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1. Learning Outcomes (Times New Roman , size 14)

After studying this module, you shall be able to

- Know what symmetry of a physical law means
- Learn a few familiar examples of geometrical continuous symmetries such as translations in space and time and be able to distinguish these from the dynamical symmetries…
- Show that invariance of Hamiltonian of a physical system under space translations leads to the conservation of linear momentum of the system, while total energy is conserved if the Hamiltonian is invariant under translations in time

2. Introduction

In this module we turn over to the topic of symmetries in quantum mechanics. After presenting a general overview of symmetries that exist in the physical laws or the phenomena occurring in nature, we shall find that a symmetry operation on a given physical system has associated with it the law of conservation of a dynamical observable. In other words, if the Hamiltonian of a physical system is invariant under a certain symmetry operation, it would then imply the constancy of a physical observable. In this module, we shall specifically study continuous geometrical symmetries such as translation (displacement) in space and time of a physical system. We shall find that conservation of the linear momentum of a physical system is a consequence of the translational invariance of its Hamiltonian. Similarly, the total energy of the system is conserved if the system is invariant under translations in time,

3. Symmetries in Quantum Mechanics

3.1 General view of symmetries

We are all familiar with the notion of symmetry from daily experience. A given object is said to display a symmetry if it is found to be invariant under a certain operation or a transformation. For instance, a sphere is symmetric because it is invariant under rotations; or a symmetrical vase of such a kind that if we reflect or turn it, it would look the same as before. Here our main interest, however, is to examine the symmetries that exist in the physical laws or the phenomena occurring in nature. For example, we all know that Newton's law of motion, $\vec{F} = m\, {d^2\vec{r}}/{dt^2}$, is symmetrical under translation in space. What it means is that if one makes a transformation, $\vec{r} \rightarrow \vec{r}' = \vec{r} + \vec{a}$, where the vector **a** is a constant displacement, then ${d^2\vec{r}'}/{dt^2}$ $= {d^2(\vec{r} + \vec{a})}/{dt^2} = {d^2\vec{r}}/{dt^2} = \vec{F}$, implying thereby that the law remains unchanged under translation in space. Similarly, one can check that under translation in time, i.e., $t \rightarrow t' = t + \alpha$, where α is a constant displacement in time, the Newton's law remains unchanged that is to say that displacement in time will have no effect on the physical law. To express in simple language, it says that we can move our entire physical apparatus from one place to another or carry out the observations at a later time without affecting the outcome of the experiment. Another important property that Newton's law possesses is that it is represented by a vector equation: $\vec{F} = m\,\vec{a}$. If, therefore, one rotates a vector or equivalently rotate the coordinate system about a given axis, the vector, $\vec{F} \rightarrow \vec{F'}$ and correspondingly the acceleration vector $\vec{a} \rightarrow \vec{a}'$. Thus, for instance, if we rotate the coordinate system about z-axis by an angle θ, then the component x of the vector $\vec{F}$ transforms as $F'_x = F_x \cos(\theta) + F_y \sin(\theta)$ and so does the x-component of the acceleration vector, i.e., $a'_x = a_x \cos(\theta) + a_y \sin(\theta)$. In other words, the law also remains covariant under rotations. These simple symmetry operations of geometrical translations and rotations manifest that ordinary **space is homogeneous and isotropic**.

The symmetries of the physical laws are found to be more interesting and exciting when we come to quantum mechanics. In quantum mechanics, there is an intimate relationship between the law of conservation of a dynamical observable and the corresponding symmetry operation of the physical system. We shall see that if the Hamiltonian of a physical system is invariant under a certain symmetry operation, it would then correspond to the constancy of a physical observable.

The symmetries may be broadly categorized in two groups: (i) the geometrical symmetries associated with space and time and (ii) the dynamical symmetries which are associated with the particular features of the interaction involved. A typical example of a dynamical symmetry is the one observed in hydrogen atom where the energy level of the atom exhibits $n^2 -$ fold degeneracy (n being the principal quantum number of the atom), which is a consequence of a special symmetry of the coulomb interaction. The continuous symmetries associated with displacement in space and time and rotation in space are to be distinguished from the **discrete symmetries** which are defined by the operations of inversion of space and time. While the continuous symmetries are known to be valid universally, independent of the nature of interaction involved, the same does not hold in the case of discrete symmetries. In the next module, we shall discuss these in some detail.

There is yet another type of symmetry, i.e., **the permutation symmetry** which has a central role in quantum mechanics. It turns out that systems containing N identical particles are either totally symmetrical under the interchange of any pair, in which case the particles are known to satisfy Bose-Einstein statistics, hence called bosons, or totally antisymmetrical, in which case they are said to satisfy Fermi-Dirac statistics and called fermions. You must have learnt in your undergraduate course that half-integer spin particles are fermions whereas the integer spin particles are bosons and may have also studied the basic elements of Bose-Einstein and Fermi-Dirac statistics.

3.2 Spatial translations and conservation of linear momentum

Let us study to analyze the connection between translational invariance in space and the conservation of linear momentum of a system. Consider the simple case of a system consisting of a single particle described at a given time by the spatial wave function $\psi(\vec{r})$. The translation of a point particle located at $\vec{r}$ with momentum $\vec{p}$ is defined by the operation

$$\vec{r} \rightarrow \vec{r'} = \vec{r} + \vec{a}\,, \qquad \vec{p} \rightarrow \vec{p'} = \vec{p} \qquad (20.1)$$

The vector $\vec{a}$ is the constant displacement vector by which the particle is displaced. Such a displacement can also be viewed equivalent to the one in which the system is undisturbed but the origin of the coordinate system is displaced by an amount $-\vec{a}$ .The translated wave function, which may be defined by simply allowing the particle to have its new position $\vec{r}'$, is the same as the original wave function at $\vec{r}$, i.e.,

$$\psi'(\vec{r}') = \psi'(\vec{r} + \vec{a}) = \psi(\vec{r}) \tag{20.2}$$

The translated wave function at the point $\vec{r}$ is then obtained by moving both the points by $-\vec{a}$:

$$\psi'(\vec{r}) = \psi(\vec{r} - \vec{a}) \tag{20.3}$$

The action of transforming $\psi(\vec{r})$ *into* $\psi'(\vec{r})$ in quantum mechanics is expressed as an operator, which is accomplished by expanding Eq.(20.3) in Taylor's series:

$$\begin{aligned} \psi'(\vec{r}) &= \psi(\vec{r}) - \vec{a}.\vec{\nabla}\psi(\vec{r}) + \frac{1}{2!}(-\vec{a}.\vec{\nabla})^2\psi(\vec{r}) - \ldots\ldots\ldots\ldots \\ &= \sum_{n=0}^{\infty} \frac{(-\vec{a}.\vec{\nabla})^n}{n!}\psi(\vec{r}) = \exp(-\vec{a}.\vec{\nabla})\psi(\vec{r}) \end{aligned} \tag{20.4}$$

The operator $\vec{\nabla}$ may be expressed through the momentum operator $\vec{p} = -i\hbar\vec{\nabla}$ to get

$$\psi'(\vec{r}) = \exp(-\frac{i}{\hbar}\vec{a}.\vec{p})\psi(\vec{r}) \tag{20.5}$$

This shows that the momentum operator is directly connected with translations in space. For small infinitesimal translations, we may expand the exponential term and write

$$\psi'(\vec{r}) = (1 - \frac{i}{\hbar}\vec{a}.\vec{p})\psi(\vec{r}) , \tag{20.6}$$

so that $\vec{p}$ may be regarded as the **generator** of infinitesimal translations. In Eq.(20.5), we have thus obtained the operator for translations

$$\hat{U}(\vec{a}) = \exp(-\frac{i}{\hbar}\vec{a}.\vec{p}) , \tag{20.7}$$

which transforms the wave function ψ to ψ' as

$$\psi'(\vec{r}) = \psi(\vec{r} - \vec{a}) = \hat{U}(\vec{a})\psi(\vec{r}) \tag{20.8}$$

To see how a position dependent operator, say, $\hat{A}(\vec{r})$ is transformed, we have to remember that $\hat{A}(\vec{r})\psi(\vec{r})$ just transforms like a wave function. Thus

$$\begin{aligned}\hat{A}'(\vec{r})\psi'(\vec{r}) &= \hat{U}(\vec{a})\{\hat{A}(\vec{r})\psi(\vec{r})\} \\ &= \hat{U}(\vec{a})\,\hat{A}(\vec{r})\hat{U}^{-1}\hat{U}\psi(\vec{r})\end{aligned} \qquad (20.9)$$

Comparison with the left hand side shows that operators are transformed as

$$\hat{A}' = \hat{U}\,\hat{A}\hat{U}^{-1} \qquad (20.10)$$

This, in fact, is a general result, which we have studied in the previous module.

Using the power series expansion in Eq.(20.7), one can immediately show that

$$\mathbf{exp}(\hat{\boldsymbol{T}})^{\dagger} = \mathbf{exp}(\hat{\boldsymbol{T}}^{\dagger}) \quad , \quad \exp(\hat{\boldsymbol{T}})^{-\mathbf{1}} = \mathbf{exp}(-\hat{\boldsymbol{T}}) \ , \qquad (20.11)$$

where the operator $\hat{T} = -\frac{i}{\hbar}\vec{p}.\vec{a}$. Since $\vec{p}$ is a Hermitian operator, its product with imaginary number changes sign under Hermitian conjugation and we get

$$\widehat{\boldsymbol{U}}^{\dagger}(\vec{\boldsymbol{a}}) = \widehat{\boldsymbol{U}}^{-\mathbf{1}}(\vec{\boldsymbol{a}}) = \widehat{\boldsymbol{U}}(-\vec{\boldsymbol{a}}) \qquad (20.12)$$

The operator $\widehat{\boldsymbol{U}}(\vec{\boldsymbol{a}})$ is therefore unitary so that the norm of the wave function is conserved.

3.3 Translational Invariance

A physical system is said to be invariant under translations if the Hamiltonian does not change under translations, i.e.,

$$\widehat{\boldsymbol{H}}'(\vec{\boldsymbol{r}}) = \widehat{\boldsymbol{H}}(\vec{\boldsymbol{r}} - \vec{\boldsymbol{a}}) = \widehat{\boldsymbol{H}}(\vec{\boldsymbol{r}}) \qquad (20.13)$$

According to Eq.(20.10), it follows that

$$\begin{aligned}&\hat{U}(\vec{a})\,\hat{H}(\vec{r})\hat{U}^{-1}(\vec{a}) = \hat{H}(\vec{r}) \\ &or \quad \hat{H}(\vec{r})\hat{U}(\vec{a}) = \hat{U}(\vec{a})\,\hat{H}(\vec{r}), \\ &i.e., \quad \left[\hat{H}(\vec{r}),\hat{U}(\vec{a})\right] = 0\end{aligned} \qquad (20.14)$$

which shows that the Hamiltonian commutes with the operator of translation for arbitrary $\vec{a}$. Using the expression, Eq.(18.7), it is clear that $\hat{U}(\vec{a})$ will commute with the operator $\hat{H}$ for any $\vec{a}$, provided the momentum operator $\vec{p}$ commutes. This leads to the condition

$$\left[\hat{H}, \hat{p}\right] = 0 \qquad (20.15)$$

3.4 Many Particle System

The above results can be easily generalized to a system of many particles. We shall find that the translation of a many particle system leads to the concept of total momentum. Translating a system of N particles by the displacement $\vec{a}$ is expressed as

$$(\vec{r}_1, \vec{r}_2, \ldots\ldots\ldots, \vec{r}_N) \to (\vec{r}_1 + \vec{a}, \vec{r}_2 + \vec{a}, \ldots\ldots\ldots, \vec{r}_N + \vec{a}) \qquad (20.16)$$

As a result, the transformation of the many body wave function is given by

$$\psi'(\vec{r}_1, \vec{r}_2, \ldots\ldots\ldots, \vec{r}_N) = \psi(\vec{r}_1 - \vec{a}, \vec{r}_2 - \vec{a}, \ldots\ldots\ldots, \vec{r}_N - \vec{a}) \qquad (20.17)$$

so that applying the translational operators for each coordinate separately, we write Eq.(20.17) as

$$\psi'(\vec{r}_1, \vec{r}_2, \ldots\ldots\ldots, \vec{r}_N) = \hat{U}_1(\vec{a})\hat{U}_2(\vec{a})\ldots\ldots\hat{U}_N(\vec{a})\psi(\vec{r}_1, \vec{r}_2, \ldots\ldots\ldots, \vec{r}_N), \qquad (20.18)$$

where the operator $\hat{U}_i(\vec{a})$ acts on coordinate i:

$$\hat{U}_i(\vec{a}) = \exp(-\vec{a}.\vec{\nabla}_i) = \exp(-\frac{i}{\hbar}\vec{a}.\vec{p}_i) \qquad (20.19)$$

Eq.(18.18) can thus be expressed using Eq.(20.19) as

$$\begin{aligned} \psi'(\vec{r}_1, \vec{r}_2, \ldots\ldots\ldots, \vec{r}_N) &= \exp\left[-\frac{i}{\hbar}\vec{a}\,(\vec{p}_1 + \vec{p}_2 + \ldots\ldots\vec{p}_N)\right]\psi(\vec{r}_1, \vec{r}_2, \ldots\ldots\ldots, \vec{r}_N) \\ &= \exp\left(-\frac{i}{\hbar}\vec{a}.\vec{P}\right)\psi(\vec{r}_1 + \vec{r}_2 + \ldots\ldots\vec{r}_N), \end{aligned} \qquad (20.20)$$

where $\vec{P}$ is the total momentum operator; $\quad \vec{P} = \sum_{i=1}^{N}\vec{p}_i \qquad (20.21)$

Thus for a system of N particles, total momentum operator appears as the operator for simultaneous infinitesimal operations of all particles. If the Hamiltonian of the system is invariant under translations, then it follows that $\left[\vec{P},\hat{H}\right]=0$, with the result that total momentum of a system of particles is a constant of motion.

For example, consider a Hamiltonian of the form

$$\hat{H}=\sum_{i=1}^{N}\frac{\hat{p}_i^2}{2m_i}+\frac{1}{2}\sum_{i\neq j=1}^{N}V(\vec{r}_i,\vec{r}_j), \qquad (20.22)$$

where the two body potential depends only on the relative co-ordinates, $\vec{r}_i-\vec{r}_j$, and therefore, under constant displacement of each co-ordinate, the two body potential remains invariant. Since the kinetic energy term does not involve any dependence on the positions of the particles, the Hamiltonian should be invariant under simultaneous translations of all particles. The total momentum of the system is therefore a constant of motion.

It should be noted that with the definition, Eq.(20.21), given for the total momentum, the canonically conjugate coordinate to the total momentum for the N particle system is the centre of mass vector:

$$\vec{R}=\frac{\sum_{i=1}^{N}m_i\vec{r}_i}{\sum_{i=1}^{N}m_i} \qquad (20.23)$$

One can then easily check that similar to the commutation relation $\left[r_i,p_j\right]=i\hbar\delta_{ij}$ obeyed by the components of position and momentum of a single particle, we would have here the corresponding commutation relations between the Cartesian components, $\hat{R}_i$ *and* P_j, viz.,

$$\left[\hat{R}_i,\hat{P}_j\right]=i\hbar\delta_{ij} \qquad (20.24)$$

3.4 Displacement in Time: Conservation of Energy

One can study, in similar fashion, translation in time of the wave function , $\psi(\vec{r},t)$ describing a particle .The wave function translated in time, which may be defined by simply allowing the particle to have its new time coordinate $t\rightarrow t'=t+\tau$, is the same as the original wave function at time t, i.e.,

$$\psi'(\vec{r},t')=\psi'(\vec{r},t+\tau)=\psi(\vec{r},t) \qquad (20.25)$$

The translated wave function at the time t is then obtained by moving both the time coordinates, t and t' by - τ :

$$\boldsymbol{\psi}'(\vec{\boldsymbol{r}},\boldsymbol{t}) = \boldsymbol{\psi}(\vec{\boldsymbol{r}},\boldsymbol{t}-\boldsymbol{\tau}) \qquad (20.26)$$

The action of transforming $\boldsymbol{\psi}(\vec{\boldsymbol{r}})$ ***into*** $\boldsymbol{\psi}'(\vec{\boldsymbol{r}})$ in quantum mechanics is expressed as an operator, which is accomplished by expanding Eq.(20.26) in Taylor's series:

$$\psi'(\vec{r},t) = \psi(\vec{r},t) - \tau\frac{\partial}{\partial t}\psi(\vec{r},t) + \frac{\tau^2}{2!}\frac{\partial^2}{\partial t^2}\psi(\vec{r},t) - \ldots\ldots\ldots\ldots\ldots\ldots$$

$$= \sum_{n=0}^{\infty}\frac{\tau^n(-\partial/\partial t)^n}{n!}\psi(\vec{r},t) = \exp(-\tau\partial/\partial t)\psi(\vec{r},t) \qquad (20.27)$$

The operator $\partial/\partial t$ may now be expressed as $\frac{-i\hat{H}}{\hbar}$, so that substituting in Eq.(20.27), we have

$$\psi'(\vec{r},t) = \exp(\frac{i\tau\hat{H}}{\hbar})\psi(\vec{r},t) \qquad (20.28)$$

We thus find that displacement in time, which is also a continuous transformation is also **unitary**. The effect of the displacement $\boldsymbol{\tau}$ on the wave function ψ(t) is given by

$$\psi'(\vec{r},t) = \hat{U}(\tau)\,\psi(\vec{r},t)\,, \qquad (20.29)$$

where $$U(\tau) = \exp(\frac{i\tau\hat{H}}{\hbar}) \qquad (20.30)$$

What it means is that events corresponding to time t in ψ, correspond to time (t+$\boldsymbol{\tau}$) in $\boldsymbol{\psi}'$.

The invariance of the Hamiltonian under translations in time requires that

$$\widehat{\boldsymbol{H}}'(\boldsymbol{t}) = \widehat{\boldsymbol{H}}(\boldsymbol{t}-\boldsymbol{\tau}) = \widehat{\boldsymbol{H}}(\boldsymbol{t}) \qquad (20.31a)$$

i.e., $$\hat{U}(\tau)\hat{H}\hat{U}^{-1}(\tau) = \hat{H} \quad \text{or} \quad \hat{U}(\tau)\hat{H} = \hat{H}\hat{U}(\tau). \qquad (20.31b)$$

Now $\widehat{\boldsymbol{H}}$ commutes with $\widehat{\boldsymbol{U}}$ if $\widehat{\boldsymbol{H}}$ is independent of t. The time independence of $\widehat{\boldsymbol{H}}$ means that the total energy of the system is conserved. *It thus follows that the total energy of the system is conserved if the system is invariant under translations in time.*

4. Summary

After studying this module, you would be able

- Define the symmetry of a physical law and come to know of different types of symmetries in quantum mechanics
- Learn a few familiar examples of geometrical continuous symmetries such as translations in space and time, their connections with homogeneity of space and time and be able to distinguish these from the dynamical symmetries
- Show that invariance of Hamiltonian of a physical system under space translations leads to the conservation of linear momentum of the system, while total energy is conserved if the Hamiltonian is invariant under translations in time