Quantum Mechanics

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V. Symmetry in Quantum Mechanics

5.1 Symmetries, Conservation Laws, and Degeneracies

5.1.1 Symmetries in Classical Physics

If the classical Lagrangian *L*, as a function of a generalized q_i and its velocity $\dot{q}_i$, is unchanged under displacement

$$q_i \to q_i + \delta q_i , \tag{5.1}$$

then we must have

$$\frac{\partial L}{\partial q_i} = 0 . \tag{5.2}$$

By virtue of the Lagrange equation

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial \dot{q}}\right) - \frac{\partial L}{\partial q_i} = 0 , \tag{5.3}$$

we have

$$\frac{\mathrm{d}p_i}{\mathrm{d}t} = 0 , \tag{5.4}$$

where

$$p_i = \frac{\partial L}{\partial \dot{q}_i} \tag{5.5}$$

is the canonical momentum. So if *L* is unchanged under displacement Eq. (5.1), we have a conserved quantity of the canonical momentum conjugated to q_i .

Likewise, it is also true if the Hamiltonian has a symmetry under Eq. (5.1).

5.1.2 Symmetry in Quantum Mechanics

In quantum mechanics, a **symmetry operator** (e.g., translation or rotation)

$$\mathscr{I} = 1 - \frac{i\varepsilon}{\hbar} G , \tag{5.6}$$

where *G* is the Hermitian generator of the symmetry operator. Supposing that *H* is invariant under $\mathscr{I}$, we have

$$\mathscr{I}^\dagger H \mathscr{I} = H , \tag{5.7}$$

which is equivalent to

$$[G, H] = 0 . \tag{5.8}$$

By virtue of the Heisenberg equation of motion, we have

$$\frac{\mathrm{d}G}{\mathrm{d}t} = 0 . \tag{5.9}$$

Therefore, *G* is a constant of the motion.

Supposing the system is in an eigenstate of *G* at time t_0, then the ket at a later time

$$|g', t_0; t\rangle = \mathscr{U}(t, t_0)|g'\rangle \tag{5.10}$$

is also an eigenket of *G* with the same eigenvalue, where $\mathscr{U}(t, t_0)$ is the time-evolution operator.

5.1.3 Degeneracies

Let us suppose that

$$[H, \mathscr{I}] = 0 \tag{5.11}$$

and $|n\rangle$ is an energy eigenket with eigenvalue E_n, then

$$H(\mathscr{I}|n\rangle) = \mathscr{I}H|n\rangle = E_n(\mathscr{I}|n\rangle), \tag{5.12}$$

which means that $\mathscr{I}|n\rangle$ is also an energy eigenket with the same eigenvalue. Therefore, $|n\rangle$ and $\mathscr{I}|n\rangle$ are degenerate eigenstates.

Consider the unitary operator of rotation $\mathscr{D}(R)$. If the Hamiltonian is rotationally invariant:

$$[\mathscr{D}(R), H] = 0 , \tag{5.13}$$

we should have

$$[\mathbf{J}, H] = 0, \quad [\mathbf{J}^2, H] = 0 . \tag{5.14}$$

The simultaneous eigenkets of *H*, $\mathbf{J}^2$, and J_z denoted by $|n; j, m\rangle$ are energetically degenerate with all states of the form $\mathscr{D}(R)|n; j, m\rangle$, which is a linear combination of $2j+1$ independent states:

$$\mathscr{D}(R)|n; j, m\rangle = \sum_{m'}|n; j, m'\rangle \mathscr{D}^{(j)}_{m'm}(R). \tag{5.15}$$

5.1.4 SO(4) Symmetry in the Coulomb Potential

As for the classical potentials with the $1/r$ form, the constant of the motion maintaining the orientation of the major axis of the elliptical orbit is the **Runge-Lenz vector**,

$$\mathbf{M} = \frac{\mathbf{p}\times\mathbf{L}}{m} - \frac{Ze^2}{r}\mathbf{r} . \tag{5.16}$$

It has the SO(4) symmetry, the group of rotation operators in four spatial dimensions. A Hermitian version of the Lenz vector is

$$\mathbf{M} = \frac{1}{2m}(\mathbf{p}\times\mathbf{L} - \mathbf{L}\times\mathbf{p}) - \frac{Ze^2}{r}\mathbf{r} , \tag{5.17}$$

which commutes with the Hamiltonian

$$H = \frac{\mathbf{p}^2}{2m} - \frac{Ze^2}{r}, \tag{5.18}$$

namely,

$$\left[\mathbf{M}, H\right] = 0 . \tag{5.19}$$

So **M** is indeed a quantum-mechanical constant of the motion. It can also be proved that

$$\begin{aligned} &\mathbf{L}\cdot\mathbf{M} = \mathbf{M}\cdot\mathbf{L} = 0 \\ &\mathbf{M}^2 = \frac{2}{m}H\left(L^2+\hbar^2\right)+Z^2e^4 \end{aligned} . \tag{5.20}$$

The algebra for the generators of this symmetry is

$$\begin{aligned} &\left[L_i, L_j\right] = i\hbar\varepsilon_{ijk}L_k \\ &\left[M_i, L_j\right] = i\hbar\varepsilon_{ijk}M_k \\ &\left[M_i, M_j\right] = -i\hbar\varepsilon_{ijk}\frac{2}{m}HL_k \end{aligned} , \tag{5.21}$$

which is not closed due to the presence of *H*. However, we can considered the bounded states with energy eigenvalue $E<0$. Replacing **M** with the scaled vector operator

$$\mathbf{N} \equiv \sqrt{-\frac{m}{2E}}\mathbf{M}, \tag{5.22}$$

Eq. (5.21) becomes the closed algebra:

$$\begin{aligned} &\left[L_i, L_j\right] = i\hbar\varepsilon_{ijk}L_k \\ &\left[N_i, L_j\right] = i\hbar\varepsilon_{ijk}N_k \\ &\left[N_i, N_j\right] = i\hbar\varepsilon_{ijk}L_k \end{aligned} . \tag{5.23}$$

Because the number of generators for rotations in *n* spatial dimensions is $n(n-1)/2$, the operators **L** and **N** in Eq. (5.23) are rotations in four spatial dimensions.

In four spatial dimensions, define

$$\begin{aligned} &N_1 \equiv \tilde{L}_{14} = x_1p_4 - x_4p_1 \\ &N_2 \equiv \tilde{L}_{24} = x_2p_4 - x_4p_2 \\ &N_2 \equiv \tilde{L}_{34} = x_3p_4 - x_4p_3 \end{aligned} , \tag{5.24}$$

which obeys Eq. (5.23). Further define the operators

$$\begin{aligned} &\mathbf{I} \equiv \left(\mathbf{L}+\mathbf{N}\right)/2 \\ &\mathbf{K} \equiv \left(\mathbf{L}-\mathbf{N}\right)/2 \end{aligned} , \tag{5.25}$$

which obeys the following algebra:

$$\begin{aligned} &\left[I_i, I_j\right] = i\hbar\varepsilon_{ijk}I_k \\ &\left[K_i, K_j\right] = i\hbar\varepsilon_{ijk}K_k \\ &\left[I_i, K_j\right] = 0 \end{aligned} . \tag{5.26}$$

Therefore, **I** and **K** obey independent angular-momentum algebra. Because it is also evident that

$$\left[\mathbf{I}, H\right] = \left[\mathbf{K}, H\right] = 0, \tag{5.27}$$

they are conserved quantities. We denote the eigenvalues of $\mathbf{I}^2$ and $\mathbf{K}^2$ by $i(i+1)\hbar$ and $k(k+1)\hbar$, respectively, with $i,k=0,\frac{1}{2},1,\frac{3}{2},\cdots$. Because $\mathbf{I}^2-\mathbf{K}^2=\mathbf{L}\cdot\mathbf{N}=0$, we must have $i=k$. On the other hand,

$$\mathbf{I}^2+\mathbf{K}^2=\frac{1}{2}\left(\mathbf{L}^2+\mathbf{N}^2\right)=\frac{1}{2}\left(\mathbf{L}^2-\frac{m}{2E}\mathbf{M}^2\right), \tag{5.28}$$

which leads to the numerical relation

$$2k(k+1)\hbar^2=\frac{1}{2}\left(-\hbar^2-\frac{m}{2E}Z^2e^4\right). \tag{5.29}$$

From the above relation, we get

$$E=-\frac{mZ^2e^4}{2\hbar^2}\frac{1}{(2k+1)^2}, \tag{5.30}$$

which is the same as the solution for the Coulomb problem with the principle quantum number n replaced by $2k+1$. Therefore, the degeneracy in the Coulomb problem arises from the two rotational symmetries represented by the operators **I** and **K**. The degree of degeneracy is

$$(2i+1)(2k+1)=(2k+1)^2=n^2. \tag{5.31}$$

Eq. (5.26) shows that this SO(4) group can also be thought of two independent SU(2) groups, namely, $\mathrm{SU}(2)\times\mathrm{SU}(2)$.

5.2 Discrete Symmetries, Parity, or Space Inversion

5.2.1 Parity Operator

One of the discrete operation is **parity**, or space inversion. For a state ket $|\alpha\rangle$, the **parity operator** π ($|\alpha\rangle\rightarrow\pi|\alpha\rangle$) changes the expectation value of the position operator $\mathbf{x}$ to be opposite in sign:

$$\langle\alpha|\pi^\dagger\mathbf{x}\pi|\alpha\rangle=-\langle\alpha|\mathbf{x}|\alpha\rangle. \tag{5.32}$$

Because π is unitary, we have

$$\pi^\dagger\mathbf{x}\pi=-\mathbf{x} \tag{5.33}$$

or equivalently

$$\{\pi,\mathbf{x}\}=0. \tag{5.34}$$

For the eigenkets of the parity operator $|\mathbf{x}'\rangle$, we have

$$\mathbf{x}\pi|\mathbf{x}'\rangle=-\pi\mathbf{x}|\mathbf{x}'\rangle=(-\mathbf{x}')\pi|\mathbf{x}'\rangle, \tag{5.35}$$

which means that $\pi|\mathbf{x}'\rangle$ is an eigenket of **x** with eigenvalue $-\mathbf{x}'$. So we may choose

$$\pi\left|\mathbf{x}'\right\rangle=\left|-\mathbf{x}'\right\rangle . \tag{5.36}$$

Because $\pi^2=1$, π is not only unitary but also Hermitian:

$$\pi^{-1}=\pi^{+}=\pi . \tag{5.37}$$

Its eigenvalue can only be $+1$ or -1.

Because for the translation operator, we also have

$$\pi\mathscr{T}\left(\mathrm{d}\mathbf{x}'\right)=\mathscr{T}\left(-\mathrm{d}\mathbf{x}'\right)\pi , \tag{5.38}$$

which is just

$$\pi\left(1-\frac{i\mathbf{p}\cdot\mathrm{d}\mathbf{x}'}{\hbar}\right)\pi^{\dagger}=1+\frac{i\mathbf{p}\cdot\mathrm{d}\mathbf{x}'}{\hbar} , \tag{5.39}$$

so

$$\pi^{\dagger}\mathbf{p}\pi=-\mathbf{p} \tag{5.40}$$

or equivalently

$$\{\pi,\mathbf{p}\}=0 . \tag{5.41}$$

For orbital angular momentum $\mathbf{L}=\mathbf{x}\times\mathbf{p}$, we clearly have

$$[\pi,\mathbf{L}]=0 . \tag{5.42}$$

Considering that the 3×3 orthogonal matrix

$$R^{(\text{parity})}=\begin{pmatrix}-1 & 0 & 0\\ 0 & -1 & 0\\ 0 & 0 & -1\end{pmatrix} \tag{5.43}$$

satisfies

$$R^{(\text{parity})}R^{(\text{rotation})}=R^{(\text{rotation})}R^{(\text{parity})} , \tag{5.44}$$

so in quantum mechanics, it is natural to *postulate* the corresponding relation for the unitary operators

$$\pi\mathscr{D}(R)=\mathscr{D}(R)\pi , \tag{5.45}$$

where $\mathscr{D}(R)=1-i\mathbf{J}\cdot\hat{\mathbf{n}}\varepsilon/\hbar$. Therefore, it follows that

$$\pi^{\dagger}\mathbf{J}\pi=\mathbf{J} \tag{5.46}$$

or equivalently

$$[\pi,\mathbf{J}]=0 . \tag{5.47}$$

Because $\mathbf{J}=\mathbf{L}+\mathbf{S}$, the spin operator **S** also transforms in the same way as **L**.

Polar vectors: Vectors that are odd under parity (e.g., **x**, **p**).

Axial vectors (**pseudovectors**): Vectors that are even under parity (e.g., **L**, **J**, **S**).

Because

$$\pi^{-1}\mathbf{S}\cdot\mathbf{x}\pi=-\mathbf{S}\cdot\mathbf{x} , \tag{5.48}$$

$\mathbf{S}\cdot\mathbf{x}$ is a **pseudoscalar**.

5.2.2 Wave Functions under Parity

For a wave function

$$\psi(\mathbf{x}') = \langle \mathbf{x}' | \alpha \rangle , \tag{5.49}$$

the space-inverted state $\pi|\alpha\rangle$ has the wave function of

$$\langle \mathbf{x}' | \pi | \alpha \rangle = \langle -\mathbf{x}' | \alpha \rangle = \psi(-\mathbf{x}') . \tag{5.50}$$

If $|\alpha\rangle$ is an eigenket of parity, then

$$\pi|\alpha\rangle = \pm|\alpha\rangle , \tag{5.51}$$

The corresponding wave function

$$\langle \mathbf{x}' | \pi | \alpha \rangle = \pm \langle \mathbf{x}' | \alpha \rangle . \tag{5.52}$$

Along with Eq. (5.50), we know that

$$\psi(-\mathbf{x}') = \pm\psi(\mathbf{x}') , \tag{5.53}$$

which means that the wave function should have either even or odd parity.

Note that not all wave functions of physical interest have definite parities. For instance, the momentum operator anticommutes with the parity operator, so the momentum eigenket is not a parity eigenket. Therefore, the plane wave, which is the wave function for a momentum eigenket, does not satisfy Eq. (5.53).

Because the orbital angular momentum operator **L** commutes with π (see Eq. (5.42)), they have simultaneous eigenkets. The transformation $\mathbf{x}' \to -\mathbf{x}'$ of its wave function

$$\langle \mathbf{x}' | \alpha, lm \rangle = R_\alpha(r) Y_l^m(\theta, \phi) \tag{5.54}$$

is accomplished by letting

$$\begin{array}{lc} r \to r & \\ \theta \to \pi - \theta & (\cos\theta \to -\cos\theta) \\ \phi \to \phi + \pi & \left(\exp(im\phi) \to (-1)^m \exp(im\phi)\right) \end{array} . \tag{5.55}$$

It can be shown that the above transformation let

$$Y_l^m \to (-1)^l Y_l^m . \tag{5.56}$$

Therefore, we conclude that

$$\pi|\alpha, lm\rangle = (-1)^l |\alpha, lm\rangle . \tag{5.57}$$

Theorem. Suppose

$$[H, \pi] = 0 \tag{5.58}$$

and $|n\rangle$ is a nondegenerate eigenket of H with eigenvalue E_n:

$$H|n\rangle = E_n|n\rangle, \tag{5.59}$$

then $|n\rangle$ is also a parity eigenket.

Proof. First considering the state

$$|\alpha\rangle \equiv \frac{1}{2}(1 \pm \pi)|n\rangle. \tag{5.60}$$

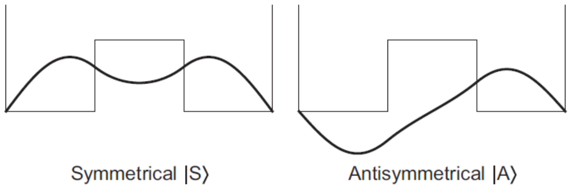
Since $\pi^2 = 1$, $\pi|\alpha\rangle = \pm|\alpha\rangle$, so $|\alpha\rangle$ is a parity eigenket. Also, since $H\pi = \pi H$, $H|\alpha\rangle = E_n|\alpha\rangle$, so $|\alpha\rangle$ is also an energy eigenket. Because $|n\rangle$ is supposed to be nondegenerate, $|n\rangle$ and $|\alpha\rangle$ must be the same. Therefore, $\pi|n\rangle = \pm|n\rangle$, namely, $|n\rangle$ is also a parity eigenket.

Let us look at the simple harmonic oscillator as an example. The ground state $|0\rangle$ has even parity because its wave function is Gaussian. The first excited state

$$|1\rangle = a^\dagger|0\rangle \tag{5.61}$$

has the odd parity because $a^\dagger$ is linear in *x* and *p*, which are both odd. In general, the parity of the *n*th excited state of the simple harmonic operator is $(-1)^n$.

5.2.3 Symmetrical Double-Well Potential



The symmetrical double well with the two lowest-lying states $|S\rangle$ (symmetrical) and $|A\rangle$ (antisymmetrical) shown.

The two lowest-lying states of the symmetrical double-well potential are the **symmetric state** $|S\rangle$ and the **anti-symmetric state** $|A\rangle$, which are simultaneous eigenkets of *H* and π with

$$E_A > E_S. \tag{5.62}$$

We can form two wave functions

$$|R\rangle = \frac{1}{\sqrt{2}}\left(|S\rangle + |A\rangle\right) \tag{5.63}$$

and

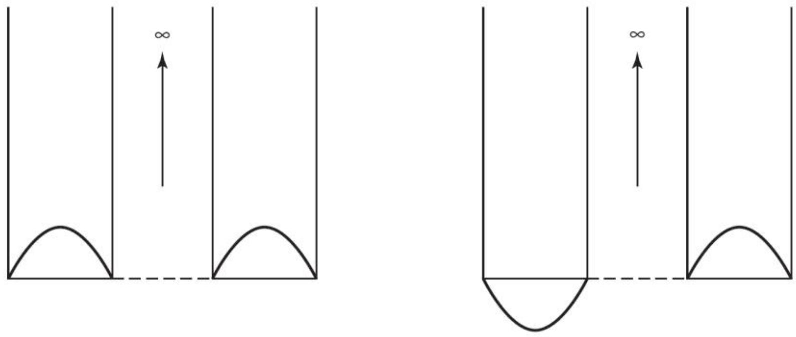
$$|L\rangle = \frac{1}{\sqrt{2}}\left(|S\rangle - |A\rangle\right) \tag{5.64}$$

largely concentrated in the right-hand side and the left-hand side, respectively. They are **non-stationary states** neither parity nor energy eigenstates. If the system is represented by $|R\rangle$ at $t = 0$, then at a later time *t*, we have

$$
\begin{aligned}
|R, t_0 = 0; t\rangle &= \frac{1}{\sqrt{2}}\left(\exp\left(-iE_S t/\hbar\right)|S\rangle + \exp\left(iE_A t/\hbar\right)|A\rangle\right) \\
&= \frac{1}{\sqrt{2}}\exp\left(-iE_S t/\hbar\right)\left(|S\rangle + \exp\left(i\left(E_A - E_S\right)t/\hbar\right)|A\rangle\right)
\end{aligned}
. \tag{5.65}
$$

At time $t = T/2 \equiv \dfrac{2\pi\hbar}{2\left(E_A - E_S\right)}$, the system is found in pure $|L\rangle$. At time $t = T$, the system is back to pure $|R\rangle$. Therefore, the angular frequency for the oscillation between $|R\rangle$ and $|L\rangle$ is

$$
\omega = \frac{E_A - E_S}{\hbar}. \tag{5.66}
$$



The symmetrical double well with an infinitely high middle barrier.

Considering the case that the middle barrier goes to infinity, the $|S\rangle$ and $|A\rangle$ states are degenerate, the symmetry of the Hamiltonian is not obeyed in this degenerate case.

5.2.4 Parity Selection Rule

Suppose $|\alpha\rangle$ and $|\beta\rangle$ are parity eigenstates:

$$
\pi|\alpha\rangle = \varepsilon_\alpha|\alpha\rangle \tag{5.67}
$$

and

$$
\pi|\beta\rangle = \varepsilon_\beta|\beta\rangle, \tag{5.68}
$$

where $\varepsilon_\alpha, \varepsilon_\beta = \pm 1$. Because

$$
\langle\beta|\mathbf{x}|\alpha\rangle = \langle\beta|\pi^{-1}\pi\mathbf{x}\pi^{-1}\pi|\alpha\rangle = \varepsilon_\alpha\varepsilon_\beta\left(-\langle\beta|\mathbf{x}|\alpha\rangle\right), \tag{5.69}
$$

we have

$$
\langle\beta|\mathbf{x}|\alpha\rangle = 0 \tag{5.70}
$$

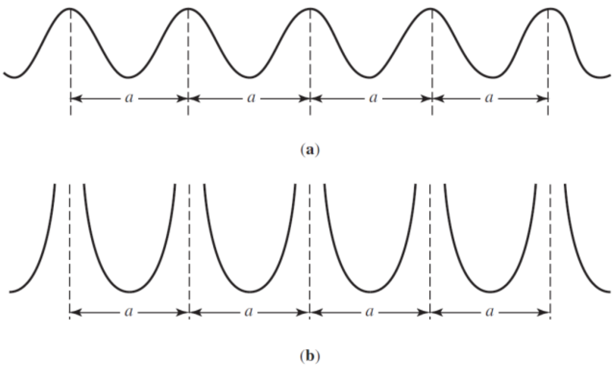
unless $\varepsilon_\alpha = -\varepsilon_\beta$. The corresponding **selection rule** for wave function is

$$
\int \psi_\beta^* \psi_\alpha \, \mathrm{d}\tau = 0 \tag{5.71}
$$

if ψ_β and ψ_α have the same parity.

The generalized conclusion is: Operators that are odd under parity, e.g., $\mathbf{p}$ or $\mathbf{S}\cdot\mathbf{x}$, have non-vanishing matrix elements only between states of opposite parity. In contrast, operators that are even under parity connect states of the same parity.

5.3 Lattice Translation as a Discrete Symmetry



(a) Periodic potential in one dimension with periodicity *a*. (b) The periodic potential when the barrier height between two adjacent lattice sites becomes infinite.

Considering a periodic potential in one dimension $V(x\pm a)=V(x)$, the Hamiltonian is generally not invariant with the translation operator $\tau(l)$ with an arbitrary *l*:

$$\tau^\dagger(l)x\tau(l)=x+l,\quad \tau(l)|x'\rangle=|x'+l\rangle. \tag{5.72}$$

However, when *l* coincides with the lattice spacing *a*, we do have

$$\tau^\dagger(a)V(x)\tau(a)=V(x+a)=V(x). \tag{5.73}$$

So

$$\tau^\dagger(a)H\tau(a)=H. \tag{5.74}$$

Because $\tau(a)$ is unitary, the above is equivalent to

$$[H,\tau(a)]=0. \tag{5.75}$$

which means that they have simultaneous eigenkets. $\tau(a)$ is unitary but non-Hermitian, so its eigenvalue is a complex number of modulus 1.

If the potential barrier height goes to infinity, we specify the ground state at the *n*th site with the ground energy of E_0 as $|n\rangle$:

$$H|n\rangle=E_0|n\rangle, \tag{5.76}$$

where $n\in(-\infty,+\infty)$. It is not an eigenket of $\tau(a)$ due to the degeneracy, because

$$\tau(a)|n\rangle=|n+1\rangle. \tag{5.77}$$

Define

$$\left|\theta\right\rangle \equiv \sum_{n=-\infty}^{\infty} \exp\left(in\theta\right)\left|n\right\rangle, \tag{5.78}$$

where $\theta \in \left[-\pi,\pi\right]$ is a real parameter. Because

$$\tau\left(a\right)\left|\theta\right\rangle = \sum_{n=-\infty}^{\infty} \exp\left(in\theta\right)\left|n+1\right\rangle = \sum_{n=-\infty}^{\infty} \exp\left(i\left(n-1\right)\theta\right)\left|n\right\rangle = \exp\left(-i\theta\right)\left|\theta\right\rangle, \tag{5.79}$$

$\left|\theta\right\rangle$ is a simultaneous eigenket of H and $\tau\left(a\right)$.

For the more realistic situation that the barrier is finite, the localize ket $\left|n\right\rangle$ has some leakage into neighboring lattice due to the tunneling effect. As a consequence, although still

$$\left\langle n\right|H\left|n\right\rangle = E_0, \tag{5.80}$$

the matrix of H is not completely diagonal. Consider the **tight-binding approximation** that the barrier is so high that only non-diagonal elements connecting neighbors are important:

$$\left\langle n'\right|H\left|n\right\rangle \neq 0, \quad n'=n \text{ or } n'=n\pm 1 . \tag{5.81}$$

Define

$$\left\langle n\pm 1\right|H\left|n\right\rangle = -\Delta, \tag{5.82}$$

obviously Δ is also independent of n. We then have

$$H\left|n\right\rangle = E_0\left|n\right\rangle - \Delta\left|n+1\right\rangle - \Delta\left|n-1\right\rangle, \tag{5.83}$$

which shows that $\left|n\right\rangle$ is no longer an energy eigenket.

Still define $\left|\theta\right\rangle$ by Eq. (5.78), which is still an eigenket of $\tau\left(a\right)$ because Eq. (5.79) still holds. Because

$$\begin{aligned} H\left|\theta\right\rangle &= H\sum \exp\left(in\theta\right)\left|n\right\rangle \\ &= E_0\sum \exp\left(in\theta\right)\left|n\right\rangle - \Delta\sum \exp\left(in\theta\right)\left|n+1\right\rangle - \Delta\sum \exp\left(in\theta\right)\left|n-1\right\rangle \\ &= E_0\sum \exp\left(in\theta\right)\left|n\right\rangle - \Delta\sum\left[\exp\left(in\theta-i\theta\right)+\exp\left(in\theta+i\theta\right)\right]\left|n\right\rangle \\ &= \left(E_0 - 2\Delta\cos\theta\right)\sum \exp\left(in\theta\right)\left|n\right\rangle \\ &= \left(E_0 - 2\Delta\cos\theta\right)\left|\theta\right\rangle \end{aligned}, \tag{5.84}$$

$\left|\theta\right\rangle$ is also an energy eigenket.

Bloch's Theorem: The wave function of $\left|\theta\right\rangle$ can be written as a plane wave $\exp\left(ikx'\right)$ times a periodic function with periodicity a.

Proof: On the one hand, we can let $\tau\left(a\right)$ operate on $\left\langle x'\right|$ to have

$$\left\langle x'\right|\tau\left(a\right)\left|\theta\right\rangle = \left\langle x'-a\middle|\theta\right\rangle; \tag{5.85}$$

On the other hand, we can let $\tau(a)$ operate on $|\theta\rangle$ and use Eq. (5.79) to have

$$\langle x'|\tau(a)|\theta\rangle = \exp(-i\theta)\langle x'|\theta\rangle \,. \tag{5.86}$$

So we get

$$\langle x'-a|\theta\rangle = \exp(-i\theta)\langle x'|\theta\rangle \,, \tag{5.87}$$

whose solution has the form

$$\langle x'|\theta\rangle = \exp(ikx')u_k(x') \,, \tag{5.88}$$

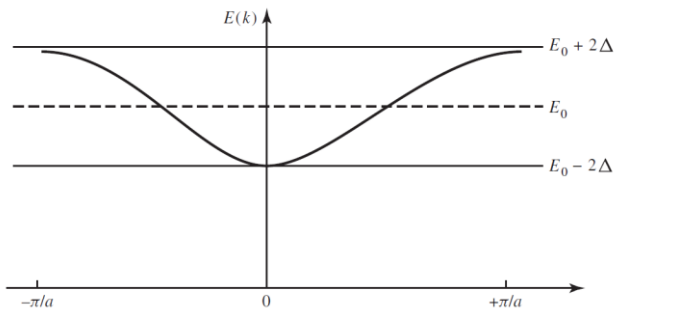
where $\theta = ka$ and $u_k(x')$ is a periodic function with period a. The validity of the above solution can be easily verified by substituting it into Eq. (5.87):

$$\exp\left[ik(x'-a)\right]u_k(x'-a) = \exp(ikx')u_k(x')\exp(-ika) \,. \tag{5.89}$$

As $\theta \in [-\pi,\pi]$, we have $k \in \left[-\frac{\pi}{a},\frac{\pi}{a}\right]$. The energy eigenvalue is

$$E(k) = E_0 - 2\Delta\cos ka \,. \tag{5.90}$$

The continuous band between $E_0 - 2\Delta$ and $E_0 + 2\Delta$ is know as the **Brillouin Zone**.



Dispersion curve for $E(k)$ versus k in the Brillouin zone $|k| \leq \pi/a$.

5.4 Time-Reversal Discrete Symmetry

5.4.1 Time-Reversal Operator

The term "time-reversal" actually means "reversal of motion". For the Schrödinger wave equation

$$i\hbar\frac{\partial\psi}{\partial t} = \left(-\frac{\hbar^2}{2m}\nabla^2 + V\right)\psi \,, \tag{5.91}$$

suppose $\psi(\mathbf{x},t)$ is a solution, then $\psi(\mathbf{x},-t)$ is not a solution, but $\psi^*(\mathbf{x},-t)$ is.

Antiunitary Transformation: For the transformation

$$|\alpha\rangle \to |\tilde{\alpha}\rangle = \theta|\alpha\rangle, \quad |\beta\rangle \to |\tilde{\beta}\rangle = \theta|\beta\rangle \,, \tag{5.92}$$

θ is an antilinear operator if

$$\begin{aligned}&\langle\tilde{\beta}|\tilde{\alpha}\rangle=\langle\beta|\alpha\rangle^{*}\\&\theta\left(c_{1}|\alpha\rangle+c_{2}|\beta\rangle\right)=c_{1}^{*}\theta|\alpha\rangle+c_{2}^{*}\theta|\beta\rangle\end{aligned}. \tag{5.93}$$

Note that θ should not act on bras from the right.

Because an antiunitary operator θ can be written as the product of a unitary operator *U* and the complex conjugate operator *K*:

$$\theta=UK\ , \tag{5.94}$$

the time-reversal operator

$$|\alpha\rangle\rightarrow\Theta|\alpha\rangle \tag{5.95}$$

satisfying the Schrödinger wave equation Eq. (5.91) is an antiunitary operator.

Consider a ket $|\alpha\rangle$ at $t=0$ evolving to a slightly later time δt. With the time-reversal operator applied, we have

$$\left(1-\frac{i}{\hbar}H\delta t\right)\Theta|\alpha\rangle=\Theta\left(1-\frac{i}{\hbar}H\left(-\delta t\right)\right)|\alpha\rangle\ , \tag{5.96}$$

leading to the requirement

$$-iH\Theta|\alpha\rangle=\Theta iH|\alpha\rangle\ . \tag{5.97}$$

On the other hand, the antiunitary feature Eq. (5.93) gives

$$\Theta iH|\alpha\rangle=-i\Theta H|\alpha\rangle\ . \tag{5.98}$$

The above two equations lead to

$$\Theta H=H\Theta\ . \tag{5.99}$$

For the act

$$|\tilde{\alpha}\rangle=\Theta|\alpha\rangle,\quad|\tilde{\beta}\rangle=\Theta|\beta\rangle\ , \tag{5.100}$$

We have the important identity:

$$\langle\beta|\otimes|\alpha\rangle=\langle\tilde{\alpha}|\Theta\otimes^{\dagger}\Theta^{-1}|\tilde{\beta}\rangle, \tag{5.101}$$

where $\otimes$ is a linear operator.

Proof: Define

$$|\gamma\rangle\equiv\otimes^{\dagger}|\beta\rangle\ . \tag{5.102}$$

By dual correspondence, we have

$$|\gamma\rangle\xleftrightarrow{\text{DC}}\langle\beta|\otimes=\langle\gamma|\ . \tag{5.103}$$

Hence,

$$\begin{aligned}&\langle\beta|\otimes|\alpha\rangle=\langle\gamma|\alpha\rangle=\langle\tilde{\alpha}|\tilde{\gamma}\rangle\\&=\langle\tilde{\alpha}|\Theta\otimes^{\dagger}|\beta\rangle=\langle\tilde{\alpha}|\Theta\otimes^{\dagger}\Theta^{-1}\Theta|\beta\rangle\ ,\\&=\langle\tilde{\alpha}|\Theta\otimes^{\dagger}\Theta^{-1}|\tilde{\beta}\rangle\end{aligned} \tag{5.104}$$

which proves the identity.

For a Hermitian observable A, we get

$$\langle\beta|A|\alpha\rangle = \langle\tilde{\alpha}|\Theta A\Theta^{-1}|\tilde{\beta}\rangle . \tag{5.105}$$

The observables are even or odd under time reversal:

$$\Theta A\Theta^{-1} = \pm A , \tag{5.106}$$

which, together with Eq. (5.105), gives a phase restriction on the matrix elements of A:

$$\langle\beta|A|\alpha\rangle = \pm\langle\tilde{\beta}|A|\tilde{\alpha}\rangle^* . \tag{5.107}$$

For expectation values, according to the above equation, we have

$$\langle\alpha|A|\alpha\rangle = \pm\langle\tilde{\alpha}|A|\tilde{a}\rangle . \tag{5.108}$$

Taken the momentum operator as an example. Because **p** is odd under time reversal, we have

$$\langle\alpha|\mathbf{p}|\alpha\rangle = -\langle\tilde{\alpha}|\mathbf{p}|\tilde{a}\rangle \tag{5.109}$$

and

$$\Theta\mathbf{p}\Theta^{-1} = -\mathbf{p} . \tag{5.110}$$

Therefore,

$$\mathbf{p}\Theta|\mathbf{p}'\rangle = -\Theta\mathbf{p}\Theta^{-1}\Theta|\mathbf{p}'\rangle = (-\mathbf{p}')\Theta|\mathbf{p}'\rangle , \tag{5.111}$$

which means that $\Theta|\mathbf{p}'\rangle$ is a momentum eigenket with eigenvalue $-\mathbf{p}'$.

Likewise, we obtain

$$\begin{aligned} &\langle\alpha|\mathbf{x}|\alpha\rangle = \langle\tilde{\alpha}|\mathbf{x}|\tilde{\alpha}\rangle \\ &\Theta\mathbf{x}\Theta^{-1} = \mathbf{x} \\ &\Theta|\mathbf{x}'\rangle = |\mathbf{x}'\rangle \end{aligned} \quad . \tag{5.112}$$

We can now check the invariance of the fundamental commutation relation

$$\left[x_i, p_j\right]|\alpha\rangle = i\hbar\delta_{ij}|\alpha\rangle . \tag{5.113}$$

Applying Θ to both sides:

$$\Theta\left[x_i, p_j\right]\Theta^{-1}\Theta|\alpha\rangle = \Theta i\hbar\delta_{ij}|\alpha\rangle , \tag{5.114}$$

which leads to

$$\left[x_i, -p_j\right]\Theta|\alpha\rangle = -i\hbar\delta_{ij}\Theta|\alpha\rangle . \tag{5.115}$$

So the fundamental commutation relation $\left[x_i, p_j\right] = i\hbar\delta_{ij}$ is preserved, which again rationalizes the setup that Θ is antiunitary.

Similarly, to preserve

$$\left[J_i, J_j\right] = i\hbar\varepsilon_{ijk}J_k , \tag{5.116}$$

We must have

$$\Theta\mathbf{J}\Theta^{-1} = -\mathbf{J} . \tag{5.117}$$

5.4.2 Time Reversal of Wave Function

Suppose a spinless single-particle stays at a state

$$|\alpha\rangle=\int d^3x'|\mathbf{x}'\rangle\langle\mathbf{x}'|\alpha\rangle, \tag{5.118}$$

where $\langle\mathbf{x}'|\alpha\rangle$ is its wave function. Applying the time-reversal operator yields

$$\Theta|\alpha\rangle=\int d^3x'\Theta|\mathbf{x}'\rangle\langle\mathbf{x}'|\alpha\rangle^*=\int d^3x'|\mathbf{x}'\rangle\langle\mathbf{x}'|\alpha\rangle^*. \tag{5.119}$$

We then recover the rule

$$\psi(\mathbf{x}')\to\psi^*(\mathbf{x}'). \tag{5.120}$$

The angular part of the wave function given by a spherical harmonic function

$$Y_l^m(\theta,\phi)\to Y_l^{m*}(\theta,\phi)=(-1)^m Y_l^{-m}(\theta,\phi). \tag{5.121}$$

Because $Y_l^m(\theta,\phi)$ is the wave function for $|l,m\rangle$, from Eq. (5.120), we deduce

$$\Theta|l,m\rangle=(-1)^m|l,-m\rangle. \tag{5.122}$$

Theorem. Suppose the Hamiltonian is invariant under time reversal and the energy eigenket $|n\rangle$ is nondegenerate, then the corresponding energy eigenfunction is real.

Proof. Note that

$$H\Theta|n\rangle=\Theta H|n\rangle=E_n\Theta|n\rangle, \tag{5.123}$$

so $|n\rangle$ and $\Theta|n\rangle$ have the same energy. The nondegeneracy requires that they are the same state.

Because their wave functions are $\langle\mathbf{x}'|n\rangle$ and $\langle\mathbf{x}'|n\rangle^*$, respectively, we must have

$$\langle\mathbf{x}'|n\rangle=\langle\mathbf{x}'|n\rangle^*, \tag{5.124}$$

which just means that the energy eigenfunction is real.

5.4.2 Time Reversal for a spin ½ system

A particle with spin ½ can have the eigenket of $\mathbf{S}\cdot\hat{\mathbf{n}}$ with eigenvalue $\hbar/2$, written as

$$|\hat{\mathbf{n}};+\rangle=\exp(-iS_z\alpha/\hbar)\exp(-iS_y\beta/\hbar)|+\rangle, \tag{5.125}$$

where $\hat{\mathbf{n}}$ is characterized by the polar and azimuthal angles β and α, respectively. Using Eq. (5.117), we have

$$\Theta|\hat{\mathbf{n}};+\rangle=\exp(-iS_z\alpha/\hbar)\exp(-iS_y\beta/\hbar)\Theta|+\rangle=\eta|\hat{\mathbf{n}};-\rangle. \tag{5.126}$$

where η stands for an arbitrary phase. On the other hand, it is easy to verify that

$$|\hat{\mathbf{n}};-\rangle=\exp(-iS_z\alpha/\hbar)\exp\left(-iS_y(\pi+\beta)/\hbar\right)|+\rangle. \tag{5.127}$$

Comparing these two equations and using Eq. (5.94) and $K|+\rangle=|+\rangle$, we obtain

$$\Theta = \eta \exp\left(-i\frac{\pi S_y}{\hbar}\right)K = -i\eta\left(\frac{2S_y}{\hbar}\right)K \tag{5.128}$$

Correspondingly, for $\chi(\hat{\mathbf{n}};+)$, the eigenspinor of $|\hat{\mathbf{n}};+\rangle$, we have that $-i\sigma_y\chi^*(\hat{\mathbf{n}};+)$ is an eigenspinor of $|\hat{\mathbf{n}};-\rangle$.

Because

$$\exp\left(-i\frac{\pi S_y}{\hbar}\right)|+\rangle = +|-\rangle, \quad \exp\left(-i\frac{\pi S_y}{\hbar}\right)|-\rangle = -|+\rangle\,, \tag{5.129}$$

for a general spin ½ ket, we have

$$\Theta\left(c_+|+\rangle + c_-|-\rangle\right) = +\eta c_+^*|-\rangle - \eta c_-^*|+\rangle\,. \tag{5.130}$$

Applying Θ again, we obtain

$$\Theta^2\left(c_+|+\rangle + c_-|-\rangle\right) = -|\eta|^2 c_+|+\rangle - |\eta|^2 c_-|-\rangle = -\left(c_+|+\rangle + c_-|-\rangle\right). \tag{5.131}$$

That is,

$$\Theta^2 = -1\,, \tag{5.132}$$

which is different from $\Theta^2 = +1$ for a spinless state, e.g., Eq. (5.122).

More generally, according to Eq. (5.128), we have

$$\begin{aligned}\Theta^2|\alpha\rangle &= \Theta\left(\Theta\sum|jm\rangle\langle jm|\alpha\rangle\right) = \Theta\left(\eta\sum\exp\left(-i\frac{\pi J_y}{\hbar}\right)|jm\rangle\langle jm|\alpha\rangle^*\right)\\ &= |\eta|^2\exp\left(-i\frac{2\pi J_y}{\hbar}\right)\sum|jm\rangle\langle jm|\alpha\rangle\end{aligned}, \tag{5.133}$$

together with

$$\exp\left(-i\frac{2\pi J_y}{\hbar}\right)|jm\rangle = (-1)^{2j}|jm\rangle\,, \tag{5.134}$$

we reach the general conclusion that the eigenvalue of Θ^2 is $(-1)^{2j}$. It takes -1 when j is half-integer and 1 when j is integer.

5.4.2 Interactions with Electric and Magnetic Fields

The Hamiltonian for an electric charge e in a static electric field is

$$H = -\frac{p^2}{2m}\nabla^2 + e\phi(\mathbf{x}), \tag{5.135}$$

where $\phi(\mathbf{x})$ is the electrostatic potential. We have

$$[\Theta, H] = 0\,, \tag{5.136}$$

which leads to the fact that $|n\rangle$ and $\Theta|n\rangle$ belong to the same energy eigenvalue E_n:

$$H\Theta|n\rangle = \Theta H|n\rangle = E_n\Theta|n\rangle \ . \tag{5.137}$$

Supposing they are the same state, then they can differ at most by a phase facor:

$$\Theta|n\rangle = \exp(i\delta)|n\rangle \ . \tag{5.138}$$

Applying Θ again to the above equation, we obtain

$$\Theta^2|n\rangle = \Theta\exp(i\delta)|n\rangle = \exp(-i\delta)\Theta|n\rangle = |n\rangle , \tag{5.139}$$

which is impossible for systems with half-integer *j* values. So $|n\rangle$ and $\Theta|n\rangle$ are distinct states for half-integer *j*, which means that there must be a **Kramers degeneracy** for half-integer *j* systems (a system containing an odd number of electrons).

For interactions with an external magnetic field, the Hamiltonian contains terms like

$$\mathbf{S}\cdot\mathbf{B}, \quad \mathbf{p}\cdot\mathbf{A}+\mathbf{A}\cdot\mathbf{p}, \quad (\mathbf{B}=\nabla\times\mathbf{A}) . \tag{5.140}$$

Because **S** and **p** are odd under time reversal, we have

$$\Theta H \neq H\Theta . \tag{5.141}$$

As an example, for a spin ½ system, $|+\rangle$ and $|-\rangle$ no longer have the same energy under an external magnetic field, so Kramers degeneracy can be lifted by an external magnetic field.