$, $T_q = U_i V_j$, is decomposed into three spherical tensor operators with rank = 0, 1, and 2, respectively,

$$
T^{(0)}_0 = -\frac{\mathbf{U} \cdot \mathbf{V}}{3} = \frac{U_{+1}V_{-1} + U_{-1}V_{+1} - U_0V_0}{3}, \quad T^{(1)}_q = \frac{\mathbf{U} \times \mathbf{V}}{i\sqrt{2}}, \tag{6.90}
$$

$$
T^{(2)}_{\pm 2} = U_{\pm 1}V_{\pm 1}, \quad T^{(2)}_{\pm 1} = \frac{U_{+1}V_{0} + U_{0}V_{+1}}{\sqrt{2}}, \quad T^{(2)}_{0} = \frac{U_{+1}V_{-1} + 2U_{0}V_{0} + U_{-1}V_{+1}}{\sqrt{6}}.
$$

Systematically, we construct irreducible tensor $T^{(k)}_q$ by multiplying two irreducible tensor operators $X^{(k)}_{q_1}$ and $Z^{(k)}_{q_2}$:

$$
T^{(k)}_q = \sum_{q_1} \sum_{q_2} \langle k_1 k_2 ; q_1 q_2 | k_1 k_2 ; q k \rangle X^{(k)}_{q_1} Z^{(k)}_{q_2}, \tag{6.91}
$$

Here $\langle k_1 k_2 ; q_1 q_2 | k_1 k_2 ; q k \rangle$ is the Clebsch-Gordan coefficients, $| k_1 - k_2 | \leq k \leq k_1 + k_2$, $q = q_1 + q_2$, runs from $-k$ to $k$. Obviously, Eq. (6.91) corresponds to

$$
| l_{12}^1 lm \rangle = \sum_{m_1} \sum_{m_2} \langle l_{12}^1 ; m_1 m_2 | l_{12}^1 lm \rangle | l_{12}^1 m_1 \rangle \otimes | l_{12}^1 m_2 \rangle. \tag{6.92}
$$

Therefore, one can construct tensor operators of higher or lower ranks from two tensor operators.

### 6.5.2 Wigner-Eckart theorem

This is one of the most important theorems in quantum mechanics, which states that the matrix elements of a tensor operator with respect to angular-momentum eigenstates satisfy
\[ \langle j' m'| T_q^{(k)} | j m \rangle = \langle jk; mq | jk; j'm' \rangle \langle j' \bigg | T_q^{(k)} \bigg | j \rangle, \]

(6.93)

where the reduced matrix elements \( \langle j' \bigg | T_q^{(k)} \bigg | j \rangle \) depend only on \( k, j \) and \( j' \). Eq. (6.93) tells us that, for a given set of \( k, j \) and \( j' \), if the matrix elements \( \langle j' m'| T_q^{(k)} | j m \rangle \) for one specific combination of \( m', m \) and \( q \) is known, then the rest of the matrix elements are determined by the CG coefficients \( \langle jk; mq | j'm' \rangle \). It allows considerable simplifications in calculating the matrix elements and leads to many interesting selection rules for non-zero matrix elements.

**Proof** of the Wigner-Eckart theorem. From Eq. (6.87) we obtain

\[ \langle j' m'| [J_\pm, T_q^{(k)}] | j m \rangle = h \sqrt{(k \mp q)(k \pm q + 1)} \langle j' m'| T_q^{(k)} | j m \rangle. \]

(6.94)

On the other hand, the left-hand side is

\[ \langle j' m'| [J_\pm, T_q^{(k)}] | j m \rangle = h \sqrt{(j' \pm m')(j' \mp m' + 1)} \langle j', m' \mp 1 | T_q^{(k)} | j m \rangle \]

\[ - h \sqrt{(j \mp m)(j \pm m + 1)} \langle j'm' | T_q^{(k)} | j, m \pm 1 \rangle. \]

(6.95)

Combining Eqs. (6.94) and (6.95), the recursion relations are derived

\[ \sqrt{(j' \pm m')(j' \mp m' + 1)} \langle j', m' \mp 1 | T_q^{(k)} | j m \rangle = \]

\[ \sqrt{(j \mp m)(j \pm m + 1)} \langle j'm' | T_q^{(k)} | j, m \pm 1 \rangle + \sqrt{(k \mp q)(k \pm q + 1)} \langle j'm' | T_q^{(k)} | j m \rangle. \]

(6.96)

This is exactly the same as Eq. 4.42, if we make the following substitutions

\[ j' \rightarrow j, \ m' \rightarrow m, \ j \rightarrow j, \ m \rightarrow m, \ k \rightarrow k, \ q \rightarrow m. \]

(6.97)

Therefore \( \langle j'm'| T_q^{(k)} | jm \rangle \) is proportional to the CG coefficient \( \langle jk; mq | jk; j'm' \rangle \) by a constant \( \lambda \), which depends only on \( k, j \) and \( j' \). We can set \( \lambda = \langle j' \bigg | T_q^{(k)} \bigg | j \rangle \), the reduced matrix elements.

This proves the Wigner-Eckart theorem.

**6.5.3 Applications of the Wigner-Eckart theorem**

**Example 1.** Prove that \( \langle j' m'| T_q^{(k)} | jm \rangle = 0 \), unless \( |j' - j| \leq k \leq j' + j \) and \( q = m' - m \).

**Example 2.** Selection rules for optical transitions within the electric dipole approximation.

Here the transition matrix elements are \( \langle j'm'| p | jm \rangle \), and the operator \( p \) is a rank 1 tensor, which can be written as a spherical tensor \( T_q^{(1)} |_{q=\pm 1, 0} \). Thus we obtain the selection rules,

\[ \Delta m \equiv m' - m = \pm 1, 0; \quad \Delta j \equiv j' - j = \begin{cases} \pm 1 \\ 0 \end{cases}. \]

(6.98)
The only exception is that the $j' = 0 \rightarrow j = 0$ transition is forbidden (Why?)

**Example 3.** The projection theorem when $j' = j$:

$$
\langle jm'|V_q|jm\rangle = \frac{\langle jm| J \cdot V |jm\rangle}{\hbar^2 j(j+1)} \langle jm'|J_q|jm\rangle,
$$

(6.99)

where $V$ is an arbitrary vector operator, and $J$ the angular momentum. Using the spherical tensor notation, $q = \pm 1, 0, k = 1$. Using the Wigner-Eckart theorem, we obtain

$$
\frac{\langle jm'|V_q|jm\rangle}{\langle jm'|J_q|jm\rangle} = \frac{\langle j|V||j\rangle}{\langle j|J||j\rangle}.
$$

(6.100)

We need to show that $\langle jm| J \cdot V |jm\rangle$ is proportional to $\langle j|V||j\rangle$. Eq. (6.90) ⇒

$$
J \cdot V = J_0 V_0 - J_+ V_- - J_- V_+,
$$

(6.101)

where $J_0 = J_z$, and $J_{\pm} = \mp \sqrt{2} (J_x \pm iJ_y) = \mp \sqrt{2} J_\pm$, based on Eq. (6.89). Since operators $J_z$ and $J_{\pm}$ do not change $j$ and $\langle jm'|V_q|jm\rangle \propto \langle j|V||j\rangle$, $\langle jm| J \cdot V |jm\rangle = c_{jm} \langle j|V||j\rangle$.

Furthermore, $c_{jm}$ is independent of $m$ because $J \cdot V$ is a scalar operator. Therefore,

$$
\langle jm| J \cdot V |jm\rangle = c_j \langle j|V||j\rangle,
$$

(6.102)

For an arbitrary vector operator $V$. If we set $V = J$, then $\langle jm|J_j^2|jm\rangle = c_j \langle j|J||j\rangle$, and Eq. (6.100) becomes

$$
\frac{\langle jm'|V_q|jm\rangle}{\langle jm'|J_q|jm\rangle} = \frac{\langle jm| J \cdot V |jm\rangle}{\langle jm|J_j^2|jm\rangle} = \frac{\langle jm| J \cdot V |jm\rangle}{\hbar^2 j(j+1)}.
$$

(6.103)

**Example 4.** A magnetic moment operator

$$
\vec{\mu} = g_1 J_1 + g_2 J_2,
$$

(6.104)

where $J_1 + J_2 = J$, the total angular momentum. We can evaluate $\langle j|\mu_0|\vec{\mu}\rangle$ using the projection theorem,

$$
\langle j|\mu_0|\vec{\mu}\rangle = \frac{\langle j|J \cdot \vec{\mu}|j\rangle}{\hbar^2 j(j+1)} \langle j|J_0|j\rangle,
$$

(6.105)

where $J \cdot \vec{\mu} = g_1 J \cdot J_1 + g_2 J \cdot J_2$, and

$$
J \cdot J_1 = (J^2 + J_1^2 - J_2^2) / 2, \quad J \cdot J_2 = (J^2 - J_1^2 + J_2^2) / 2.
$$

(6.106)
Here the $|j\rangle$ state is the addition of eigenstates of $J_1^2$ and $J_2^2$, i.e., $|j\rangle = |j_1,j_2; j, m = j\rangle$, and $\langle j| J_0 |j\rangle = j\hbar$, we finally obtain

$$
\langle j| J_0 |j\rangle = \frac{\hbar}{2(j+1)} [j(j+1)(g_1 + g_2) + j_1(j_1 + 1)(g_1 - g_2) + j_2(j_2 + 1)(g_2 - g_1)] .
$$

(6.107)

Lande g-factor:

$$
\tilde{\mu} = gJ,
$$

(6.108)

where $J = J_1 + J_2$. We obtain

$$
\langle j| J_0 |j\rangle = gj\hbar.
$$

(6.109)

Combining Eqs. (6.107) and (6.109), we find that

$$
g = \frac{j(j+1) + j_1(j_1 + 1) - j_2(j_2 + 1)}{2j(j+1)} g_1 + \frac{j(j+1) + j_2(j_2 + 1) - j_1(j_1 + 1)}{2j(j+1)} g_2 .
$$

(6.110)