Chapter 5

Symmetries II

In Chapter 2 we had already defined that an operator A, which does not explicitly depend on the time, i.e., $\frac{\partial A}{\partial t} \; = \; 0$, is then and only then a **constant of motion** if $[H, A] \; = \; 0$.

Let us define a unitary operator

$$U(t) = e^{-\frac{i}{\hbar}Ht} \tag{5.1}$$

for translations with respect to time.

Differentiation with respect to time gives

$$\frac{d}{dt}\,U(t) \;=\; -\,\frac{i}{\hbar}\,H\;e^{-\frac{i}{\hbar}Ht}\;. \tag{5.2}$$

This operation is allowed since all quantities commute, i.e., one has $[U(t), H] \; = \; 0$. Thus $U(t)$ fulfills the following differential equation

$$i\hbar\,\frac{d\,U(t)}{dt} \;=\; H\;U(t)\;. \tag{5.3}$$

This equation has formal similarity with the time-dependent Schrödinger equation, however, the wave function ψ is here replaced by the operator U. Thus (5.3) can be viewed as **Operator- Schrödinger equation**. Eq. (5.3) can also be viewed as defining equation for $U(t)$. With the initial condition $U(0) = \mathbf{1}$, one obtains (5.1).

5.1 Translations

In Section 4.12, we showed by using the commutation relation between $\vec{X}$ and $\vec{P}$ that an operator

$$U(\vec{a}) \; = \; e^{-\frac{i}{\hbar}\, \vec{a}\cdot\vec{P}} \tag{5.4}$$

has the properties of a translation operator. We now want to construct this result systematically.

A translation in space is given by

$$\vec{x}\,' \; = \; \vec{x} \; + \; \vec{a} \; , \tag{5.5}$$

where $\vec{a}$ is an arbitrary vector $\in \mathbf{R}^3$. Analogously we define the translation of the $\vec{X}$-operator as

$$\vec{X}\,' \; = \; \vec{X} \; + \; \vec{a}\mathbf{1} \; , \tag{5.6}$$

and try to find a unitary translation operator $U(\vec{a})$ with

$$U^\dagger(\vec{a}) \; \vec{X} \; U(\vec{a}) \; = \; \vec{X} \; + \; \vec{a}\mathbf{1} \; . \tag{5.7}$$

With

$$\begin{aligned} U^\dagger(\vec{a}_2)\; U^\dagger(\vec{a}_1)\; \vec{X}\; U(\vec{a}_1)\; U(\vec{a}_2) \; &= \; \vec{X} \; + \; (\vec{a}_1 + \vec{a}_2)\; \mathbf{1} \\ &= \; U^\dagger(\vec{a}_1 + \vec{a}_2)\vec{X}\; U(\vec{a}_1 + \vec{a}_2) \end{aligned} \tag{5.8}$$

one has the following property of $U(\vec{a})$:

$$U(\vec{a}_2)\; U(\vec{a}_1) \; = \; U(\vec{a}_1 + \vec{a}_2) \; . \tag{5.9}$$

From

$$U(\vec{a}_1 + \vec{a}_2) \; = \; U(\vec{a}_2 + \vec{a}_1) \tag{5.10}$$

follows

$$[U(\vec{a}_1),\; U(\vec{a}_2)] \; = \; 0 \; . \tag{5.11}$$

Furthermore, one has

$$U(\vec{0}) \; = \; \mathbf{1} \; . \tag{5.12}$$

Because of (5.9), the relation

$$\vec{a} \longmapsto U(\vec{a}) \tag{5.13}$$

is a Homomorphism, namely the representation of the Abelian translation group with the unitary operators $U(\vec{a})$. In order to draw conclusions from the above given properties, we consider (because of simplicity) the one-dimensional problem. One has

$$U(a_2)\, U(a_1) \;=\; U(a_1)\, U(a_2) \;=\; U(a_1 + a_2) \tag{5.14}$$

and thus differentiating with respect to a_1 or a_2 gives

$$\begin{aligned} U(a_2)\, \frac{dU(a_1)}{da_1} \;&=\; \frac{dU(a)}{da} \\ \frac{dU(a_2)}{da_2}\, U(a_1) \;&=\; \frac{dU(a)}{da} \end{aligned} \tag{5.15}$$

where $a = a_1 + a_2$. Thus one has

$$U(a_2)\, \frac{dU(a_1)}{da_1} \;=\; \frac{dU(a_2)}{da_2}\, U(a_1) \tag{5.16}$$

or

$$\frac{dU(a_1)}{da_1}\, U^{-1}(a_1) \;=\; U^{-1}(a_2)\, \frac{dU(a_2)}{da_2} \;. \tag{5.17}$$

Since (5.17) has to be valid for different values a_1, a_2, follows that

$$\frac{dU(a)}{da}\, U^{-1}(a) \;=\; U^{-1}(a)\, \frac{dU(a)}{da} \;=\; -iK \tag{5.18}$$

has to be independent of a. The operator K still has to be determined. The solution of

$$\frac{dU(a)}{da} \;=\; -iK\; U(a) = U(a)(-iK) \tag{5.19}$$

is obviously

$$U(a) \;=\; e^{-iKa} \;, \tag{5.20}$$

where (5.12) has to be taken into account. From the unitarity of U follows that K is self-adjoint and vice versa. For an infinitesimal value da, one can expand (5.20)

$$U(da) \;=\; \mathbf{1} \;-\; i\; da\; K \tag{5.21}$$

and

$$U^\dagger(da) \;=\; \mathbf{1} \;+\; i\; da\; K \; . \tag{5.22}$$

Inserting (5.21) and (5.22) in (5.7) gives

$$\begin{aligned} U^\dagger(da) X\; U(da) &= (\mathbf{1} + i\; da\; K) X\; (\mathbf{1} - i\; da\; K) \\ &= X + i\; da[K, X] \\ &\equiv X + da\; \mathbf{1} \; . \end{aligned} \tag{5.23}$$

Thus

$$i[K, X] \;=\; \mathbf{1} \; . \tag{5.24}$$

Comparing (5.24) with the Heisenberg commutation relation gives that

$$\hbar K \;=\; P \; , \tag{5.25}$$

i.e., one obtains for $U(a)$

$$U(a)\; e^{-\frac{i}{\hbar}\; aP} \; . \tag{5.26}$$

The same considerations are valid for the three-dimensional case. Thus, one has here

$$U(\vec{a}) \;=\; e^{-\frac{i}{\hbar}\; \vec{a}\cdot\vec{P}} \; . \tag{5.27}$$

Remarks: In the above derivation, the commutation relation $i\hbar[P, X] = \mathbf{1}$ was assumed. Taking a more general point of view, one could have defined the momentum operator $\vec{P}$ as "infinitesimal generator" of the translation (5.21). Then one would have automatically obtained the commutation relation (5.24). Thus, up to the factor $\hbar$, the definition of $U(\vec{a})$ based on group theory determines the momentum operator $\vec{P}$.

5.2 Application of $U(a)$ on Quantum States

At the beginning of the Chapter, we already indicated that $U(t)$ can be applied on operators or quantum mechanical states:

$$\begin{aligned} \langle A(t)\rangle_\psi &= \langle \psi \mid A(t) \mid \psi\rangle \;=\; \langle \psi \mid U^\dagger(t)\; A(0)\; U(t) \mid \psi\rangle \\ &= \langle U(t)\psi \mid A(0) \mid U(t)\psi\rangle \\ &= \langle \psi(t) \mid A(0) \mid \psi(t)\rangle \; . \end{aligned} \tag{5.28}$$

Specifically, (5.28) indicates going from the Heisenberg representation to the Schrödinger representation with respect to time dependence. Analogously translations can be viewed as

$$\langle\psi \mid U^\dagger(a) A U(a) \mid \psi\rangle \;=\; \langle U(a)\psi \mid A \mid U(a)\psi\rangle \;. \tag{5.29}$$

Thus $U(a)$ could be defined via its action on states $\mid \varphi_{\vec{x}} \,\rangle$. Here we use

$$\vec{X} \mid \varphi_{\vec{x}} \,\rangle \;=\; \vec{x} \;\mid \varphi_{\vec{x}} \,\rangle \tag{5.30}$$

to define the eigenstates and eigenvalues of the position operator $\vec{X}$. Multiplication of (5.30) with $U(\vec{a})$ gives with (5.7)

$$\begin{aligned} U(\vec{a})\vec{X} \;\mid \varphi_{\vec{x}} \,\rangle &= \vec{x}\, U(\vec{a}) \mid \varphi_{\vec{x}} \,\rangle \\ &= \vec{X}\, U(\vec{a}) \mid \varphi_{\vec{x}} \,\rangle \;-\; \vec{a}\, U(\vec{a}) \mid \varphi_{\vec{x}} \,\rangle \end{aligned} \tag{5.31}$$

from which follows

$$\vec{X}\, U(\vec{a}) \mid \varphi_{\vec{x}} \,\rangle \;=\; (\vec{x} \;+ \vec{a})\, U(\vec{a}) \mid \varphi_{\vec{x}} \,\rangle \;. \tag{5.32}$$

Thus, applying $U(\vec{a})$ on a state $\mid \varphi_{\vec{x}} \,\rangle$ to eigenvalue $\vec{x}$ results in a state to eigenvalue $(\vec{x} \;+ \vec{a})$, i.e.,

$$U(\vec{a}) \mid \varphi_{\vec{x}} \,\rangle \;= \mid \varphi_{\vec{x}+\vec{a}} \,\rangle \;. \tag{5.33}$$

One could have chosen (5.33) as alternative to the definition (5.7) for defining the translation operator $U(\vec{a})$. Obviously one has

$$U(\vec{a}_2)\; U(\vec{a}_1) \mid \varphi_{\vec{x}} \,\rangle \;= \mid \varphi_{\vec{x}+\vec{a}_1+\vec{a}_2}\rangle \;=\; U(\vec{a}_1 + \vec{a}_2) \mid \varphi_{\vec{x}} \,\rangle \;, \tag{5.34}$$

from which we obtain again (5.9)

$$U(\vec{a}_2)\; U(\vec{a}_1) \;=\; U(\vec{a}_1)\; U(\vec{a}_2) \;=\; U(\vec{a}_1 + \vec{a}_2) \;. \tag{5.35}$$

This relation together with $U(\vec{0}) \;=\; \mathbf{1}$ lead to the specific solution (5.20) of the differential equation. This means, even when starting from the definition (5.33) for the translation operator, one would end up with the explicit form

$$U(\vec{a}) \;=\; e^{-\frac{i}{\hbar}\; \vec{a}\cdot\vec{P}} \;. \tag{5.36}$$

Let us consider the expectation value of (5.7)

$$\langle\psi \mid U^\dagger(\vec{a})\; \vec{X}\; U(\vec{a}) \mid \psi\rangle \;=\; \langle\psi \mid \vec{X} \mid \psi\rangle \;+\; \vec{a} \;. \tag{5.37}$$

In the Schrödinger-type picture, one has

$$\begin{aligned}\langle U(\vec{a})\psi \mid \vec{X} \mid U(\vec{a})\psi\langle &= \int d\vec{x}\,' \int d\vec{x}\, \langle \psi \mid \varphi_{\vec{x}\,'}\rangle\langle U(\vec{a})\varphi_{\vec{x}\,'} \mid \vec{X} \mid U(\vec{a})\varphi_{\vec{x}}\rangle\langle\varphi_{\vec{x}} \mid \psi\rangle \\ &= \int d\vec{x}\,' \int d\vec{x}\, \langle \psi \mid \varphi_{\vec{x}\,'}\rangle\langle\varphi_{\vec{x}\,'+a} \mid \vec{X} \mid \varphi_{\vec{x}+\vec{a}}\rangle\langle\varphi_{\vec{x}} \mid \psi\rangle \\ &= \int d\vec{x}\,' \int d\vec{x}\, \langle \psi \mid \varphi_{\vec{x}\,'}\rangle(\vec{x}+\vec{a})\, \delta(\vec{x}\,'-\vec{x})\langle\varphi_{\vec{x}} \mid \psi\rangle \\ &= \int d\vec{x}\, \langle \psi \mid \varphi_{\vec{x}}\rangle\vec{x}\,\langle\varphi_{\vec{x}} \mid \psi\rangle + \vec{a}\end{aligned} \tag{5.38}$$

and thus

$$\langle U(\vec{a})\psi \mid \vec{X} \mid U(\vec{a})\psi\rangle = \langle \psi \mid \vec{X} \mid \psi\rangle + a\,, \tag{5.39}$$

which shows that $U(\vec{a})$ applied either on the position operator $\vec{X}$ or on the state $\mid \psi\rangle$ leads to a shift of the expectation value by $\vec{a}_1$ as it was expected.

5.3 Transition Operator in Coordinate Space Representation

It is instructive to study the translation operator in its coordinate representation. With (5.33) follows

$$\langle\varphi_{\vec{x}} \mid U(\vec{a}) \mid \psi\rangle = \langle U^\dagger(\vec{a})\, \varphi_{\vec{x}} \mid \psi\rangle\,. \tag{5.40}$$

The explicit form of $U^\dagger(\vec{a})$ follows from (5.36):

$$U^\dagger(a) = e^{\frac{i}{\hbar}\,\vec{a}\,\vec{P}} = e^{-\,\frac{i}{\hbar}\,(-\vec{a})\cdot\vec{P}}\,. \tag{5.41}$$

Thus $U^\dagger(\vec{a})$ acts similar to $U(\vec{a})$; however, here $\vec{a}$ is replaced by $(-\vec{a})$. This also follows directly from the definition (5.33). Because of $U(\vec{a})$ being unitary, i.e.,

$$U^\dagger(\vec{a})\, U(\vec{a}) = \mathbf{1} \tag{5.42}$$

one has

$$U^\dagger(\vec{a})\, U(\vec{a}) \mid \varphi_{\vec{x}}\rangle = \mid \varphi_{\vec{x}}\rangle \tag{5.43}$$

and thus

$$U^\dagger(\vec{a}) \mid \varphi_{\vec{x}+\vec{a}}\rangle = \mid \varphi_{\vec{x}}\rangle\,. \tag{5.44}$$

If one replaces here $\vec{x}\,' = \vec{x} - \vec{a}$, then

$$U^{\dagger}(\vec{a}) \mid \varphi_{\vec{x}} \rangle = \mid \varphi_{\vec{x}-\vec{a}} \rangle \,, \tag{5.45}$$

and (5.40) becomes

$$\langle \varphi_{\vec{x}} \mid U(\vec{a}) \mid \psi \rangle = \langle \varphi_{\vec{x}-\vec{a}} \mid \psi \rangle \,. \tag{5.46}$$

This, in turn, means that in the coordinate space representation $U(\vec{a})$ takes the form

$$U(\vec{a})\, \psi(\vec{x}) = \psi(\vec{x}-\vec{a}) \,. \tag{5.47}$$

The relation (5.47) is often used as **definition of the translation operator**. From

$$U(\vec{a}_2)\, U(\vec{a}_1)\, \psi(\vec{x}) = \psi(\vec{x}-\vec{a}_1-\vec{a}_2) = U(\vec{a}_1+\vec{a}_2)\, \psi(\vec{x}) \tag{5.48}$$

follows again the relation (5.9) from which we started. A relation as (5.9) conserves the algebraic structure of an operator and is called Homomorphism. In this example, the algebraic structure of translations in $\mathbf{R}^3$ is mapped on unitary operators in the Hilbert space. In coordinate space, one has the explicit representation

$$U(\vec{a}) = e^{-\frac{i}{\hbar}\,\vec{a}\cdot\vec{P}} = e^{-\vec{a}\cdot\vec{\nabla}} \,. \tag{5.49}$$

5.4 Representation of the Translation Group in the Hilbert Space

Let G be a group with elements $\{g_1, g_2, g_3 \cdots\}$. Further, one has a map from the elements of the group on to other mathematical quantities, e.g., operators of a Hilbert space:

$$g \longmapsto U(g) \,. \tag{5.50}$$

If this map is a Homomorphism, so that

$$U(g_1 g_2) = U(g_1)\, U(g_2) \tag{5.51}$$

holds, then $U(G)$ is called a representation of the Group G. Obviously, translations form a group in $\mathbf{R}^3$. With

$$T_{\vec{a}}\, \vec{x} := \vec{x} + \vec{a} \,, \tag{5.52}$$

one has

$$T_{\vec{a}_1} T_{\vec{a}_2}\, \vec{x} = T_{a_1}(\vec{x}+\vec{a}_2) = \vec{x}+\vec{a}_2+\vec{a}_1 = T_{\vec{a}_1+\vec{a}_2}\, \vec{x} \,. \tag{5.53}$$

Starting from (5.53), one can easily show all other group properties. If one writes (5.13) as

$$T_{\vec{a}} \longmapsto U(T_{\vec{a}}) \tag{5.54}$$

in analogy to (5.50), then (5.9) or (5.35), one written as

$$U(T_{\vec{a}_1})\, U(T_{\vec{a}_2}) \;=\; U(T_{\vec{a}_1} T_{\vec{a}_2}) \tag{5.55}$$

and a comparison with (5.51) shows the group homomorphism quite clearly.

Remark: Addition of the vectors $\vec{x}$ and $\vec{a}$ results in the vector $\vec{x} + \vec{a}$. However, adding the eigenvectors $|\,\varphi_{\vec{x}}\,\rangle$ and $|\,\varphi_{\vec{a}}\,\rangle$ of the operator $\vec{X}$ does **not** lead to the eigenvector $|\,\varphi_{\vec{x}\,+\vec{a}}\,\rangle$. One has

$$\vec{X}\,|\,\varphi_{\vec{x}+\vec{a}}\,\rangle \;=\; (\vec{x}+\vec{a})\,|\,\varphi_{\vec{x}+\vec{a}}\,\rangle \tag{5.56}$$

and

$$\vec{X}[|\,\varphi_{\vec{x}}\,\rangle + \;|\,\varphi_{\vec{a}}\,\rangle] \;=\; \vec{x}\,|\,\varphi_{\vec{x}}\,\rangle + \vec{a}\,|\,\varphi_{\vec{a}}\,\rangle \;\neq\; (\vec{x}+\vec{a})[|\,\varphi_{\vec{x}}\,\rangle + |\,\varphi_{\vec{a}}\,\rangle]\ , \tag{5.57}$$

i.e.,

$$|\,\varphi_{\vec{x}\,+\vec{a}}\,\rangle \;\neq |\,\varphi_{\vec{x}}\,\rangle + |\,\varphi_{\vec{a}}\,\rangle\ . \tag{5.58}$$

5.5 Translational Invariance

Like in classical mechanics, translational invariance will be defined via properties of the Hamiltonian, i.e.,

$$H(\vec{P}, \vec{X} + \vec{a}\;\mathbf{1}) \;=\; H(\vec{P}, \vec{X})\ . \tag{5.59}$$

Considering that $U(\vec{a})$ and $\vec{P}$ commute and that for the scalar product the following relation holds

$$\begin{aligned}(\vec{X} + \vec{a}\;\mathbf{1})\cdot\ \cdots\ \cdot(\vec{X} + \vec{a}\mathbf{1}) \;&=\; U^\dagger(\vec{a})\;\vec{X}\;U(\vec{a})\;\cdots\;U^\dagger(\vec{a})\;\vec{X}\;U(\vec{a}) \\ &=\; U^\dagger(\vec{a})\;\{\vec{X}\;\cdot\;\cdots\;\cdot\;\vec{X}\;\}\;U(\vec{a})\ ,\end{aligned} \tag{5.60}$$

then one can show that

$$H(\vec{P}, \vec{X} + \vec{a}\;\mathbf{1}) \;=\; U^\dagger(\vec{a})\;H(\vec{P}, \vec{X})\;U(\vec{a})\ . \tag{5.61}$$

Thus the translational invariance of H can be written as

$$U^\dagger(\vec{a})\ H(\vec{P}, \vec{X})\ U(\vec{a}) \;=\; H(\vec{P}, \vec{X})\ . \tag{5.62}$$

In this case $U(\vec{a})$ commutes with H, i.e.,

$$[H, U(\vec{a})] \;=\; 0\ . \tag{5.63}$$

If one considers infinitesimal translations, this means

$$[H, \vec{P}] \;=\; 0\ . \tag{5.64}$$

In the Heisenberg-representation, one had

$$\dot{\vec{P}} \;=\; \frac{i}{\hbar}\ [H, \vec{P}]\ . \tag{5.65}$$

If the Hamiltonian is invariant under translations, then $[H, \vec{P}] = 0$ and thus $\dot{\vec{P}} = 0$, i.e., $\vec{P}$ is a conserved quantity.

In the so-far considered one-body problems, H was of the form

$$H \;=\; \frac{\vec{P}^{\ 2}}{2m} \;+\; V(\vec{x})\ . \tag{5.66}$$

Thus invariance of H under translations put the restriction

$$V(\vec{X} + \vec{a}\ \mathbf{1}) \;=\; V(\vec{x}) \tag{5.67}$$

on the interaction V. This is only the case if V is independent of $\vec{X}$. In that case V can be set to zero. Thus conservation of the linear momentum $\vec{P}$ (with a Hamiltonian of the form (5.66)) can only occur if there is no potential V, i.e., for the free motion. Translational invariance of H and the resulting conservation of the **total** momentum will only become important for systems with two or more particle.

5.6 Rotations in $\mathbf{R}^3$

A linear map

$$\vec{x}\ ' \;=\; \mathbf{R}\ \vec{x} \tag{5.68}$$

in $\mathbf{R}^3$ is called rotation in this space if it leaves the there defined scalar product invariant, i.e., if for two vectors $\vec{x}$ and $\vec{y}$

$$(R\vec{y}) \cdot (R\vec{x}) \;=\; \vec{y} \cdot \vec{x}\ . \tag{5.69}$$

Introducing the canonical basis in $\mathbf{R}^3, \vec{e}_i, i = 1, 2, 3$ with $\vec{e}_i \cdot \vec{e}_j \; = \; \delta_{ij}$ and associating via

$$(\vec{e}_j \cdot R \; \vec{e}_k) \; \equiv \; R_{jk} \tag{5.70}$$

the matrices R_{jk} with the map R, then (5.68) takes the usual matrix form

$$x'_j \; = \; \sum_{k=1}^{3} \; R_{jk} \; x_k \; . \tag{5.71}$$

The invariance of the scalar product leads to

$$\sum_j \sum_{k\ell} \; R_{jk} y_k \; R_{j\ell} x_\ell \; = \; \sum_k \; y_k x_k \tag{5.72}$$

and thus

$$\sum_j \; R_{jk} \; R_{j\ell} \; = \; \delta_{k\ell} \tag{5.73}$$

or if one uses that $R^T_{kj} \; = \; R_{jk}$ describes the transpose matrix of (R_{jk})

$$\sum_j \; R^T_{kj} R_{j\ell} \; = \; \delta_{k\ell} \quad \text{or} \quad R^T R \; = \; \mathbf{1} \; . \tag{5.74}$$

The matrices fulfilling (5.74) build a group, the rotational group or the orthogonal group in three dimensions $O(3)$. For the determinants, one finds

$$\det(R^T R) \; = \; (\det \; R^T)(\det \; R) \; = \; (\det \; R)^2 \; = \; \det \; \mathbf{1} \; = \; \mathbf{1} \tag{5.75}$$

and thus

$$detR \; = \; \pm \mathbf{1} \; . \tag{5.76}$$

From this follows immediately the existence of the inverse R^{-1} to R and

$$R^T \; = \; R^{-1} \; , \tag{5.77}$$

which characterizes orthogonal matrices.

The orthogonal matrices with determinant $+1$ build a subgroup of $O(3)$, the special orthogonal group $SO(3)$. $SO(3)$ contains all matrices which can be transformed continuously to the unit matrix, thus the rotations.

The matrix

$$\hat{R} \; = \; (-\delta_{jk}) \tag{5.78}$$

is an element of $O(3)$ with $\det \hat{R} = -1$, and thus does **not** belong to $SO(3)$. The transformation (5.71) takes the form

$$\sum_k \hat{R}^T_{jk} \, x_k \;=\; -x_j \;=\; x'_j \tag{5.79}$$

and describes an inversion (as discussed in Chapter 2). If one multiplies elements of $SO(3)$ with $\hat{R}$, one obtains orthogonal matrices, which because of

$$\det(R\hat{R}) \;=\; (\det\; R)(\det\; \hat{R}) \;=\; -1 \tag{5.80}$$

do not belong to $SO(3)$.

Parameters of $O(3)$: In general 3×3 matrices have nine matrix elements. Because of (5.74) and *det* $R = 1$, they are not all independent. All orthogonal matrices can be represented in the form

$$R \;= e^{A} \; . \tag{5.81}$$

Because of

$$R^T R \;=\; e^{A^T} \, e^{A} \;=\; \mathbf{1} \tag{5.82}$$

follows

$$A^T \;=\; -A \tag{5.83}$$

and thus for the matrix elements of A

$$A_{kj} \;=\; -A_{jk} \; , \tag{5.84}$$

i.e., only three elements are independent. This means $O(3)$ can be characterized by **three** parameters (e.g., by explicitly fixing elements A_{12}, A_{13} and A_{23}).

The Euler angles are another way of fixing the three parameters. Here the rotation of a vector $\vec{x}$ is given by

$$\vec{x}_A{}' \;=\; A(\alpha, \beta, \gamma) \, \vec{x} \tag{5.85}$$

and A is given as

$$A(\alpha, \beta, \gamma) \;=\; A_3(\alpha) \; A_2(\beta) \; A_3(\gamma) \; , \tag{5.86}$$

where the subscripts specify the axis about which the rotation is made. Explicitly:

$$A_3(\alpha) \;\equiv\; \begin{pmatrix} \cos\alpha & -\sin\alpha & 0 \\ \sin\alpha & \cos\alpha & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{5.87}$$

$$A_2(\beta) \;=\; \begin{pmatrix} \cos\beta & 0 & \sin\beta \\ 0 & 1 & 0 \\ -\sin\beta & 0 & \cos\beta \end{pmatrix} \;. \tag{5.88}$$

Note: The matrix describes the **active** rotation of the vector $\vec{x}$.

For completeness,

$$A_1(\gamma) \;=\; \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\gamma & -\sin\gamma \\ 0 & \sin\gamma & \cos\;\gamma \end{pmatrix} \;. \tag{5.89}$$

5.7 Rotations around the 3-Axis

As general form of (5.87), one can write

$$R \;=\; \begin{pmatrix} R_{11} & R_{12} & 0 \\ R_{21} & R_{22} & 0 \\ 0 & 0 & 1 \end{pmatrix} \;. \tag{5.90}$$

One obtains the subgroup $O(2)$, which is given by the 2×2 matrix

$$\begin{pmatrix} R_{11} & R_{12} \\ R_{21} & R_{22} \end{pmatrix} \;. \tag{5.91}$$

The orthogonality condition now reads

$$\sum_{j=1}^{2} R_{jk} R_{j\ell} \;=\; \delta_{k\ell} \quad k, \ell = 1, 2 \tag{5.92}$$

and shows that only one matrix element, e.g., R_{11}, is independent. Because of $R_{11}R_{11} + R_{21}R_{21} = 1$, it is suggestive to put

$$R_{11} \;=\; \cos\alpha \;. \tag{5.93}$$

Then $R_{21} \;=\; \pm\; \sin\alpha$. The choice $R_{21} = \sin\alpha$ leads to the form (5.87), which describes an active rotation of a vector $\vec{x}$. An argument for the choice of R_{11} in (5.93) is the requirement, that for $\alpha = 0, R$ should be the identity matrix. (Note that (5.92) would allow to choose $R_{11} = \sin\beta$, e.g.).

It can be easily shown that $SO(2)$ is a group. In addition, it is an Abelian group, i.e.,

$$R(\alpha_2)\; R(\alpha_1) \;=\; R(\alpha_2 + \alpha_1) \;=\; R(\alpha_1 + \alpha_2) \;=\; R(\alpha_1)\; R(\alpha_2) \;. \tag{5.94}$$

(Note: $SO(3)$ is **not** Abelian.)

Similar to the translation, one can write $R(\alpha)$ in the form

$$R(\alpha) \;=\; e^{-i\alpha\ I_3} \;, \tag{5.95}$$

where I_3 is a 3×3 matrix. To prove this, we differentiate (5.94) with respect to α_1 and α_2 and obtain

$$R(\alpha_2)\,\frac{dR(\alpha_1)}{d\alpha_1} \;=\; \frac{dR(\alpha_1+\alpha_2)}{d(\alpha_1+\alpha_2)} \tag{5.96}$$

and

$$\frac{dR(\alpha_2)}{d\alpha_2}\,R(\alpha_1) \;=\; \frac{dR(\alpha_1+\alpha_2)}{d(\alpha_1+\alpha_2)} \;. \tag{5.97}$$

Since both expressions (5.96) and (5.97) are equal, one obtains

$$\frac{dR(\alpha_1)}{d\alpha_1}\,R^{-1}(\alpha_1) \;=\; R^{-1}(\alpha_2)\,\frac{dR(\alpha_2)}{d\alpha_2} \;\equiv\; -iI_3 \;, \tag{5.98}$$

where I_3 is a matrix, which is **independent** of α. The solution of (5.98) with $R(\alpha = 0) = 1$ is given by (5.95).

Let us now consider **infinitesimal** rotations around the 3-axis. If one replaces in (5.87) the angle α with an infinitesimal small angle $d\alpha$, then

$$\begin{aligned} \cos(d\alpha) &\;\cong\; \cos 0 \;=\; 1 \\ \sin(d\alpha) &\;\cong\; d\alpha \;. \end{aligned} \tag{5.99}$$

That is for infinitesimal angles $d\alpha$ the rotation matrix becomes

$$R(d\alpha) \;=\; \begin{pmatrix} 1 & -d\alpha & 0 \\ d\alpha & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \;=\; \mathbf{1} - id\alpha \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \;. \tag{5.100}$$

Expanding (5.95) up to the same order yields

$$R(d\alpha) \;=\; \mathbf{1} - id\alpha\ I_3 \;, \tag{5.101}$$

and thus

$$I_3 \;=\; \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \;. \tag{5.102}$$

By using infinitesimal angles of rotation for the other Euler angles in (5.88) one obtains

$$I_2 \;=\; \begin{pmatrix} 0 & 0 & i \\ 0 & 0 & 0 \\ -i & 0 & 0 \end{pmatrix} \qquad (5.103)$$

and

$$I_1 \;=\; \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix} \; . \qquad (5.104)$$

This result can be summarized in one single equation

$$(I_k)^\ell_{\;m} \;=\; -i\; \varepsilon_{k\ell m} \; . \qquad (5.105)$$

Under rotation the infinitesimal rotations $I_k, k = 1, 2, 3$ behave in the same way as the coordinate vectors $\vec{e}_k$, i.e.,

$$R I_k R^{-1} \;=\; \sum_\ell \; I_\ell R^\ell_{\;k} \; . \qquad (5.106)$$

The proof can be done directly by matrix multiplication using (5.87), (5.88), (5.89) and the explicit representation of the I_k. Thus the generator of rotations (infinitesimal rotation) of an arbitrary rotation around an axis $\vec{n}$ can be written as

$$I \;=\; \sum_k \; I_k n_k \qquad (5.107)$$

where $\vec{n} \;=\; \sum_k \; n_k \vec{e}_k$. Thus I_1, I_2, I_3 form a basis for the generators of all the one-parameter Abelian subgroups of $SO(3)$, and one can write for an arbitrary rotation

$$R_n(\alpha) \;=\; e^{-i\alpha \; \sum_k \; I_k n_k} \; . \qquad (5.108)$$

Similarly, the Euler angle representation of (5.87) - (5.89) can be written in terms of the generators

$$A(\alpha, \beta, \gamma) \;=\; e^{-i\alpha I_3} \; e^{-\beta I_2} \; e^{-i\gamma I_3} \; . \qquad (5.109)$$

Therefore, for all practical purposes, it suffices to work with the three **basis-generators** I_k rather than the 3-fold infinity of group elements $A(\alpha, \beta, \gamma)$.

The three basis generators I_k satisfy the **Lie algebra**

$$[I_k, I_\ell] \;=\; i\; \varepsilon_{k\ell m} \; I_m \; . \qquad (5.110)$$

5.8 Rotation of Position and Momentum Vectors

If one rotates the expectation values of $\vec{X}$, one obtains, according to (5.71),

$$\langle \psi \mid X'_j \mid \psi \rangle \;=\; \sum_k R_{jk} \, \langle \psi \mid X_k \mid \psi \rangle \;, \tag{5.111}$$

i.e., one has for the components of the $\vec{X}$-operator

$$X'_j \;=\; \sum_k R_{jk}(\alpha) \; X_k \tag{5.112}$$

and correspondingly for the components of the $\vec{P}$-operator

$$P'_j \;=\sum_k R_{jk}(\alpha) \; P_k \;. \tag{5.113}$$

Similar to (5.7) one can try to construct unitary operators $U(R(\alpha))$, which, when applied on $\vec{X}$ and $\vec{P}$, give the results (5.112) and (5.113)

$$\begin{aligned} U^\dagger(R(\alpha)) \; X_j \; U(R(\alpha)) \;&=\; \sum_k R_{jk}(\alpha) \; X_k \\ U^\dagger(R(\alpha)) \; P_j \; U(R(\alpha)) \;&=\; \sum_k R_{jk}(\alpha) \; P_k \;. \end{aligned} \tag{5.114}$$

These definitions lead to

$$\begin{aligned} U^\dagger(R(\alpha_2))U^\dagger(R(\alpha_1))X_jU(R(\alpha_1))U(R(\alpha_2)) \;&=\; \sum_{k\ell} R_{jk}(\alpha_1) \; R_{k\ell}(\alpha_2) \;\; X_\ell \\ &=\; \sum_\ell \, [R(\alpha_1) \; R(\alpha_2)]_{j\ell} \; X_\ell \\ &=\; U^\dagger(R(\alpha_1) \; R(\alpha_2)) \; X_j \; U(R(\alpha_1) \; R(\alpha_2)) \;. \end{aligned} \tag{5.115}$$

This means that

$$U[R(\alpha_1)R(\alpha_2)] \;=\; U(R(\alpha_1)) \; U(R(\alpha_2)) \;. \tag{5.116}$$

Thus the in (5.114) defined map

$$R(\alpha) \;\mapsto\; U(R(\alpha)) \tag{5.117}$$

is a Homomorphism, a **representation** of the rotation group with unitary operators in a Hilbert space.

Introducing the abbreviation

$$U(R(\alpha)) \equiv U(\alpha) \tag{5.118}$$

and remembering that rotations around a fixed axis form a Abelian group, one has similar to (5.94)

$$U(\alpha_2)\, U(\alpha_1) = U(\alpha_2 + \alpha_1) = U(\alpha_1)\, U(\alpha_2) \; . \tag{5.119}$$

Thus one can conclude that $u(\alpha)$ has to be of the form

$$U(\alpha) = e^{-i\alpha L_3} \; , \tag{5.120}$$

with L_3 being a self-adjoint operator (since $U(\alpha)$ is unitary). For infinitesimal rotations, one has

$$U(\alpha_2) = 1 - i(d\alpha)\, L_3 \; . \tag{5.121}$$

If one inserts the matrix I_3 (5.102) into the right side of the definition (5.114) and the operator (5.121) into the left side, then follows

$$(1 + i(d\alpha)L_3)\; X_j\; (1 - i(d\alpha)L_3) = \sum_k \left[\delta_{jk} - i(d\alpha)(I_3)_{jk}\right] X_k \; . \tag{5.122}$$

Comparing the terms of first order in $d\alpha$ gives

$$[L_3, X_j] = -\sum_k (I_3)_{jk}\, X_k \; . \tag{5.123}$$

Inserting the matrix I_3 gives explicitly

$$\begin{aligned} [L_3, X_1] &= iX_2 \\ [L_3, X_2] &= -iX_1 \\ [L_3, X_3] &= 0 \end{aligned} \tag{5.124}$$

or

$$[L_3, X_k] = i \sum_m \varepsilon_{3km}\, X_m \; . \tag{5.125}$$

Instead of considering rotations around the 3-axis, which should be labeled as $R^3(\alpha)$ to be more precise, we could have considered rotations $R'(\alpha)$ around the 1-axis and $R^2(\alpha)$ around the 2-axis. Then we would have obtained unitary operators

$$U(R^1(\alpha)) \equiv U^1(\alpha) = e^{-i\alpha L_1} \tag{5.126}$$

$$U(R^2(\alpha)) \equiv U^2(\alpha) = e^{-i\alpha L_2} \; . \tag{5.127}$$

Repeating the considerations leading to (5.124) and (5.125) leads to the generalization of (5.125)

$$[L_j, X_k] \;=\; i \sum_m \varepsilon_{jkm}\; X_k \;. \tag{5.128}$$

Similar consideration lead from (5.114) to

$$[L_j, P_k] \;=\; i \sum_m \varepsilon_{jkm}\; P_m \;. \tag{5.129}$$

Thus, starting from the definitions (5.114) of the unitary operator $U(R(\alpha))$, we obtained the relations (5.128) and (5.129). The definition (5.114) makes no statement about the existence of $U(R(\alpha))$. However, the existence is given by the fact that the components L_j of the **orbital angular momentum**

$$L_j \;=\; \frac{1}{\hbar} \sum_m \varepsilon_{jkm}\; X_k P_m \tag{5.130}$$

fulfill the commutation relations (5.128) and (5.129). In summary, the components L_j of the angular momentum operator $\vec{L}$ allow to introduce unitary operators

$$U(R^j(\alpha)) \;=\; e^{-i\alpha L_j} \;, \tag{5.131}$$

which, when applied on X_j or P_j, lead to the rotated components:

$$\begin{aligned} U^\dagger(R^j(\alpha))\; X_l\; U(R^j(\alpha)) \;&=\; \sum_k R^j_{lk}(\alpha)\; X_k \\ U^\dagger(R^j(\alpha))\; P_l\; U(R^j(\alpha)) \;&=\; \sum_k R^j_{lk}(\alpha)\; P_k \;. \end{aligned} \tag{5.132}$$

If one considers a general rotation around an arbitrary axis $\vec{\xi}$ with angle α, characterized by

$$\vec{\alpha} \;\equiv\; \alpha\vec{\xi} \tag{5.133}$$

and consider a general rotation matrix $R(\alpha)$, e.g., (5.86), then one can write as generalization of (5.131)

$$U(R(\vec{\alpha})) \;=\; e^{-i\vec{\alpha}\,\cdot\vec{L}} \;. \tag{5.134}$$

In case of the Euler-angle scheme, one would have

$$U(\alpha,\beta,\gamma) \;=\; e^{-i\alpha L_3}\; e^{-i\beta L_2}\; e^{-i\gamma L_3} \;. \tag{5.135}$$

The relations (5.132) are then generalized to

$$
\begin{aligned}
U^\dagger(R(\vec{\alpha}))\ X_j\ U(R(\vec{\alpha})) &= \sum_k R_{jk}(\vec{\alpha})\ X_k \\
U^\dagger(R(\vec{\alpha}))\ P_j\ U(R(\vec{\alpha})) &= \sum_k R^{jk}(\vec{\alpha})\ P_k\ .
\end{aligned} \tag{5.136}
$$

If one applies (5.136) on eigenvectors $\mid \varphi_{\vec{x}}\ \rangle$ of $\vec{X}$, then

$$
U^\dagger(R(\vec{\alpha}))\ X_j\ U(R(\vec{\alpha})) \mid \varphi_{\vec{x}}\ \rangle\ =\ \sum_k R_{jk}(\vec{\alpha})\ x_k \mid \varphi_{\vec{x}}\ \rangle \tag{5.137}
$$

and thus

$$
X_j\ U(R(\vec{\alpha})) \mid \varphi_{\vec{x}}\ \rangle\ =\ \sum_k R_{jk}(\vec{\alpha})\ x_k\ U(R(\vec{\alpha})) \mid \varphi_{\vec{x}}\ \rangle\ . \tag{5.138}
$$

Multiplication with $\vec{e}_j$ and summation over j gives

$$
\vec{X}\ U(R(\vec{\alpha})) \mid \varphi_{\vec{x}}\ \rangle\ =\ (R(\vec{\alpha})\vec{x})\ \ U(R(\vec{\alpha}))\ \ \mid \varphi_{\vec{x}}\ \rangle\ . \tag{5.139}
$$

Thus, applying $U(R(\vec{\alpha}))$ on $\mid \varphi_{\vec{x}}\ \rangle$ gives an eigenstate to the rotated eigenvalue

$$
\vec{x}\ '\ =\ R(\vec{\alpha})\vec{x}\ , \tag{5.140}
$$

i.e.,

$$
U(R(\vec{\alpha})) \mid \varphi_{\vec{x}}\ \rangle\ = \mid \varphi_{(R(\vec{\alpha})\vec{x})}\rangle\ . \tag{5.141}
$$

For the expectation values, one obtains

$$
\begin{aligned}
\langle\psi \mid U^\dagger(R(\alpha))\ \vec{X}\ U(R(\vec{\alpha})) \mid \psi\rangle &= \langle U(R(\vec{\alpha}))\psi \mid \vec{X}\ \ \mid U(R(\vec{\alpha}))\psi\rangle \\
&= R(\vec{\alpha})\vec{x} \\
&= x'\ .
\end{aligned} \tag{5.142}
$$

This also means that the result does not depend if one uses rotated operators or rotated states. For the momentum eigenstates, a similar result to (5.141) holds

$$
U(R(\vec{\alpha})) \mid \varphi_{\vec{p}}\ \rangle\ = \mid \varphi_{(R(\vec{\alpha})\vec{p})}\rangle\ . \tag{5.143}
$$

5.9 Coordinate Space Representation

We need to consider

$$\langle \vec{x} \mid U(\vec{\alpha}) \mid \psi \rangle \;=\; \langle U^{\dagger}(\vec{\alpha})\vec{x} \mid \psi \rangle \;. \tag{5.144}$$

With

$$U^{\dagger}(\vec{\alpha}) \mid \vec{x}\, \rangle \;= \mid R^{-1}(\vec{\alpha})\vec{x}\, \rangle \tag{5.145}$$

Eq. (5.144) becomes

$$\langle \vec{x} \mid U(\vec{\alpha})\psi \rangle \;=\; \langle R^{-1}(\vec{\alpha})\vec{x} \mid \psi \rangle \;. \tag{5.146}$$

Thus in the coordinate space representation, $U(\vec{\alpha})$ is defined as

$$U(\vec{\alpha})\; \psi(\vec{x}) \;=\; \psi(R^{-1}(\vec{\alpha})\vec{x}) \;. \tag{5.147}$$

This result can be viewed as a **definition** of a representation of $SO(3)$, here in $\mathcal{L}^2(\mathbf{R}^3)$.

For an infinitesimal rotation around the 3-axis follows

$$\begin{aligned} U(R^3(d\alpha))\; \psi(x_1,x_2,x_3) &= \psi(x_1 + d\alpha x_2, x_2 - d\alpha x_1, x_3) \\ &= \psi(x_1,x_2,x_3) \;+\; d\alpha \left(x_2 \frac{\partial}{\partial x_1} \;-\; x_1 \frac{\partial}{\partial x_2} \right) \psi(x_1,x_2,x_3) \\ &= \left\{ \mathbf{1} - id\alpha \left[x_1 \frac{1}{i} \frac{\partial}{\partial x_2} \;-\; x_1 \frac{1}{i} \frac{\partial}{\partial x_1} \right] \right\} \psi(x_1,x_2,x_3) \;. \end{aligned} \tag{5.148}$$

With

$$U(R^3(d\alpha)) \;\equiv\; \mathbf{1} - id\alpha\; L_3 \;, \tag{5.149}$$

we obtain for the generator of the rotation operator in coordinate space representation

$$L_3 \;=\; \left[x_1 \frac{1}{i} \frac{\partial}{\partial x_2} \;-\; x_2 \frac{1}{i} \frac{\partial}{\partial x_1} \right] \;. \tag{5.150}$$

In general

$$\begin{aligned} L_j &= \frac{1}{2} \sum_{k,m} \varepsilon_{jkm} \left[x_k \frac{1}{i} \frac{\partial}{\partial x_m} \;-\; x_m \frac{1}{i} \frac{\partial}{\partial x_k} \right] \\ &= \frac{1}{2} \sum_{k,m} \varepsilon_{jkm} \frac{1}{\hbar} \left(X_k P_m - X_m P_k \right) \;, \end{aligned} \tag{5.151}$$

which is

$$\vec{L} = \frac{1}{\hbar} \vec{X} \times \vec{P} . \tag{5.152}$$

Again, one sees that the orbital angular momentum operators are the generators of the rotation operation $U(\vec{\alpha})$.

5.10 Vector Operators in Coordinate Space

Rotating a vector operator $\vec{X}$ gives

$$\vec{X}\,' = R\vec{X} , \tag{5.153}$$

i.e.,

$$X_j' = \sum_k R_{jk} X_k . \tag{5.154}$$

With

$$P_j' = m\dot{X}'j = \sum_k R_{jk}\, m\dot{X}_k = \sum_k R_{jk} P_k , \tag{5.155}$$

one has also

$$P_j' = \sum_k R_{jk} P_k . \tag{5.156}$$

If one constructs with $\vec{X}$ and $\vec{P}$ an operator $\vec{A}\,(\vec{X}, \vec{P})$ for which holds

$$\vec{A}\,(R\vec{X}, R\vec{P}) = R\vec{A}\,(\vec{X}, \vec{P}) , \tag{5.157}$$

then $\vec{A}$ is called vector operator. Its components have the transformation behavior under rotations

$$A_j' = A_j(R\vec{X}, R\vec{P}) = \sum_k R_{jk} A_k(\vec{X}, \vec{P}) . \tag{5.158}$$

An example is the orbital angular momentum operator, for which we already showed that

$$\begin{aligned} L_j' &= \frac{1}{\hbar} \sum_{k,m} \varepsilon_{jkm}\, X_k' P_m' \\ &= \frac{1}{\hbar} \sum_{k,m} \varepsilon_{jkm}\, R_{k\ell} R_{mn}\, X_\ell P_n \\ &= \sum_k R_{jk} L_k \end{aligned} \tag{5.159}$$

One also has

$$
\begin{aligned}
L'_j &= \frac{1}{\hbar} \sum_{k,m} \varepsilon_{jkm} \, U^\dagger(R) X_k \, U(R) \, U^\dagger(R) P_m \, U(R) \\
&= U^\dagger(R) \left(\frac{1}{\hbar} \sum_{k,m} \varepsilon_{jkm} \, X_k P_m \right) U(R) \\
&= U^\dagger(R) L_j \, U(R) \; .
\end{aligned}
\tag{5.160}
$$

Comparing (5.159) and (5.160) gives

$$
U^\dagger(R) L_j \, U(R) \;=\; \sum_k R_{jk} L_k \; . \tag{5.161}
$$

In general, the following relation holds for vector operators in coordinate space

$$
U^\dagger(R) \; A_j(\vec{X}, \vec{P}) \; U(R) \;=\; \sum_k R_{jk} A_k(\vec{X}, \vec{P}) \; . \tag{5.162}
$$

Definition: An operator $C(\vec{X}, \vec{P})$ is called **scalar operator** in coordinate space if

$$
C(R\vec{X}, R\vec{P}) \;=\; C(\vec{x}, \vec{p}) \; . \tag{5.163}
$$

Since

$$
\begin{aligned}
C(R\vec{X}, R\vec{P}) &= C(U^\dagger(R)\vec{X} \, U(R), \; U^\dagger(R)\vec{P} \, U(R)) \\
&= U^\dagger(R) \; C(\vec{X}, \vec{P}) \; U(R) \; ,
\end{aligned}
\tag{5.164}
$$

this means that an operator constructed from the operators $\vec{X}$ and $\vec{P}$ is a scalar operator if

$$
U^\dagger(R) \; C(\vec{X}, \vec{P}) \; U(R) \;=\; C(\vec{X}, \vec{P}) \tag{5.165}
$$

or if

$$
[C(\vec{X}, \vec{P}), L_j] \;=\; 0 \tag{5.166}
$$

as can be shown when considering infinitesimal rotations. Consider the scalar product

$$
\begin{aligned}
\vec{A}\,' \cdot \vec{B}\,' \;=\; \sum_j A'_j B'_j &= \sum_{jkm} R_{jk} A_k \; R_{jm} B_m \\
&= \sum_{km} \delta_{km} \; A_k B_m \;=\; \sum_k A_k B_k \;=\; \vec{A} \cdot \vec{B}
\end{aligned}
\tag{5.167}
$$

and

$$\sum_j \quad U^\dagger(R) \quad A_j\, U(R)\, U^\dagger(R) B_j\, U(R)$$
$$= \quad U^\dagger(R) \left(\sum_j \, A_j B_j \right) \, U(R) \; = \; \vec{A} \cdot \vec{B} \tag{5.168}$$

then follows

$$[\vec{A} \cdot \vec{B}, U(R)] \; = \; 0 \tag{5.169}$$

or

$$[\vec{A} \cdot \vec{B}, \vec{L}] \; = \; 0 \; . \tag{5.170}$$

Remark: In (5.162) vector operators were defined with respect to finite rotations. If one applies in the definition infinitesimal rotation, then follows

$$[L_k, A_j] \; = \; -\sum_m \, (I_k)_{jm} A_m \tag{5.171}$$

and thus

$$[L_k, A_j] \; = \; i \, \sum_m \, \varepsilon_{kjm} A_m \; . \tag{5.172}$$

This result was introduced in Chapter 3 as definition of vector operators, and (5.170) was verified by explicit calculation. The above consideration show the deeper reason why $\vec{A} \cdot \vec{B}$ commutes with the generators L_j of rotations in coordinate space.

In Chapter 3 we had also considered the eigenvalue equations for $\vec{L}^2$ and L_k (3.67) - (3.70)

$$\begin{aligned} \vec{L}^2 \mid \ell m \rangle &= \ell(\ell+1) \mid \ell m \rangle \\ L_3 \mid \ell m \rangle &= m \mid \ell m \rangle \\ L_\pm \mid \ell m \rangle &= \sqrt{\ell(\ell+1) - m(m \pm 1)} \;\; \mid \ell \; m \pm 1 \rangle \; . \end{aligned} \tag{5.173}$$

Now we can say that the irreducible representations of the Lie algebra of $SO(3)$ are each characterized by an **angular momentum** eigenvalue ℓ from the set of positive integers and half-integers. The orthonormal basis vectors are specified by (5.173).
The normalization factor was calculated in (3.78).

It should be pointed out that in principal one has the freedom to multiply the normalization constant by an additional arbitrary (m-dependent) **phase factor** (i.e., complex number of unit modulus). The resulting set of vectors would be equally acceptable as a basis. The basis defined in (5.173) is referred to as **canonical basis**.

Knowing how the generators act on the basis vectors, one can immediately derive the matrix elements in the various irreducible representations.

5.11 The Spherical Basis

Usually vectors are represented in the **Cartesian** basis with the unit vectors e_x, e_y, and e_z, pointing into the direction of the Cartesian x, y, and z-axis. The **Spherical** basis is an equivalent basis, often useful when considering rotations in quantum mechanics. The basis vectors are defined as

$$\begin{aligned} \epsilon_1^0 &= e_z \\ \epsilon_1^1 &= -\frac{1}{\sqrt{2}}(e_x + i\ e_y) \\ \epsilon_1^{-1} &= \frac{1}{\sqrt{2}}(e_x - i\ e_y) \end{aligned} \tag{5.174}$$

Any vector $\vec{A}$ can be expressed as

$$\begin{aligned} \vec{A} &= A_x e_x + A_y e_y + A_z e_z = \sum_{i=1}^{3} A_i e_i \\ &= -A_1^1 \epsilon_1^{-1} + A_1^0 \epsilon_1^0 - A_1^{-1} \epsilon_1^1 = \sum_{\mu=-1,0,1} (-1)^\mu A_1^\mu \epsilon_1^{-\mu}\ , \end{aligned} \tag{5.175}$$

with

$$\begin{aligned} A_1^1 &= -\frac{1}{\sqrt{2}}(A_x + iA_y) \\ A_1^0 &= A_z \\ A_1^{-1} &= \frac{1}{\sqrt{2}}(A_x - iA_y)\ . \end{aligned} \tag{5.176}$$

In addition we have $A_1^{\mu^\star} = (-1)^\mu A_1^{-\mu}$.

Apply this to the position vector $\vec{r} = -r_1^1 \epsilon_1^{-1} + r_1^0 \epsilon_1^0 - r6{-}1_1 \epsilon_1^1$ with

$$\begin{aligned} r_1^1 &= -\frac{1}{\sqrt{2}}(r_x + ir_y) \\ r_1^0 &= r_z \end{aligned}$$

$$r_1^{-1} = \frac{1}{\sqrt{2}}(r_x - ir_y) , \tag{5.177}$$

where the position vector can be a function $\vec{r}(x, y, z)$ or $\vec{r}(r, \theta, \phi)$. Using the relations

$$\begin{aligned} x &= r \sin\theta \cos\phi \\ y &= r \sin\theta \sin\phi \\ z &= r \cos\theta \end{aligned}$$

one calculates

$$\begin{aligned} r_1^1 &= -\frac{r}{\sqrt{2}} \sin\theta e^{i\phi} = \sqrt{\frac{4\pi}{3}} r Y_1^1(\hat{r}) \\ r_1^{-1} &= \frac{r}{\sqrt{2}} \sin\theta e^{-i\phi} = \sqrt{\frac{4\pi}{3}} r Y_1^{-1}(\hat{r}) \\ r_1^0 &= \frac{r}{\sqrt{2}} \cos\theta = \sqrt{\frac{4\pi}{3}} r Y_1^0(\hat{r}) \end{aligned} \tag{5.178}$$

leading to the well known spherical harmonics of order 1

$$\begin{aligned} Y_1^1(\hat{r}) &= -\sqrt{\frac{3}{8\pi}} \sin\theta e^{i\phi} \\ Y_1^{-1}(\hat{r}) &= \sqrt{\frac{3}{8\pi}} \sin\theta e^{-i\phi} \\ Y_1^0(\hat{r}) &= \sqrt{\frac{3}{8\pi}} \cos\theta \end{aligned} \tag{5.179}$$

which leads to the representation of the position vector in terms of spherical harmonics of order 1

$$\vec{r} = \sqrt{\frac{4\pi}{3}} r \sum_{\mu} (-1)^{\mu} Y_1^{\mu} \epsilon_1^{-\mu} \tag{5.180}$$

5.11.1 Transformation of a spherical vector under rotation of the coordinate system

Consider a rotation of a vector $\vec{A}$ around the z-axis with angle α. In Cartesian coordinates this is given as

$$\begin{pmatrix} A_{x'} \\ A_{y'} \\ A_{z'} \end{pmatrix} = \begin{pmatrix} \cos\alpha & \sin\alpha & 0 \\ -\sin\alpha & \cos\alpha & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} A_x \\ A_y \\ A_z \end{pmatrix} . \tag{5.181}$$

In spherical components one obtains

$$\begin{aligned} (A_1^1)' &= -\frac{1}{\sqrt{2}}(A_{x'} + A_{y'}) = -\frac{1}{\sqrt{2}}(A_x e^{-i\alpha} + iA_y e^{-i\alpha}) = A_1^1 e^{-i\alpha} \\ (A_1^0)' &= A_1^0 \\ (A_1^{-1})' &= A_1^{-1} e^{i\alpha} \end{aligned} \tag{5.182}$$

so that

$$\begin{pmatrix} A_1^1 \\ A_1^0 \\ A_1^{-1} \end{pmatrix}' = \begin{pmatrix} e^{-i\alpha} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & e^{i\alpha} \end{pmatrix} \begin{pmatrix} A_1^1 \\ A_1^0 \\ A_1^{-1} \end{pmatrix} . \tag{5.183}$$

Consider now the rotation of the vector $\vec{A}'$ around the y'-axis with angle β. In Cartesian coordinates one obtains

$$\begin{pmatrix} A_{x''} \\ A_{y''} \\ A_{z''} \end{pmatrix} = \begin{pmatrix} \cos\beta & 0 & -\sin\beta \\ 0 & 1 & 0 \\ \sin\beta & 0 & \cos\beta \end{pmatrix} \begin{pmatrix} A_{x'} \\ A_{y'} \\ A_{z'} \end{pmatrix} . \tag{5.184}$$

while for spherical coordinates one obtains the transformation matrix

$$M_{y'}(\beta) \equiv \begin{pmatrix} \frac{1}{2}(1+\cos\beta) & \sqrt{\frac{1}{2}}\sin\beta & \frac{1}{2}(1-\cos\beta) \\ -\sqrt{\frac{1}{2}}\sin\beta & \cos\beta & \sqrt{\frac{1}{2}}\sin\beta \\ \frac{1}{2}(1-\cos\beta) & -\sqrt{\frac{1}{2}}\sin\beta & \frac{1}{2}(1-\cos\beta) \end{pmatrix} . \tag{5.185}$$

so that

$$\vec{A}'' = M_{y'}(\beta)\vec{A}' = M_{y'}(\beta)M_z(\alpha)\vec{A} . \tag{5.186}$$

One needs one more rotation about the new z-axis to obtain a complete rotation with the Euler angles α, β, and γ,

$$M(\alpha\beta\gamma) = M_{z''}(\gamma)M_{y'}(\beta)M_z(\alpha) , \tag{5.187}$$

so that

$$\vec{A}' = M(\alpha\beta\gamma)\vec{A} , \tag{5.188}$$

or in components

$$A'_\mu = \sum_\nu M_{\mu\nu}(\alpha\beta\gamma)A_\nu . \tag{5.189}$$

The D-function or rotation matrix $D^1(\alpha\beta\gamma)$ is defined as the transpose of the matrix $M(\alpha\beta\gamma)$, so that

$$A'_\mu = \sum_\nu D^1_{\nu\mu}(\alpha\beta\gamma)A_\nu , \tag{5.190}$$

with

$$D^1(\alpha\beta\gamma) = \begin{pmatrix} e^{-i\gamma}\frac{(1+\cos\beta)}{2}e^{-i\alpha} & -\frac{\sin\beta}{\sqrt{2}}e^{-i\alpha} & e^{i\gamma}\frac{(1-\cos\beta)}{2}e^{-i\alpha} \\ e^{-i\gamma}\frac{\sin\beta}{\sqrt{2}} & \cos\beta & -e^{i\gamma}\frac{\sin\beta}{\sqrt{2}} \\ e^{-i\gamma}\frac{(1-\cos\beta)}{2}e^{i\alpha} & \frac{\sin\beta}{\sqrt{2}}e^{i\alpha} & e^{i\gamma}\frac{(1+\cos\beta)}{2}e^{i\alpha} \end{pmatrix} . \tag{5.191}$$

Remarks: The matrices D are called *representation corefficients of the rotation group*, and abbreviated as D-matrices. When using the parameterization based on Euler angles, one should note that the usual definition in quantum mechanics is not identical with the one traditional choice made in classical mechantics. When consulting literature, one has to be careful about the choice if phase conventions, which is unfortunately not unique.

5.11.2 Rotation of quantum mechanical states

When representing the rotation of a state $\psi_{jm}(\vec{r})$, where j is an arbitrary angular momentum, and m the respective quantum number, one has

$$\psi_{jm}(\vec{r}') = M(\alpha\beta\gamma)\psi_{jm}(\vec{r}) \tag{5.192}$$

where

$$\begin{aligned} D^j_{m'm}(\alpha\beta\gamma) &= \langle\psi_{jm'}(\vec{r}) \mid M(\alpha\beta\gamma) \mid \psi_{jm}(\vec{r})\rangle \\ &\equiv \langle jm'|\ M(\alpha\beta\gamma)\ |jm\rangle \end{aligned} \tag{5.193}$$

Rotations around the z-axis are relatively simple to represent,

$$\begin{aligned} D^j_{m'm}(\alpha\beta\gamma) &= \langle jm'|\ e^{-i\alpha J_z}e^{-i\beta J_y}e^{-i\gamma J_z}\ |jm\rangle \\ &= e^{-i\alpha m'}\langle jm'|\ e^{-i\beta J_y}\ |jm\rangle e^{-i\gamma m} \end{aligned} \tag{5.194}$$

The representation of J_y is purely imaginary, thus the matrix element in (5.194) is real. Thus

$$D^j_{m'm}(\alpha\beta\gamma) = e^{-i\alpha m'}d^j_{m'm}(\beta)e^{-i\gamma m} , \tag{5.195}$$

where the functions $d^j_{m'm}(\beta)$ are the *Wigner d-matrices*. In general, in the the canonical basis J_y is always represented by an imaginary anti-symmetric matrix (5.103), hence the d^j matrices are real (and orthogonal).

Their special form is determined by the value of j, which can be integer or half-integer.

Let us consider j having integer values ℓ and define

$$U(\alpha,\beta,\gamma) \mid \ell m\rangle = D^\ell(\alpha,\beta,\gamma)_{m'm} \mid \ell m\ \rangle , \tag{5.196}$$

where U is the operator representing the group element $A(\alpha, \beta, \gamma)$. Then (5.195) reads

$$D^\ell(\alpha, \beta, \gamma)_{m'm} \;=\; e^{-i\alpha m'}\; d^\ell(\beta)_{m'm}\; e^{-i\gamma m} \tag{5.197}$$

and

$$d^\ell(\beta)_{m'm} \;=\; \langle \ell m' \mid e^{-i\beta J_y} \mid \ell m\rangle \; . \tag{5.198}$$

Since $U(\alpha, \beta, \gamma)$ is supposed to be a unitary operator, the D^ℓ matrices have to be unitary:

$$D^\dagger(\alpha, \beta, \gamma) \;=\; D^{-1}(\alpha, \beta, \gamma) \;=\; D(-\gamma, -\beta, -\alpha)\; , \tag{5.199}$$

where the index ℓ has been omitted in (5.199). For the d^ℓ matrices, one has

$$d^{-1}(\beta) \;=\; d(-\beta) \;=\; d^T(\beta) \tag{5.200}$$

where d^T denotes the transpose of the matrix. The real matrices d^ℓ satisfy a number of symmetry relations, e.g.,

$$\begin{aligned} d^\ell(\beta)_{m'm} &= d^\ell(-\beta)_{mm'} \\ &= d^\ell(\pi-\beta)_{-m'm}\;(-1)^{\ell-m'} \\ &= d^\ell(\beta)_{-m-m'}\;(-1)^{m'-m}\; . \end{aligned} \tag{5.201}$$

For integer values of ℓ the D-functions are closely related to the spherical harmonics $Y_{\ell m}$ and Legendre functions. Specifically

$$\begin{aligned} Y_{\ell m}(\theta, \phi) &= \left(\frac{2\ell+1}{4\pi}\right)^{\frac{1}{2}}\; [D^\ell(\phi, \theta, 0)_{m0}]^* \\ P_{\ell m}(\cos\theta) &= (-1)^m\; \left(\frac{(\ell+m)!}{(\ell-m)!}\right)^{\frac{1}{2}}\; d^\ell(\theta)_{m0} \\ P_\ell(\cos\theta) &= P_{\ell 0}(\cos\theta) \;=\; d^\ell(\theta)_{00}\; . \end{aligned} \tag{5.202}$$

5.12 Special Galilei Transformations: Determination of the Unitary Operator Representing the Transformation

Two observers O and O' describing the same physical system S use reference frames moving with velocity $\vec{v}_0$ with respect to each other. The reference frames coincide at $t = 0$. O and O' compare their measurements at the same instant of time, and their clocks are identical. Thus, the transformation law for the classical dynamical variables is given by

$$\begin{aligned} \vec{r}_i(O') &= \vec{r}_i(O) - \vec{v}_0 t \\ \vec{P}_i(O') &= \vec{p}_i(O) - m_i \vec{v}_0 \\ &= t(O') \;=\; t(O) \;, \end{aligned} \tag{5.203}$$

where m_i is the mass of the ith particle of the system $S, i = 1, 2, \cdots, N$. Eqs. (5.203) define the special Galilei transformations of non-relativistic mechanics.

If U_G is the operator that gives in the quantum mechanical case the translation from the variables used by O to those used by O', then it must satisfy

$$\begin{aligned} U_G^\dagger \, \vec{r}_i \, U_G &= \vec{r}_i - \vec{v}_0 t \\ U_G^\dagger \, \vec{p}_i \, U_G &= \vec{p}_i - \vec{v}_0 m_i \\ U_G^\dagger \, U_G &= U_G \, U^\dagger \;=\; \mathbf{1} \;. \end{aligned} \tag{5.204}$$

Remark: Spin variables, if present, are supposed to remain unaltered, since this happens for any orbital angular momentum intrinsic to the system. Thus we can ignore spin variables in the following discussion.

From (5.204) follows

$$\begin{aligned} [U_G^\dagger \, \vec{r}_i \, U_G, U_G^\dagger \, \vec{p}_i \, U_G] &= [\vec{r}_i - \vec{v}_0 t, \vec{p}_i - \vec{v}_0 m_i] \\ &= [\vec{r}_i, \vec{p}_i] \;. \end{aligned} \tag{5.205}$$

Since U_G does not commute with both $\vec{r}_i$ and $\vec{p}_i$, it has to be a function of both dynamical variables. The simple structure of (5.204) together with the unitary of U_G suggest that U_G can be written as a product

$$U_G \;=\; U_G^r \, U_G^p \tag{5.206}$$

where U_G^p is only a function of $\vec{p}_i$ and U_G^r only a function of $\vec{r}_i$. With

$$\begin{aligned} U_G^{p\dagger}\ \vec{r}_i\ U_G^p &= \vec{r}_i - \vec{v}_0 t \\ U_G^{r\dagger}\ \vec{p}_i\ U_G^r &= \vec{p}_i - \vec{v}_0 m_i \end{aligned} \tag{5.207}$$

(5.204) follows. From (5.207) follows

$$\begin{aligned} [U_G^p, \vec{r}_i] &= \vec{v}_0 t\ U_G^p \\ [U_G^r, \vec{p}_i] &= \vec{v}_0 m_i\ U_G^r\ . \end{aligned} \tag{5.208}$$

Remembering that the commutator acts like a derivative, (4.129), this is

$$\begin{aligned} -i\hbar\,\frac{\partial U_G^p}{\partial p_{ik}} &= v_{0,k} t\ U_G^p \\ i\hbar\,\frac{\partial U_G^r}{\partial r_{ik}} &= v_{0,k} m_i\ U_G^r\ . \end{aligned} \tag{5.209}$$

Since U_G^p is only a function of $\vec{p}_i$ and U_G^r only of $\vec{r}_i$, (5.209) can be immediately integrated

$$\begin{aligned} U_G^p &= e^{\frac{i}{\hbar}\vec{P}\cdot\vec{v}_0 t} \\ U_G^r &= e^{-\frac{i}{\hbar}\sum_i m_i \vec{r}_i\cdot\vec{v}_0}\ . \end{aligned} \tag{5.210}$$

Thus

$$U_G = \gamma(t,\vec{v}_0)\ e^{\frac{i}{\hbar}\ \vec{P}\cdot v_0 t}\ e^{-\frac{i}{\hbar}\ M\vec{R}\cdot\vec{v}_0}\ , \tag{5.211}$$

where M is the total mass of the system, $\vec{P}$ the total linear momentum and $\vec{R}$ the operator describing the c.m. position. Because of the unitary of U_G, the modulus of $\gamma(t,\vec{v}_0)$ is 1. The order of U_G^r and U_G^p in (5.211) is not essential, since with $e^A e^B = e^{[A,B]}\ e^B e^A$ follows

$$e^{-\frac{i}{\hbar}\ M\vec{R}\cdot\vec{v}_0}\ e^{\frac{i}{\hbar}\ \vec{P}\cdot\vec{v}_0 t} = e^{\frac{i}{\hbar}\ M v_0^2 t}\ e^{\frac{i}{\hbar}\ \vec{P}\cdot\vec{v}_0 t}\ e^{-\frac{i}{\hbar}\ M\vec{R}\cdot\vec{v}_0}\ . \tag{5.212}$$

5.13 Invariance Under Special Galilei Transformations

The operator U_G of (5.211) still contains the undetermined factor $\gamma(t,\vec{v}_0)$ of modulus 1, which may depend on t and $\vec{v}_0$. In the following, this factor is determined and explicitly shown that it can **not** be set to 1. (If it would be 1, we would obtain that a quantum mechanical system containing only free particles is not invariant under special Galilei transformations.) This essential difference from the other cases considered so far stems from the fact that the transformation, which U_G represents, is explicitly time dependent.

The theory is invariant under special Galilei transformations if

$$i\hbar \, \frac{\partial U_G(t)}{\partial t} \; + \; [U_G(t), H(t)] \; = \; 0 \; , \tag{5.213}$$

where $H = H_0 + V(t)$ with $H_0 = \sum_i \frac{p_i^2}{2m_i}$ being the free Hamiltonian and $V(t)$ the interaction Hamiltonian. In ordinary quantum mechanics, the theory of free particles should be invariant under special Galilei transformations, i.e.,

$$i\hbar \, \frac{\partial U_G(t)}{\partial t} \; + \; [U_G(t), H_0] \; = \; 0 \; . \tag{5.214}$$

Inserting (5.211) into (5.214) yields

$$\left[\sum_i \frac{p_i^2}{2m_i} \, , U_G \right] \; = \; i\hbar \, \frac{d\gamma(t,\vec{v}_0)}{dt} \, \gamma^{-1}(t,\vec{v}_0) \, U_G - \; (\vec{v}_0 \cdot \vec{P}) \, U_G \; . \tag{5.215}$$

Evaluating the commutator gives

$$-\, \frac{1}{2} \, (\vec{v}_0 \cdot \vec{P} \, U_G \; + \; U_G \, \vec{v}_0 \cdot \vec{P}) \; = \; i\hbar \, \frac{d\gamma(t,\vec{v}_0)}{dt} \, \gamma^{-1}(t,\vec{v}_0) \, U_G \; - \; (v_0 \cdot \vec{P}) \, U_G \tag{5.216}$$

or

$$\frac{1}{2} \, [(v_0 \cdot P), \; U_G] \; = \; i\hbar \, \frac{d\gamma(t,\vec{v}_0)}{dt} \, \gamma^{-1} \, (t,\vec{v}_0) \, U_G \; . \tag{5.217}$$

Considering that $\frac{i}{\hbar} \, [M\vec{v}_0 \cdot \vec{R}, \; \vec{P} \cdot \vec{v}_0] = Mv_0^2$, one can obtain

$$i\hbar \, \frac{d\gamma(t,\vec{v}_0)}{dt} \; = \; - \, \frac{1}{2} \, Mv_0^2 \, \gamma(t,\vec{v}_0) \tag{5.218}$$

which has as solution

$$\gamma(t,\vec{v}_0) \; = \; c(\vec{v}_0) \, e^{\frac{i}{\hbar} \, \frac{1}{2} \, Mv_0^2 t} \tag{5.219}$$

with $\mid c(\vec{v}_0) \mid = \mathbf{1}$. Since (5.214) still leaves a free, time independent phase factor in U_G, we can choose $c(\vec{v}_0) = 1$. Then we obtain for U_G

$$\begin{aligned} U_G(t) \; &= \; e^{\frac{i}{\hbar} \, \frac{1}{2} \, Mv_0^2 t} \, e^{\frac{i}{\hbar} \vec{P} \cdot \vec{v}_0 t} \, e^{-\frac{i}{\hbar} M\vec{R} \cdot \vec{v}_0} \\ &= \; e^{-\frac{i}{\hbar} \, \frac{1}{2} \, Mv_0^2 t} \, e^{-\frac{i}{\hbar} \, M\vec{R} \cdot \vec{v}_0} \, e^{\frac{i}{\hbar} \, \vec{P} \cdot \vec{v}_0 t} \; . \end{aligned} \tag{5.220}$$

Using $e^{A+B} = e^{-\frac{1}{2}[A,B]} e^A e^B$, we can write (5.220) as

$$U_G(t) \;=\; e^{\frac{i}{\hbar}(\vec{P}t \;-\; M\vec{R})\cdot\vec{v}_0} \tag{5.221}$$

Finally, we need to discuss the transformation properties of the energy when going from Observer O to Observer O'. If for O the time evolution

$$i\hbar \, \frac{d\psi_0(t)}{dt} \;=\; H(t)\;\psi_0(t) \tag{5.222}$$

is valid, then one has for O':

$$i\hbar \, U_G(t)\, \frac{d\psi_0(t)}{dt} \;=\; (U_G(t)\;H(t)\;U_G^\dagger(t))\;U_G(t)\;\psi_0(t)\;. \tag{5.223}$$

With $\psi_{0'}(t) \;=\; U_G(t)\;\psi_0(t)$, we have

$$\begin{aligned} H'(t) \;&=\; U_G(t)\;H(t)\;U_G^\dagger(t) \;+\; i\hbar\,\frac{\partial U_G(t)}{\partial t}\;U_G^\dagger(t) \\ &=\; U_G(t)\;H(t)\;U_G^\dagger(t) \;-\; \frac{1}{2}\,Mv_0^2 - (\vec{v}_0\cdot\vec{P})\;. \end{aligned} \tag{5.224}$$

For the latter the explicit representation of $U_G(t)$ was used. We get then for the expectation values of the energy operator for the observers O and O'

$$\langle E\rangle_0 \;=\; \langle E\rangle_{0'} \;+\; \vec{v}_0\cdot\langle\vec{P}\,\rangle_{0'} \;+\; \frac{1}{2}\,Mv_0^2 \tag{5.225}$$

which simplifies if $\langle\vec{P}\,\rangle_{0'} = 0$, i.e., if $0'$ is at rest relative to the c.m. of the system.

Eq. (5.224) is useful if one wants to obtain conserved quantities. If we require invariance of the theory under the group of **special Galilei transformations**, then we get with (5.221)

$$\frac{d}{dt}\,(\vec{P}\,t - M\vec{R}) \;=\; 0\;. \tag{5.226}$$

If in addition invariance under space translations is assumed, i.e., $\vec{P}\,(t) = $ const., this gives

$$\frac{d}{dt}\,\vec{R}\,(t) \;=\; \frac{1}{M}\,\vec{P}\;, \tag{5.227}$$

which shows that the center of mass moves with uniform velocity.

5.14 General Considerations

5.14.1 Exponential Form of the Representation

Given a Lie group of order n, one defines a one-parameter subgroup in the following way: It is a subgroup of G whose elements $g(t)$ depend continuously on a real parameter $t(-\infty < t < +\infty)$. By properly changing the parameterization, one obtains for the element $g(t)$ the simple composition law:

$$\begin{aligned} g(t_1)\; g(t_2) &= g(t_1 + t_2) \\ g(0) &= \mathbf{1}\ . \end{aligned} \tag{5.228}$$

In such a case, t is said to be a canonical parameter. (Since group elements are characterized by values of parameters $a_1, a_2, \cdots, a_n$, a one-parameter subgroup is obtained by properly expressing a_i in terms of t.

Example: Every arbitrary rotation in $\mathbf{R}^3$ can be expressed by rotations around fixed axes, like in case of Euler angles. One can then write the operators corresponding to the elements of the one-parameter subgroup as $T(a_1(t), a_2(t), \cdots, a_n(t))$, and has with (5.228)

$$T(t_1)\; T(t_2) \;=\; T(t_1 + t_2)\ . \tag{5.229}$$

Evaluating the derivative of $T(t)$ at $t = 0$ gives

$$\begin{aligned} \frac{dT(t)}{dt}\;|_{t=0} &= \sum_k \left(\frac{\partial T(t)}{\partial a_k}\, \frac{\partial a_k}{\partial t} \right)\;|_{t=0} \\ &= \sum_k J_k\; c_k \end{aligned} \tag{5.230}$$

where $c_k = \frac{\partial a_k}{\partial t}\;|_{t=0}$. Here we used the fact that the value $t = 0$ of the parameter corresponds to the identity element $a_i = 0$.

The operator

$$\frac{dT(t)}{dt}\;|_{t=0} = \sum_k J_k\; c_k \tag{5.231}$$

is called the **infinitesimal generator** of the one-parameter subgroup in the considered representation and is a linear combination of the infinitesimal generators J_k. The generators, in turn, constitute a representation of the Lie algebra associated with the group. Using (5.229) and (5.230) one can express the general element $T(t)$ in term of the J_k's. Differentiating (5.229) with respect to t_1 and putting $t_1 = 0, t_2 = t$ gives

$$\frac{dT(t)}{dt} = \frac{dT}{dt}\ |_{t=0}\ T(t) = \left(\sum_k c_k J_k\right) T(t) , \tag{5.232}$$

with the solution

$$T(t) = e^{\sum_k J_k c_k t} . \tag{5.233}$$

Thus, a generic element of the one-parameter subgroup is expressed in terms of the infinitesimal generator $\sum_k J_k c_k$. The important part is that for a connected Lie group it can be proved that every element of the group belongs to a one-parameter subgroup $G(t)$. Since we are interested in the unitary representation of the Lie groups, it follows that the operators J_k must be skew hermitian. It is then customary to write

$$T(t) = e^{i \sum_k I_k c_k t} \tag{5.234}$$

where I_k is self-adjoint.

5.14.2 Casimir Operators

A very useful concept in the theory of group representation is that of Casimir operators. Consider the Lie algebra associated with the group

$$[\lambda_i, \lambda_j] = \sum_k c_{ij}^k \lambda_k . \tag{5.235}$$

We call Casimir operator for the considered algebra every expression c in the λ_i's that commutes with all the basic elements of the algebra

$$[c, \lambda_k] = 0 . \tag{5.236}$$

Note, that c does in general **not** belong to the algebra, since it is not linear in the λ_i's. The importance of determining the Casimir operators is obvious. c is an operator, expressed in terms of the generators which commutes with all the generators and thus with all the operators representing elements of the group. If the considered representation is irreducible, c must then be a constant multiple of the identity in the linear vector space carrying the representation. The irreducible representations can then be labeled by the eigenvalues of a sufficiently large number of Casimir operators.

Insert:
The elements c_{ij}^k in (5.235) are called structure constants of the Lie algebra. The **rank** of a Lie algebra is defined to be the maximum number of independent elements of the algebra that commute among themselves. If the algebra has rank r, the corresponding group is also said to be of rank r.

Cartan's Theorem Consider the $n \times n$ matrix

$$g_{ij} = \sum_{k\ell} c_{ik}^{\ell} \, c_{j\ell}^{k} \, . \tag{5.237}$$

A sufficient condition for an algebra to be semi-simple is that

$$\det | \, g_{ij} \, | \neq 0 \, . \tag{5.238}$$

Moreover, if (5.238) is satisfied, the necessary and sufficient condition that the corresponding group is compact is that g_{ij} be a negative definite matrix.

Cartan's theorem guarantees that g_{ij} is non-singular. Then one can define a matrix g^{ij}

$$\sum_{j} g^{ij} \, g_{ij} = \delta_{ij} \, . \tag{5.239}$$

Define a Casimir operator by

$$C = \sum_{ij} g^{ij} \, \lambda_i \lambda_j \, . \tag{5.240}$$

Evaluating $[C, \lambda_k]$ gives that the so-defined C commutes with all λ_k. Eq (5.240) is the so-called **quadratic** Casimir operator.

It can be shown that the minimum number of Casimir operators required to have a complete set, i.e., to specify completely the irreducible representations, equals the rank of the algebra.

5.15 Projection Operators

Definition: An operator P is called projection operator when it is

1. self-adjoint, i.e., $P^\dagger = P$

2. and

$$P^2 = P\ . \tag{5.241}$$

An example is the operator

$$P_\varphi \ = \mid \varphi\rangle\langle\varphi \mid \tag{5.242}$$

with $\parallel \varphi \parallel = 1$. If P_φ is applied on a state $\mid \psi\rangle$, it creates a state vector $\mid \varphi\rangle$ with a proportionality factor $\langle\varphi \mid \psi\rangle$

$$P_\varphi \mid \psi\rangle \ = \mid \varphi\rangle\langle\varphi \mid \psi\rangle\ , \tag{5.243}$$

i.e., $\mid \psi\rangle$ is projected into the direction of $\mid \varphi\rangle$.

One has the matrix elements

$$\begin{aligned} \langle\chi \mid P_\varphi \mid \psi\rangle &= \langle\chi \mid \varphi\rangle\langle\varphi \mid \psi\rangle \\ &= \langle\psi \mid \varphi\rangle^*\langle\varphi \mid \chi\rangle^* \\ &= (\langle\psi \mid \varphi\rangle\langle\varphi \mid \chi\rangle)^* \\ &= \langle\psi \mid P_\varphi \mid \chi\rangle^* \\ &= \langle P_\varphi\chi \mid \psi\rangle\ . \end{aligned} \tag{5.244}$$

Since $\langle\chi \mid$ and $\mid \psi\rangle$ are arbitrary states, it follows that $P_\varphi = P_\varphi^\dagger$ as required by (5.241). Furthermore,

$$P_\varphi^2 \ = \mid \varphi\rangle\langle\varphi \mid \varphi\rangle\langle\varphi \mid = \mid \varphi\rangle\langle\varphi \mid = \ P_\varphi \tag{5.245}$$

as required by (5.241). Thus P_φ is a projection operator. Similarly one shows that

$$P \ = \ \sum_\nu \ \mid \varphi_\nu\rangle\langle\varphi_\nu \mid \ + \ \int d\lambda \ \mid \varphi_\lambda\rangle\langle\varphi_\lambda \mid \tag{5.246}$$

with $\langle\varphi_{\nu'} \mid \varphi_\nu\rangle \ = \ \delta_{\nu'\nu}$, $\langle\varphi_{\lambda'} \mid \varphi_\lambda\rangle \ = \ \delta(\lambda' - \lambda)$ and $\langle\varphi_\nu \mid \varphi_\lambda\rangle = 0$ is a projection operator.

In fact (5.246) is the most general form of a projection operator. On the one hand, every self-adjoint operator can be represented in a spectral decomposed form. On the other hand, the eigenvalue fulfill

$$P \mid \varphi_\nu\rangle \ = \ c_\nu \mid \varphi_\nu\rangle \tag{5.247}$$

and with (5.241) one has

$$P^2 \mid \varphi_\nu\rangle \;=\; c_\nu^2 \mid \varphi_\nu\rangle \;=\; c_\nu \mid \varphi_\nu\rangle \;=\; P \mid \varphi_\nu \,\rangle \;. \tag{5.248}$$

From this follows that

$$c_\nu(c_\nu - 1) \;=\; 0 \;. \tag{5.249}$$

This means that $c_\nu = 1$ or $c_\nu = 0$. Thus one has

$$\begin{aligned} P \;&=\; \sum_\nu \mid \varphi_\nu\rangle \; c_\nu \; \langle\varphi_\nu \mid \;+\; \int d\lambda \;\mid \varphi_\lambda\rangle \; c_\lambda \; \langle\varphi_\lambda \mid \\ &=\; \sum_\nu \mid \varphi_\nu\rangle\langle\varphi_\nu \mid \;+\; \int d\lambda \;\mid \varphi_\lambda\rangle\langle\varphi_\lambda \mid \end{aligned} \tag{5.250}$$

where the sum (integral) has to be taken over all $\nu(\lambda)$ for which $c_\nu = c_\lambda = 1$.

With these preliminaries, one can write the probability to measure the value a_ν of an observable A as expectation value of an operator. If one defines for the eigenvalues a_ν of the discrete spectrum of A

$$P_{a_\nu} \;=\; \int\!\sum \; d\lambda \;\mid \varphi_{a_{\nu,\lambda}}\rangle\langle\varphi_{a_{\nu,\lambda}} \mid \;, \tag{5.251}$$

then the probability to find a_ν in the state $\mid \psi\rangle$ is given by

$$\langle\psi \mid P_{a_\nu} \mid \psi\rangle \;=\; \int\!\sum \; d\lambda \;\mid \langle\varphi_{a_{\nu,\lambda}} \mid \psi\rangle \mid^2 \,=\; p_\psi(a_\nu) \;. \tag{5.252}$$

Thus the probability is given as

$$p_\psi(a_\nu) \;=\; \langle\psi \mid P_{a_\nu} \mid \psi\rangle \;. \tag{5.253}$$