Notes on Symmetries in Quantum Mechanics

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September 16, 2021

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1. Unitary Transformations

Let $\mathcal{B} := \{|\phi_i\rangle\,; i = 1, 2, \dots\}$ be an orthonormal basis of the space of states of some quantum system

$$\langle\phi_i|\phi_j\rangle = \delta_{ij} \tag{1}$$

and $\hat{U}$ a linear operator, so that $|\phi_i\rangle \to |\psi_i\rangle$ with

$$|\psi_i\rangle = \hat{U}\,|\phi_i\rangle \tag{2}$$

Under what conditions is $\mathcal{C} := \{|\psi_i\rangle\,; i = 1, 2, \dots\}$ a new orthonormal basis, $\langle\psi_i|\psi_j\rangle = \delta_{ij}$?

We require

$$\langle\psi_i|\psi_j\rangle = \langle\phi_i|\,\hat{U}^\dagger\hat{U}\,|\phi_j\rangle = \delta_{ij} = \langle\phi_i|\phi_j\rangle \tag{3}$$

As this has to hold for any i, we must have $\hat{U}^\dagger\hat{U}\,|\phi_j\rangle = |\phi_j\rangle$ for all j ; since $\boldsymbol{\mathcal{B}}$ is a basis, this means

$$\hat{U}^\dagger U = 1 \tag{4}$$

This equation defines a *unitary transformation.* The argument shows that a change of basis can be realized by such a linear transformation. If

$$|\psi\rangle = \sum_i \lambda_i\,|\phi_i\rangle = \sum_i |\phi_i\rangle\,\langle\phi_i|\psi\rangle, \tag{5}$$

in another basis, the same ket is

$$|\psi\rangle = \sum_i \eta_i\,|\psi_i\rangle = \sum_i |\psi_i\rangle\,\langle\psi_i|\psi\rangle \tag{6}$$

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and

$$\langle\psi_i|\psi\rangle = \eta_i = \sum_j \langle\psi_i|\phi_j\rangle\langle\phi_j|\psi\rangle \tag{7}$$

$$= \sum_j \langle\psi_i|\phi_j\rangle\langle\phi_j|\psi\rangle = \sum_j \langle\phi_i|\,\hat{U}^\dagger\,|\phi_j\rangle\,\lambda_j \tag{8}$$

or

$$\eta_i = \left[U^\dagger\right]_{ij}\lambda_j \qquad \text{(repeated indexes summed)} \tag{9}$$

Considered as a basis change, a unitary transformation changes neither the states, nor the observables, only the matrices that represent them, as these depend on the basis (representation) chosen.

Nevertheless, a different outlook is possible and convenient when discussing symmetries. One can envision *doing something* to a physical system, like shifting its position, rotating it, etc. These are actual physical transformations that change the state of the system and its observable properties. One does not expect such transformations to change the norm of a ket, and if they are linear they will also be expressed by unitary transformations.

Exercise 1.
Show that if a linear operator preserves the norm of any ket, it is unitary.

This way of looking at unitary transformations is called an *active viewpoint.* One envisions transforming a state

$$|\psi\rangle \to \left|\tilde{\psi}\right\rangle := \hat{U}\,|\psi\rangle \tag{10}$$

A physical quantity like the average of $\hat{A}$ changes

$$\langle A\rangle = \langle\psi|\,\hat{A}\,|\psi\rangle \to \left\langle\tilde{\psi}\right|\hat{A}\left|\tilde{\psi}\right\rangle$$

But if we change observables by the same physical transformation $\hat{A} \to \tilde{A}$ the average of $\tilde{A}$ in the new state is the same as the average of $\hat{A}$ in the old one

$$\langle A\rangle = \langle\psi|\,\hat{A}\,|\psi\rangle = \left\langle\tilde{\psi}\right|\tilde{A}\left|\tilde{\psi}\right\rangle \tag{11}$$

The RHS is

$$\langle\psi|\,U^\dagger\tilde{A}U\,|\psi\rangle = \langle\psi|\,\hat{A}\,|\psi\rangle \tag{12}$$

As this must hold for any ket, $U^\dagger\tilde{A}U = \hat{A}$, or

$$\tilde{A} = \hat{U}\hat{A}U^\dagger, \tag{13}$$

the transformation law for observables.

Exercise 2.

Show that if $\langle\psi|\,\hat{A}\,|\psi\rangle = \langle\psi|\,\hat{B}\,|\psi\rangle$ for *any* ket, one has $\hat{A} = \hat{B}$,

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In summary, under a physical transformation represented by the unitary operator $\hat{U}$, states and observables transform as

$$|\psi\rangle \to \left|\tilde{\psi}\right\rangle := U\,|\psi\rangle \tag{14}$$

$$\hat{A} \to \tilde{A} = \hat{U}\hat{A}\hat{U}^{\dagger} \tag{15}$$

and physical quantities are unchanged if we transform states and the operators representing observables.

$$\langle A\rangle = \langle\psi|\,\hat{A}\,|\psi\rangle = \left\langle\tilde{\psi}\right|\tilde{A}\left|\tilde{\psi}\right\rangle$$

The reader may wonder why we are reducing the physical content of the theory to averages, while in general we have to deal with probability distributions. Quantum mechanical probabilities take the form

$$p_{\phi}\left[\psi\right] := |\langle\phi|\psi\rangle|^2$$

which one can read as the probability of measuring a system to be in state $|\phi\rangle$ when it has been prepared in state $|\psi\rangle$ .One can write this in the form

$$\begin{aligned} p_{\phi}\left[\psi\right] &:= |\langle\phi|\psi\rangle|^2 = \langle\psi|\phi\rangle\langle\phi|\psi\rangle = \langle\psi|\left(|\phi\rangle\,\langle\phi|\right)|\psi\rangle \\ &= \langle\hat{P}_{\phi}\rangle \end{aligned}$$

with the observable $\hat{P}_{\phi} := |\phi\rangle\,\langle\phi|$, the projector onto state $|\phi\rangle$. This shows that averages of hermitian operators exhaust the physical content of the theory.

2. Space symmetries and Groups

Our discussion starts with space symmetries. According to the active viewpoint we are considering spatial transformations from $\mathbb{E}^3 \to \mathbb{E}^3$ in which a point $\mathbf{r}$ is actually changed to another $\mathbf{r}'$,

$$\mathbf{r} \to \mathbf{r}' = \mathbf{f}(\mathbf{r}) \tag{16}$$

The transformations that maintain distances and angles are:

- reflections: this includes inversion about an origin

$$\mathbf{r} \to \mathbf{r}' = -\mathbf{r} \tag{17}$$

  or reflections about planes such as

$$(x, y, z) \to \left(x', y', z'\right) = (x, y, -z)\,; \qquad \text{reflection on } Oxy \tag{18}$$

- Translations

$$\mathbf{r} \to \mathbf{r}' = \mathbf{r} + \mathbf{a} \tag{19}$$

- Rotations

$$\mathbf{r} \to \mathbf{r}' = \mathbf{R} \cdot \mathbf{r} \tag{20}$$
$$x_i \to x_i' = R_{ij} x_j \tag{21}$$

where $\mathbf{R}$ is an orthogonal matrix. Denoting the unit vectors along cartesian coordinate axis by $\mathbf{e}_i$

$$\mathbf{e}_i \to \mathbf{e}_i' \tag{22}$$

we have

$$x_i' \mathbf{e}_i = x_j \mathbf{e}_j' \tag{23}$$

and

$$x_i' = x_j \left(\mathbf{e}_i \cdot \mathbf{e}_j' \right) \tag{24}$$
$$\mathbf{e}_i \cdot \mathbf{e}_j' = R_{ij}$$

which shows that the inverse transformations $\mathbf{e}_i' \to \mathbf{e}_i$ is defined by the matrix

$$R_{ij}^{-1} = \mathbf{e'}_i \cdot \mathbf{e}_j = R_{ji} \tag{25}$$

thus confirming that the rotation matrix is orthogonal.

$$\mathbf{R}^{-1} = \mathbf{R}^T \tag{26}$$

One consequence of orthogonality concerns the determinant of R

$$\begin{aligned} \det\left(\mathbf{R}^T \cdot \mathbf{R}\right) &= \det\left(\mathbf{R}^T\right) \det(\mathbf{R}) \\ &= \det(\mathbf{R})^2 = 1 \end{aligned} \tag{27}$$

The determinant of an orthogonal matrix is $\det(\mathbf{R}) = \pm 1$. Proper rotations are defined as having a positive determinant.

These transformations can be composed

$$\mathbf{r} \underset{\mathbf{f}}{\to} \mathbf{r}' \underset{\mathbf{g}}{\to} \mathbf{r}'' = (\mathbf{g} \circ \mathbf{f})(\mathbf{r}) \tag{28}$$

giving a natural definition of the *product* two transformations, which is, by nature, associative. Also we can include in the set of transformations the identity (doing nothing)

$$\mathbf{r} \to \mathbf{r}' = \mathbf{r} \tag{29}$$

The product of the identity e with any transformation $e \circ f = f \circ e = f$[1]. Finally, all the transformations we considered, being bijective in $\mathbb{E}^3$, have an inverse

$$f \circ f^{-1} = f^{-1} \circ f = e \tag{30}$$

In Algebra a set G with a product operation $G \otimes G \to G$ with the following properties:

[1] Take notice of the notation. These transformations are defined by functions $\mathbf{f}$ which map vectors to vectors $\mathbf{r}' = \mathbf{f}(\mathbf{r})$. But when we are referring the transformation itself we may use the corresponding letter in normal type, f.

G	E	I
E	E	I
P	I	E

Table 1: Multiplication Table of $G = \{E, I\}$

i) for any $g, h \in G$, $gh \in G$ (closure);

ii) For any $f, g, h \in G$ $(fg)h = f(gh) := fgh$ (associativity);

iii) There exists one element $e \in G$ such that for all $g \in G$, $eg = ge = g$ (identity);

iv) for any $f \in G$ there exists $f^{-1} \in G$ such that $f^{-1} \circ f = e$ (Inverse),

is called a *group*. Quite naturally, our symmetry transformations define abstract groups.

A simple example is given by the inversion transformation

$$I : \mathbf{r} \to \mathbf{r}' = -\mathbf{r} \tag{31}$$

with the identity

$$E : \mathbf{r} \to \mathbf{r}' = \mathbf{r} \tag{32}$$

The inverse of I is I itself

$$I^2 : \mathbf{r} \to \mathbf{r}' = -(-\mathbf{r}) = \mathbf{r} \tag{33}$$

This is the simplest possible group (except for the trivial one containing one element, the identity) and has only two elements. Its multiplication table is shown in Table 1. It is easy to see that the group properties imply that this is the only table compatible with a group of only two elements. But, of course, this does not mean that there is only one set of transformations with this multiplication table. For instance reflection about a plane and the identity have the same abstract multiplication table.

Exercise 3.

The $\mathbb{Z}_2$ group has two elements $\{0, 1\}$ and the group product is the addition modulo 2. Show it has the same multiplication table as the inversion group.

This is an example of a *discrete* group, with a finite number of elements. The other transformations mentioned above, translations and rotations, are *continuous* groups. Each element of the group is defined by a set of variables $g(a_1, \ldots, a_r) = g(\mathbf{a})$ that take values in some continuous space. For translations, for instance, $\mathbf{a} \in \mathbb{E}^3$. Later on we will have the opportunity to discuss the space of parameters of rotations, which is more interesting. But for now we want to discuss how these spatial transformations translate to transformations of states and observables in quantum mechanics.

2.1. Spatial transformations in Quantum States Space

In this section we consider (one-particle) systems for which a we have a position basis

$$\left\{|\mathbf{r}\rangle : \mathbf{r} \in \mathbb{E}^3\right\} \tag{34}$$

Under inversion, seen as a physical transformation,

$$\mathbf{r} \to -\mathbf{r} \tag{35}$$

it appears natural to define

$$|\mathbf{r}\rangle \to \hat{I}\,|\mathbf{r}\rangle = |-\mathbf{r}\rangle \tag{36}$$

which defines a unitary transformation, if we assume it to be also linear

$$|\psi\rangle = \int d^3r \psi(\mathbf{r})\,|\mathbf{r}\rangle \tag{37}$$

$$\hat{I}\,|\psi\rangle = \int d^3r \psi(\mathbf{r})\,|-\mathbf{r}\rangle \tag{38}$$

A simple change of variable $\mathbf{r} \to \mathbf{r'} = -\mathbf{r}$ leads to [2]

$$|\psi\rangle = \int d^3r' \psi(-\mathbf{r'})\,\left|\mathbf{r'}\right\rangle \tag{39}$$

for which we identify the transformed wave function

$$\psi_I(\mathbf{r}) = \psi(-\mathbf{r}) \tag{40}$$

By construction, this transformation is linear and preserves the norm

$$\int d^3r \left[\psi_I(\mathbf{r})\right]^* \left[\psi_I(\mathbf{r})\right] = \int d^3r \left[\psi(-\mathbf{r})\right]^* \left[\psi(-\mathbf{r})\right] = \int d^3r \left[\psi(\mathbf{r})\right]^* \left[\psi(\mathbf{r})\right] \tag{41}$$

and, therefore, is unitary. All the transformations we enumerated above, $\mathbf{r} \to \mathbf{r'} = g(\mathbf{r})$, have unit Jacobian in modulus, and this very same argument implies

$$|\psi\rangle \to |\psi\rangle = \hat{U}(g)\,|\psi\rangle \tag{42}$$

with

$$\hat{U}(g)\,|\mathbf{r}\rangle = |g(\mathbf{r})\rangle \tag{43}$$

and

$$\psi_g(\mathbf{r}) = \langle\mathbf{r}|\,\hat{U}(g)\,|\psi\rangle \tag{44}$$

Since

$$\left(\hat{U}^\dagger(g)\,|\mathbf{r}\rangle\right)^\dagger = \langle\mathbf{r}|\,\hat{U}(g) \tag{45}$$

[2] The determinant of the Jacobian of this transformation is -1, so $\int d^3r'(\dots) = \int d^3r\,|J|\,(\dots)$

we have

$$\psi_g(\mathbf{r}) = \langle \mathbf{r}| \hat{U}(g) |\psi\rangle = \langle g^{-1}(\mathbf{r})|\psi\rangle = \psi\left(g^{-1}(\mathbf{r})\right) \tag{46}$$

We take this last equation as a definition of the unitary transformation associated with the spatial transformation.

$$\begin{aligned} \mathbf{r} \to & \mathbf{r}' = g(\mathbf{r}) \\ \psi(\mathbf{r}) \to & \psi_g(\mathbf{r}) = \psi\left(g^{-1}(\mathbf{r})\right) \end{aligned}$$

In plain wording, the new wave-function at $\mathbf{r}$ has the value of the original one at the point that was mapped to $\mathbf{r}$. This is entirely consistent with our active viewpoint.

2.2. Transforming observables

If we have defined the unitary transformation, albeit with recourse to a specific basis, we should be able to determine the transformation of any observable

$$\hat{A} \to \hat{A}_g := \hat{U}\hat{A}\hat{U}^\dagger \tag{47}$$

Dealing with the position observables $\hat{\mathbf{r}}$, or with any function $V(\hat{\mathbf{r}})$, is easy since these are diagonal in the position representation:

$$\hat{\mathbf{r}}\psi(\mathbf{r}) = \mathbf{r}\psi(\mathbf{r}) \tag{48}$$

$$V(\hat{\mathbf{r}})\,\psi(\mathbf{r}) = V(\mathbf{r})\,\psi(\mathbf{r}) \tag{49}$$

The RHS of these equations are the wave functions of $\hat{\mathbf{r}}\,|\psi\rangle$ and $V(\hat{\mathbf{r}})\,|\psi\rangle$ computed at $\mathbf{r}$.

$$\langle \mathbf{r}|\,\hat{\mathbf{r}}\,|\psi\rangle = \mathbf{r}\psi(\mathbf{r}) \tag{50}$$

$$\langle \mathbf{r}|\,V(\hat{\mathbf{r}})\,|\psi\rangle = V(\mathbf{r})\,\psi(\mathbf{r}) \tag{51}$$

Accordingly

$$\hat{U}_g\left[\hat{\mathbf{r}}\psi(\mathbf{r})\right] = \mathbf{g}^{-1}(\mathbf{r})\psi\left(\mathbf{g}^{-1}(\mathbf{r})\right) = \mathbf{g}^{-1}(\mathbf{r})\psi_g(\mathbf{r}) \tag{52}$$

Or

$$\begin{aligned} \hat{U}_g\hat{\mathbf{r}}\hat{U}_g^\dagger U_g\psi(\mathbf{r}) &= \hat{U}_g\hat{\mathbf{r}}\hat{U}_g^\dagger\psi_g(\mathbf{r}) \\ &= \mathbf{g}^{-1}(\mathbf{r})\psi_g(\mathbf{r}) \\ &= \mathbf{g}^{-1}(\hat{\mathbf{r}})\psi_g(\mathbf{r}) \end{aligned} \tag{53}$$

which means

$$\hat{U}_g\hat{\mathbf{r}}\hat{U}_g^\dagger = \mathbf{g}^{-1}(\mathbf{r}) \tag{54}$$

One may ask if this somewhat unexpected. After all, we are physically mapping $\mathbf{r} \to g(\mathbf{r})$; should we not expect the same transformation for the observable $\hat{\mathbf{r}} \to g(\hat{\mathbf{r}})$, instead of $\hat{\mathbf{r}} \to \mathbf{g}^{-1}(\hat{\mathbf{r}})$, as found above? Remember that the transformed observable must have the same expectation value in the transformed states as the original one has

in the original, un-transformed, states. A state with $\langle\hat{\mathbf{r}}\rangle = \langle\psi|\,\hat{\mathbf{r}}\,|\psi\rangle = \mathbf{r}_0$, after the transformation will have mean $\langle\hat{\mathbf{r}}\rangle_g = \langle\psi_g|\,\hat{\mathbf{r}}\,|\psi_g\rangle = \mathbf{g}(\mathbf{r}_0)$. Therefore

$$\langle\psi_g|\,\hat{\mathbf{r}}_g\,|\psi_g\rangle = \mathbf{r}_0 = \mathbf{g}^{-1}\left(\mathbf{g}(\mathbf{r}_0)\right)$$

which implies $\hat{\mathbf{r}}_g = \mathbf{g}^{-1}(\hat{\mathbf{r}})$.

While this takes care, in a rather general manner, of operators which are diagonal in the position representation, we still have to consider other observables. For the simple system we are considering, dealing with the momentum operator is sufficient. The matrix elements of the momentum operator in the $\mathbf{r}$ representation are rather singular distributions, and is is easier to work out the transformation of the eigenstates of $\hat{\mathbf{p}}$,

$$\hat{\mathbf{p}}Ae^{i\mathbf{k}\cdot\mathbf{r}} = \hbar\mathbf{k}Ae^{i\mathbf{k}\cdot\mathbf{r}}. \tag{55}$$

Hence

$$\hat{U}_g\left[\hat{\mathbf{p}}Ae^{i\mathbf{k}\cdot\mathbf{r}}\right] = \hbar\mathbf{k}Ae^{i\mathbf{k}\cdot\mathbf{g}^{-1}(\mathbf{r})} \tag{56}$$

and

$$\hat{U}_g\hat{\mathbf{p}}\hat{U}_g^\dagger Ae^{i\mathbf{k}\cdot\mathbf{g}^{-1}(\mathbf{r})} = \hbar\mathbf{k}Ae^{i\mathbf{k}\cdot\mathbf{g}^{-1}(\mathbf{r})}. \tag{57}$$

At this juncture it is convenient to specify the various transformations.

- Inversion

$$\hat{U}_I\hat{\mathbf{p}}\hat{U}_I^\dagger Ae^{i\mathbf{k}\cdot(-\mathbf{r})} = \hbar\mathbf{k}Ae^{-i\mathbf{k}\cdot\mathbf{r}} \tag{58}$$

  or

$$\hat{U}_I\hat{\mathbf{p}}\hat{U}_I^\dagger = -\hat{\mathbf{p}} \tag{59}$$

- Translation

$$\hat{U}_{\mathbf{a}}\hat{\mathbf{p}}\hat{U}_{\mathbf{a}}^\dagger Ae^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{a})} = \hbar\mathbf{k}Ae^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{a})}$$

  so

$$\hat{U}_{\mathbf{a}}\hat{\mathbf{p}}\hat{U}_{\mathbf{a}}^\dagger = \hat{\mathbf{p}} \tag{60}$$

Rotation

$$\begin{aligned}\hat{U}_R\hat{p}_l\hat{U}_R^\dagger Ae^{ik_i\cdot R^T_{ij}x_j} &= \hat{U}_R p_l\hat{U}_R^\dagger Ae^{i(R_{ji}k_i)x_j}\\ &= \hbar k_l Ae^{i(R_{ji}k_i)x_j}\end{aligned} \tag{61}$$

which requires

$$\hat{U}_R p_l\hat{U}_R^\dagger = R^T_{lj}\hat{p}_j \tag{62}$$

since

$$\hat{p}_j\left[Ae^{i(R_{ji}k_i)x_j}\right] = \hbar\left(R_{ji}k_i\right)Ae^{i(R_{ji}k_i)x_j} \tag{63}$$

The transformation law stated by Eq.(62) defines $\hat{\mathbf{p}} = (\hat{p}_x, \hat{p}_y, \hat{p}_z)$ to be a *vector operator*. Is is straightforward to check that $\hat{\mathbf{r}} = (\hat{x}, \hat{y}, \hat{z})$, under rotation, has exactly the same transformation law (Eq.(54)) and is also a vector operator.

3. Symmetries and representations

These transformations can be defined for any physical system. Their existence gives no physical information on the system properties, *unless,* the all important observable, which defines the system dynamics, namely the Hamiltonian, remains invariant under a specific set (Group) of transformations. We approach the consequences of the *symmetry* of the Hamiltonian step by step.

1. If $\mathcal{H}$ is invariant under the unitary transformations of a given symmetry group, G, it commutes with all the unitary transformations $\hat{U}_g$ with $g \in G$.

   Invariance means simply
   $$\hat{U}_g \mathcal{H} \hat{U}_g^\dagger = \mathcal{H} \tag{64}$$
   and multiplying on the right by U_g
   $$\hat{U}_g \mathcal{H} = \mathcal{H} \hat{U}_g \tag{65}$$
   $$\left[\hat{U}_g, \mathcal{H}\right] = 0 \tag{66}$$

2. If $|\psi_E\rangle$is an eigenstate of $\mathcal{H}$ with energy E, $\hat{U}_g |\psi_E\rangle$ is also an eigenstate with the same energy.

   By hypothesis
   $$\mathcal{H} |\psi_E\rangle = E |\psi_E\rangle \tag{67}$$
   and
   $$\begin{aligned} \mathcal{H}\hat{U}_g |\psi_E\rangle &= \hat{U}_g \mathcal{H} |\psi_E\rangle , \qquad \left[\hat{U}_g, \mathcal{H}\right] = 0 \\ &= \hat{U}_g E |\psi_E\rangle \\ &= E\hat{U}_g E |\psi_E\rangle , \qquad \hat{U} \text{ is linear} \end{aligned} \tag{68}$$

3. Each energy level is by itself a vector sub-space of the total space of states, since any linear combinations of degenerate eigenstates is an eigenstate of the same energy. Each of these sub-spaces is *invariant* under the action of the transformations of the symmetry group of $\mathcal{H}$. In effect, if
   $$|\psi\rangle = \sum_{i=1}^{r} \lambda_i |\phi_i\rangle , \tag{69}$$
   where $\{|\phi_i\rangle ; i = 1, \ldots, r\}$ is any basis of the energy level with energy E, it follows from the previous property, that $\hat{U}_g |\psi\rangle$ has the same energy E and must be expressible as a linear combination of the basis of this energy level
   $$\hat{U}_g |\psi\rangle = \sum_{i=1}^{r} \eta_i(g) |\phi_i\rangle \tag{70}$$
   In other words, transforming a state of this energy level gives a state of the same energy level, *for any* $\hat{U}_g$ which leaves $\mathcal{H}$ invariant.

4. Each energy level provides a linear representation of matrices of the symmetry group of $\mathcal{H}$.

   Since

$$\hat{U}_g |\psi\rangle = \sum_{i=1}^{r} \eta_i(g) |\phi_i\rangle$$

$$\hat{U}_g |\phi_i\rangle = \sum_{j=1}^{r} M_{ji}(g) |\phi_j\rangle \qquad i = 1, \ldots, r$$

   Composing two transformations $h \circ g = hg$ gives

$$\hat{U}_h \hat{U}_g |\phi_i\rangle = \sum_{j=1}^{r} M_{kj}(h) M_{ji}(g) |\phi_k\rangle$$

   so that

$$h \to \mathbf{M}(h)$$
$$g \to \mathbf{M}(g)$$

   and

$$hg \to \mathbf{M}(h) \cdot \mathbf{M}(g)$$

   This map for the symmetry group to a set of matrices of dimension $r \times r$ that preserves the group property as a matrix product is a *linear representation of the Group*. In this language each energy level of the Hamiltonian provides a linear unitary representation of the symmetry group of the Hamiltonian.

These very simple statements lie at the heart of the importance of symmetries in Quantum Mechanics. If we understand and classify the representations of a given group, we learn a lot about the structure of energy levels of *any* Hamiltonian which is invariant under that group. As we will see, most of the quantum numbers that we use to characterize the eigenstates of Hamiltonians express the transformation properties of the states under its symmetries. But before this can be fully appreciated, we need to put some flesh into these bare bones.

3.1. The Inversion Symmetry

The linear operator representing the inversion transformation satisfies

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

since

$$\hat{I}^2 \psi(\mathbf{r}) = \hat{I} \psi(-\mathbf{r}) = \psi(\mathbf{r})$$

which implies that $\hat{I}$ in both unitary and hermitian. In any space that gives a linear representation of the group $\left\{\hat{E}, \hat{I}\right\}$($\hat{E}$ is the identity), we can always find basis in which $\hat{I}$ is diagonal, since it is hermitian. Its eigenvalues are

$$\hat{I}\left|\psi\right\rangle = \lambda\left|\psi\right\rangle$$
$$\hat{I}^2\left|\psi\right\rangle = \lambda^2\left|\psi\right\rangle = \left|\psi\right\rangle$$

or

$$\lambda^2 = \pm 1.$$

Hence, with a proper choice of basis, $\{\left|\phi_i\right\rangle, i = 1, \ldots, n\}$ in any energy level of the Hamiltonian, both group elements can be represented by diagonal matrices

$$\hat{E} \to M_{ij}(E) = \delta_{ij}$$
$$\hat{I} \to M_{ij}(I) = \lambda_i \delta_{ij} \qquad \lambda_i = \pm 1$$

That means that each subspace generated by each vector in this basis is itself invariant under the group transformations. The original $n \times n$ representation has been *reduced* to a direct sum of one dimensional representations. This language requires further clarification.

1. A linear representation of a symmetry group, generated by a vector space of states $\mathcal{E}$ (like an energy level of $\mathcal{H}$) is called *irreducible,* if there is no proper sub-space $\mathcal{E}'$ (other than $\mathcal{E}$ or the null vector) which is itself invariant under the group transformations. Otherwise it is called reducible.

2. A reducible representation can be reduced, by a basis choice, to a form where every matrix of the representation is block diagonal.

   Assume $\{\left|\phi_1\right\rangle, \ldots, \left|\phi_n\right\rangle\}$ is an orthonormal basis for a space $\mathcal{E}$ of a reducible representation, and $\{\left|\phi_1\right\rangle, \ldots, \left|\phi_r\right\rangle\}$, with $r < n$, a basis for an invariant subspace $\mathcal{F}$. The complement of $\mathcal{F}$ in $\mathcal{E}$ is $\overline{\mathcal{F}}$ generated by the basis $\{\left|\phi_{r+1}\right\rangle, \ldots, \left|\phi_n\right\rangle\}$ The invariance of $\mathcal{F}$ means that any group transformation acting on $\left|\phi_i\right\rangle$ for $i \leq r$ gives a state of $\mathcal{F}$

   $$\hat{U}_g\left|\phi_i\right\rangle = \sum_{j=1}^{r} M_{ji}(g)\left|\phi_j\right\rangle$$

   and for $k > r$

   $$\left\langle\phi_k\right|\hat{U}_g\left|\phi_i\right\rangle = \sum_{j=1}^{r} M_{ji}(g)\langle\phi_k|\phi_j\rangle = 0; \qquad k > r$$

   For any $i \leq r$ and $k > r$, and for all g,

   $$\left\langle\phi_k\right|\hat{U}_g\left|\phi_i\right\rangle = \left\langle\phi_i\right|\hat{U}_g^\dagger\left|\phi_k\right\rangle = 0$$

All matrix elements between states$\{|\phi_1\rangle, \ldots, |\phi_r\rangle\}$ with states$\{|\phi_{r+1}\rangle, \ldots, |\phi_n\rangle\}$ are zero. The spaces generated by these sets ,$\mathcal{F}$ and $\overline{\mathcal{F}}$ yield two representations of the symmetry group, of dimensions r and $n-r$. The original representations is called a direct sum of these two. An example of the form of all matrices of symmetry transformations for $n=3$ and $r=2$ is

$$\begin{array}{c|ccc} & |\phi_1\rangle & |\phi_2\rangle & |\phi_3\rangle \\ \langle\phi_1| & a_{11} & a_{12} & 0 \\ \langle\phi_2| & a_{12} & a_{22} & 0 \\ \langle\phi_3| & 0 & 0 & a_{33} \end{array} .$$

3. A representation of a symmetry group is either irreducible or a direct sum of irreducible representations.

   The procedure outlined above in $\mathcal{E}$ can also be carried out in $\mathcal{F}$ and its complement, until we are left with representations that can no longer be reduced, *i.e.,* with subspaces which have no invariant proper sub-spaces.

In summary:

> *An energy level of a Hamiltonian is either an irreducible representation of its symmetry group, or a direct sum of irreducible representations.*

This shows the advantage of knowing and classifying the irreducible representations of the symmetry groups. In the example of the group of inversion, there are only two inequivalent one dimensional representations. One with the matrices

$$\begin{aligned} E &\to [1] \\ I &\to [1] \end{aligned}$$

induced by even parity states

$$\hat{I}\,|\phi\rangle = |\phi\rangle$$

and second one

$$\begin{aligned} E &\to [1] \\ I &\to [-1] \end{aligned}$$

generated by odd parity states

$$\hat{I}\,|\phi\rangle = -\,|\phi\rangle$$

In any energy level we can choose a basis where all states have definite parity. Things get more interesting for higher dimensional representations, because states belonging to the same irreducible representation of the symmetry group of the Hamiltonian are *necessarily (by symmetry)* degenerate.

4. Continuous Groups

Physicists tend to think as continuous groups as transformations labeled by parameters in a continuous space. Mathematicians define them as manifolds endowed with a group property and would probably cringe in disgust at the cavalier treatment that follows. Nevertheless it will get us far.

4.1. Translation group

Our first example is the translation group. A translation is defined by a vector $\mathbf{a} \in \mathbb{E}^3$

$$\hat{T}_{\mathbf{a}} |\mathbf{r}\rangle = |\mathbf{r} + \mathbf{a}\rangle \tag{71}$$

For a wave function

$$\begin{aligned} \hat{T}_{\mathbf{a}} |\psi\rangle &= \int d^d r \psi(\mathbf{r}) \hat{T}_{\mathbf{a}} |\mathbf{r}\rangle \\ &= \int d^d r \psi(\mathbf{r}) |\mathbf{r} + \mathbf{a}\rangle \\ &= \int d^d r \psi(\mathbf{r} - \mathbf{a}) |\mathbf{r}\rangle \end{aligned} \tag{72}$$

$$\hat{T}_{\mathbf{a}} \psi(\mathbf{r}) = \psi(\mathbf{r} - \mathbf{a}) \tag{73}$$

Obviously

$$\hat{T}_{\mathbf{a}} \hat{T}_{\mathbf{b}} = \hat{T}_{\mathbf{a}+\mathbf{b}} = \hat{T}_{\mathbf{b}} \hat{T}_{\mathbf{a}} \tag{74}$$

Translations commute among themselves and the group is Abelian. Since

$$\hat{T}_{\mathbf{a}} = \hat{T}_{a_x \hat{\mathbf{e}}_x} \hat{T}_{a_y \hat{\mathbf{e}}_y} \hat{T}_{a_z \hat{\mathbf{e}}_z} \tag{75}$$

we start by considering translations along a single direction , which we leave unspecified.

4.1.1. Exponentiation

We want to argue that we can write

$$\hat{T}_a = e^{-ia\hat{p}/\hbar} \tag{76}$$

where $\hat{p}$ is an hermitian operator with an eigenbasis

$$\hat{p} |k\rangle = \hbar k |k\rangle \tag{77}$$

and this basis has wave functions (un-normalized)

$$\langle x|k\rangle = e^{ikx} \tag{78}$$

we will arrive there in several ways.

1. In a general, more abstract fashion, for each $a \in \mathbb{R}$, $\hat{T}_a$ is a linear map from $\mathcal{E} \to \mathcal{E}$

$$|\phi\rangle \to |\psi(a)\rangle = \hat{T}_a |\phi\rangle \tag{79}$$

we can differentiate this map as

$$\frac{d}{da} |\psi(a)\rangle = \frac{d\hat{T}_a}{da} |\phi\rangle \tag{80}$$

The map $d\hat{T}_a/da$, is thus defined by

$$\frac{d\hat{T}_a}{da} : \quad |\phi\rangle \to \frac{d}{da} |\psi(a)\rangle \tag{81}$$

Imagine we have chosen a basis and kets are column vectors and linear operator matrices

$$|\phi\rangle \to [\lambda_1, \ldots, \lambda_n]^T \tag{82}$$

$$\hat{T}_a |\phi\rangle \to [\eta_1, \ldots, \eta_n]^T \tag{83}$$

$$\eta_i = M_{ij}(a)\lambda_j \tag{84}$$

We are assuming that the matrix elements of $\mathbf{M}$ are differentiable functions of a and, in this representation,

$$\frac{d\hat{T}_a}{da} \to \frac{d}{da}\mathbf{M}(a) \tag{85}$$

Since the translations are a one-parameter additive group $\hat{T}_a\hat{T}_b = \hat{T}_{a+b}$, we have

$$\hat{T}_{a+b} - T_a = (T_b - 1)\hat{T}_a \tag{86}$$

and

$$\frac{d\hat{T}_a}{da} = \left.\frac{dT_a}{da}\right|_{a=0} \hat{T}_a \tag{87}$$

denoting (the $-i$ will be shortly explained)

$$-i\hat{L} := \left.\frac{dT_a}{da}\right|_{a=0} \tag{88}$$

$$\frac{dT_a}{da} = -i\hat{L}\hat{T}_a \tag{89}$$

which is solved as

$$\hat{T}_a = e^{-ia\hat{L}} \tag{90}$$

The $-i$ factor was introduced to make $\hat{L}$ an hermitian operator. The identity is $\hat{T}_0$, since $T_{a+0} = T_aT_0 = T_0T_a = T_a$. But $T_{a+(-a)} = T_aT_{-a} = 1$, so $T_{-a} = T_a^\dagger$. This means

$$\left(\frac{dT_a}{da}\right)^\dagger = \frac{dT_a^\dagger}{da} = -\left.\frac{dT_b}{db}\right|_{b=-a} \tag{91}$$

and

$$\left(-i\hat{L}\right)^{\dagger} = i\hat{L}^{\dagger} = i\hat{L}. \tag{92}$$

The hermitian operator $\hat{L}$ is called the generator of the group $\left\{\hat{T}_a : a \in \mathbb{R}\right\}$. For translations

$$\hat{T}_a\psi(x) = \psi(x-a) \tag{93}$$

$$\left.\frac{dT_a}{da}\right|_{a=0} \psi(x) = -\partial_x\psi(x) \tag{94}$$

and

$$\hat{L} = \frac{1}{i}\partial_x = \frac{\hat{p}_x}{\hbar} \tag{95}$$

$$\hat{T}_a = e^{-ia\hat{p}/\hbar} \tag{96}$$

2. Assume a state which gives a 1D representation of $\hat{T}_a$. Because this is unitary

$$\begin{aligned} \hat{T}_a\left|\lambda\right\rangle &= e^{-i\lambda(a)}\left|\lambda\right\rangle \qquad \lambda(a) \in \mathbb{R} \\ \hat{T}_b\hat{T}_a\left|\lambda\right\rangle &= e^{i\lambda(b)}e^{i\lambda(a)}\left|\lambda\right\rangle \\ &= e^{i[\lambda(b)+\lambda(a)]}\left|\lambda\right\rangle \\ &= e^{i[\lambda(b+a)]}\left|\lambda\right\rangle \end{aligned} \tag{97}$$

because $\hat{T}_b\hat{T}_a = \hat{T}_{a+b}$. We conclude

$$\lambda(b+a) = \lambda(b) + \lambda(a) \tag{98}$$

and the linearity of λ means

$$\lambda(a) = ka \tag{99}$$

or changing label

$$\hat{T}_a\left|k\right\rangle = e^{-ika}\left|k\right\rangle \tag{100}$$

We can define an operator through its action on the states $\left|k\right\rangle$

$$\hat{p}\left|k\right\rangle := \hbar k\left|k\right\rangle \tag{101}$$

and by definition of function of an operator

$$\hat{T}_a = e^{-ia\hat{p}/\hbar} \tag{102}$$

The operator $\hat{p}$ has real eigenvalues. If its eigenstates are a complete basis it is an observable. In the position representation

$$\hat{T}_a\psi_k(x) = \psi_k(x-a) = e^{-ika}\psi_k(x) \tag{103}$$

and, choosing $a = x$,

$$\psi_k(x) = \psi_k(0)e^{ikx} \tag{104}$$

These are plane waves and

$$\hat{p}e^{ikx} = \frac{\hbar}{i}\partial_x e^{ikx} \tag{105}$$

Plane waves are a basis and, therefore,

$$\hat{p} = \frac{\hbar}{i}\partial_x \tag{106}$$

3. By expanding in series

$$\begin{aligned}\psi(x-a) &= \psi(x) - a\frac{d\psi}{dx} + \frac{1}{2}a^2\frac{d^2\psi}{dx^2} + \dots \\ &\sum_{n=0}^{\infty}\frac{(-a)^n}{n!}\frac{d^n}{dx^n}\psi(x) \\ &= e^{-a\partial_x}\psi(x)\end{aligned} \tag{107}$$

$$\psi(x-a) = e^{-a\partial_x}\psi(x) \tag{108}$$

$$\psi(x-a) = e^{-ia\hat{p}/\hbar}\psi(x) \tag{109}$$

$$\hat{T}_a = e^{-ia\hat{p}/\hbar} \tag{110}$$

4. Commutation relations

$$[\hat{x}, \hat{p}_x] = i\hbar \tag{111}$$

$$[\hat{x}, \hat{p}_x^n] = i\hbar n\left[\hat{x}, \hat{p}_x^{n-1}\right] \tag{112}$$

$$[\hat{x}, f(\hat{p}_x)] = i\hbar \left.\frac{df}{dp}\right|_{p\to\hat{p}_x} \tag{113}$$

or

$$\left[\hat{x}, e^{iap_x/\hbar}\right] = -ae^{iap_x/\hbar} \tag{114}$$

giving

$$e^{-iap_x/\hbar}\hat{x}e^{iap_x/\hbar} = e^{-iap_x/\hbar}e^{iap_x/\hbar}\hat{x} + e^{-iap_x/\hbar}ae^{iap_x/\hbar} \tag{115}$$

$$= \hat{x} - a \tag{116}$$

exactly as obtained form the definition of translations. This shows again that

$$\hat{T}_a = e^{-ia\hat{p}_x/\hbar} \tag{117}$$

The first derivation makes clear that the concept of a generator is quite general for a one-parameter additive group property

$$\hat{T}_a\hat{T}_b = \hat{T}_{a+b} \tag{118}$$

This implies

$$\hat{T}_a := e^{-ia\hat{L}} \tag{119}$$

with $\hat{L}$ hermitian.

These considerations are easily generalized for the full translation group in $\mathbb{R}^3$ which now has 3 generators $\hat{\mathbf{p}} = (\hat{p}_x, \hat{p}_y, \hat{p}_z)$. They obviously inherit the commutation of the unitary transformations which they generate.

$$[\hat{p}_i, \hat{p}_j] = 0 \tag{120}$$

From Eq.(119) one can arrive at the notion of an *infinitesimal transformation* as the first order expansion in a

$$\hat{T}_\epsilon = \mathbb{1} - i\epsilon\hat{L} + \mathcal{O}(a^2) \tag{121}$$

In the vicinity of the identity, the transformation is defined by the generator. For a finite a we can split the transformations into products of n translations of a/n

$$\hat{T}_a = \overbrace{T_{a/n} \dots \hat{T}_{a/n}}^{n\,terms} \tag{122}$$

in the limit

$$\hat{T}_a = \lim_{n\to\infty} \left(\mathbb{1} - i\frac{a}{n}\hat{L}\right)^n = e^{-ia\hat{L}} \tag{123}$$

thus justifying the name of $\hat{L}$ as the infinitesimal generator of translations.

4.2. Translation symmetry

Having dealt with the translation transformation, we can now focus on the implications of translation symmetry. A translational invariant Hamiltonian satisfies

$$\hat{T}_a \mathcal{H} \hat{T}_a^\dagger = \mathcal{H} \tag{124}$$

or

$$\hat{T}_a \mathcal{H} = \mathcal{H} \hat{T}_a \tag{125}$$

$$\left[\hat{T}_a, \mathcal{H}\right] = 0 \tag{126}$$

This implies that the commutator with the generator is also zero

$$\left[\hat{L}, \mathcal{H}\right] = 0 \tag{127}$$

In the case of translations this means that stationary states can be chosen as momentum eigenstates. Momentum is named a *good quantum number*. Note that the momentum eigenvalue defines the different one-dimensional representations of the translation symmetry.

$$\hat{T}_a |k\rangle = e^{-ika} |k\rangle \tag{128}$$

This is trivially generalized for a many particle system. We define

$$\langle \mathbf{r}_1, \ldots, \mathbf{r}_N | \, \hat{T}_{\mathbf{a}} \, | \psi \rangle = \psi(\mathbf{r}_1 - \mathbf{a}, \ldots, \mathbf{r}_N - \mathbf{a}) \tag{129}$$

This means

$$\hat{T}_{\mathbf{a}} = e^{-i\mathbf{a}\cdot(\sum_i \hat{\mathbf{p}}_i)/\hbar} = e^{-i\mathbf{a}\cdot\hat{\mathbf{P}}/\hbar} \tag{130}$$

which is the product of the translation operators in each variable. The total momentum $\hat{\mathbf{P}}/\hbar$ is the generator, and translational invariance means that

$$\left[\hat{\mathbf{P}}, \mathcal{H}\right] = 0 \tag{131}$$

This means the $\hat{\mathbf{P}}$ is a conserved quantity, since its average, by Heisenberg's Equation of motion is

$$\frac{d}{dt}\langle \hat{\mathbf{P}} \rangle_t = \langle \left[\hat{\mathbf{P}}, \mathcal{H}\right] \rangle = 0$$

Momentum conservation is a consequence of translational invariance.

5. The Rotation Group

Generators

$$R_{ij} = \delta_{ij} + \Omega_{ij} + \mathcal{O}(\Omega^2) \tag{132}$$

$$RR^T = 1 \Rightarrow \Omega_{ij} = -\Omega_{ji} \tag{133}$$

$$\Omega_{ij} = \begin{bmatrix} 0 & -\Omega_{21} & \Omega_{13} \\ \Omega_{21} & 0 & -\Omega_{32} \\ -\Omega_{13} & \Omega_{32} & 0 \end{bmatrix} = -i \left[\Omega_{21}\mathbf{M}^3 + \Omega_{13}\mathbf{M}^2 + \Omega_{32}\mathbf{M}^1\right] \tag{134}$$

$$\mathbf{M}^1 = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{bmatrix} \tag{135}$$

$$\mathbf{M}^2 = \begin{bmatrix} 0 & 0 & i \\ 0 & 0 & 0 \\ -i & 0 & 0 \end{bmatrix} \tag{136}$$

$$\mathbf{M}^3 = \begin{bmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \tag{137}$$

or

$$M^i_{jl} = -i\epsilon_{ijl} \tag{138}$$

The commutators of the generators

$$\begin{aligned}\left[\mathbf{M}^i, \mathbf{M}^j\right]_{kl} &= M^i_{km}M^j_{ml} - M^j_{km}M^i_{ml} \\ &= -\epsilon_{ikm}\epsilon_{jml} + \epsilon_{jkm}\epsilon_{iml} \\ &= -\left(\delta_{il}\delta_{kj} - \delta_{ij}\delta_{kl}\right) + \left(\delta_{jl}\delta_{ki} - \delta_{ji}\delta_{kl}\right) \\ &= -\delta_{il}\delta_{jk} + \delta_{jl}\delta_{ik} = -\epsilon_{ijm}\epsilon_{lkm} \\ &= i\epsilon_{ijm}M^m_{kl} \end{aligned} \tag{139}$$

We can state

$$\left[\mathbf{M}^i, \mathbf{M}^j\right] = i\epsilon_{ijm}\mathbf{M}^m \tag{140}$$

as the commutation relations between the three infinitesimal generators. By defining

$$\omega_i := -\frac{1}{2}\epsilon_{ijk}\Omega_{jk}, \tag{141}$$

which amounts to

$$\omega_1 = -\Omega_{23} = \Omega_{32}, \tag{142}$$

$$\omega_2 = -\Omega_{31} = \Omega_{13}, \tag{143}$$

$$\omega_3 = -\Omega_{12} = \Omega_{21}, \tag{144}$$

the infinitesimal rotation matrix becomes,

$$R_{ij} = 1 - i\omega_k M^k_{ij} + \mathcal{O}(\omega^2) \tag{145}$$

$$\mathbf{R} = \lim_{n\to\infty}\left(1 - i\frac{\omega_k\mathbf{M}^k}{n}\right)^n \tag{146}$$

by exponentiation

$$R_{ij}(\boldsymbol{\omega}) = \left[e^{-i\omega_k\mathbf{M}^k}\right]_{ij} \tag{147}$$

defining a unit vector $\mathbf{n}$ and [3]

$$n_k = \frac{\omega_k}{\theta} \tag{148}$$

$$\theta = \sqrt{\omega_1^2 + \omega_2^2 + \omega_3^2} \tag{149}$$

$$R_{ij}(\boldsymbol{\omega}) = \left[e^{-i\omega_k\mathbf{M}^k}\right]_{ij} = \left[e^{-i\theta n_k\mathbf{M}^k}\right]_{ij} \tag{150}$$

We can now prove an important geometric characteristic of rotations. The matrix

$$\mathbf{R} := \left[e^{-i\theta\hat{n}_k\mathbf{M}^k}\right] \tag{151}$$

defines a rotation with axis along $\mathbf{n}$ with an angle θ.

[3] Note that it would be a serious mistake to write $R_{ij}(\boldsymbol{\omega}) = \left[e^{-i\omega_k\mathbf{M}^k_{ij}}\right]$. Can you see why?

For an arbitrary vector $\mathbf{u}$

$$\mathbf{u}(\theta) := \left[e^{-i\theta\hat{n}_k\mathbf{M}^k}\right]\cdot\mathbf{u} \tag{152}$$

$$\begin{aligned}\frac{d}{d\theta}u_i(\theta) &= -in_kM^k_{il}\left[e^{-i\theta\hat{n}_k\mathbf{M}^k}\right]_{lj}u_j \\ &= -\epsilon_{kil}n_ku_l(\theta) \\ &= (\mathbf{n}\times\mathbf{u})_i\end{aligned} \tag{153}$$

or

$$\frac{d}{d\theta}\mathbf{u}(\theta) = \mathbf{n}\times\mathbf{u}(\theta) \tag{154}$$

This defines geometrically a rotation where $\mathbf{n}$ is invariant, with $\mathbf{u}(\theta)$ rotated by θ about $\mathbf{n}$ from $\mathbf{u}(0)$.

This so far is pure geometry. No reference has been made to Quantum Mechanics. We have determined that SO(3) the group of orthogonal matrices of unit determinant:

1. Is a three parameter group $\boldsymbol{\omega} = (\omega_1, \omega_2, \omega_3)$ with three generators $\mathbf{M}^k, k = 1, 2, 3$
2. The generators satisfy the commutation relations

$$\left[\mathbf{M}^i, \mathbf{M}^j\right] = i\epsilon_{ijm}\mathbf{M}^m \tag{155}$$

3. The general rotation leaves an direction invariant, the axis of rotation, and has the form

$$\mathbf{R} := \left[e^{-i\theta n_k\mathbf{M}^k}\right] \tag{156}$$

with

$$n_k = \frac{\omega_k}{\theta} \tag{157}$$

$$\theta = \sqrt{\omega_1^2 + \omega_2^2 + \omega_3^2} \tag{158}$$

where $\mathbf{n}$ is the unit vector along the axis and θ the angle of rotation.

5.1. Rotations and Angular Momentum

We now consider the unitary representations of SO(3). We will denote by $\hat{U}(\boldsymbol{\omega})$ the unitary transformation associated with rotation parametrized $\boldsymbol{\omega} = \theta\mathbf{n}$. For an infinitesimal transformation ($\theta \to 0$)

$$\mathbf{R}(\boldsymbol{\omega}) = 1 - i\omega_k\mathbf{M}^k + \mathcal{O}(\omega^2), \tag{159}$$

we must have

$$\hat{U}(\boldsymbol{\omega}) = \hat{1} - i\omega_k\hat{J}^k + \mathcal{O}(\omega^2) \tag{160}$$

where the operators $\hat{J}^k, k = 1, 2, 3$ are hermitian

$$\hat{U}^\dagger(\boldsymbol{\omega}) = \hat{1} + i\omega_k\left(\hat{J}^k\right)^\dagger + \mathcal{O}(\omega^2)$$

and

$$\hat{U}^{\dagger}(\boldsymbol{\omega})U(\boldsymbol{\omega}) = \hat{1} + \omega_k \left(\hat{J}^k - \left(\hat{J}^k \right)^{\dagger} \right) + \mathcal{O}(\omega^2) = \hat{1} \tag{161}$$

$$\hat{J}^k = -\left(\hat{J}^k \right)^{\dagger} \tag{162}$$

By definition, the group property must be preserved

$$\begin{aligned} \mathbf{R}\left(\boldsymbol{\alpha}\right)\mathbf{R}\left(\boldsymbol{\omega}\right)\mathbf{R}^T\left(\boldsymbol{\alpha}\right) &= \left(1 - i\alpha_k \mathbf{M}^k\right)\left(1 - i\omega_l \mathbf{M}^l\right)\left(1 + i\alpha_m \mathbf{M}^m\right) \\ &= 1 - i\omega_l \mathbf{M}^l - \alpha_k\omega_l \left[\mathbf{M}^k, \mathbf{M}^l\right] + \mathcal{O}(\alpha^2, \omega^2) \\ &= 1 - i\omega_l \mathbf{M}^l - i\epsilon_{klm}\alpha_k\omega_l \mathbf{M}^m + \mathcal{O}(\alpha^2, \omega^2) \\ &= 1 - i\omega'_k \mathbf{M}^k + \mathcal{O}(\alpha^2, \omega^2) \end{aligned} \tag{163}$$

where

$$\boldsymbol{\omega}' = \boldsymbol{\omega} + \boldsymbol{\alpha} \times \boldsymbol{\omega} \tag{164}$$

we must have to order $\omega\alpha$

$$\begin{aligned} \hat{U}\left(\boldsymbol{\alpha}\right)\hat{U}\left(\boldsymbol{\omega}\right)\hat{U}^{\dagger}\left(\boldsymbol{\alpha}\right) &= 1 - i\omega_l \hat{J}^l - i\alpha_k\omega_l \left[\hat{J}^k, \hat{J}^l\right] \\ &= 1 - i\omega_l \hat{J}^l - i\epsilon_{klm}\alpha_k\omega_l \hat{J}^m + \mathcal{O}(\alpha^2, \omega^2) \\ &= 1 - i\omega'_k \hat{J}^k + \mathcal{O}(\alpha^2, \omega^2) \end{aligned} \tag{165}$$

and the hermitian generators must have the commutation relations

$$\left[\hat{J}^i, \hat{J}^j\right] = i\epsilon_{ijk}\hat{J}^k \tag{166}$$

and

$$\hat{U}\left(\boldsymbol{\omega}\right) = e^{-i\omega_k \hat{J}^k} = e^{-i\theta n_k \hat{J}^k} \tag{167}$$

5.1.1. Vector Operators

We briefly mentioned above the concept of vector operators as sets $\hat{V}^k$, $k = (1, 2, 3)$ or $k = (x, y, z)$ that transform as

$$\hat{U}(\boldsymbol{\omega})\hat{V}^k\hat{U}^{\dagger}(\boldsymbol{\omega}) = R^T_{kl}(\boldsymbol{\omega})\hat{V}^l \tag{168}$$

We will now see that this translates into specific commutation relations with the angular momentum operators, and furthermore, $\hat{\mathbf{J}} = \left(\hat{J}^x, \hat{J}^y, \hat{J}^z\right)$ is itself a vector operator set.

For an infinitesimal transformation Eq.(168) reads

$$\left(1 - i\omega_i \hat{J}^i\right)\hat{V}^k\left(1 + i\omega_l \hat{J}^l\right) = 1 + i\omega_i M^i_{kl}\hat{V}^l \tag{169}$$

or

$$-i\omega_i \left[\hat{J}^i, \hat{V}^k\right] = i\omega_i M^i_{kl}\hat{V}^l \tag{170}$$

Since this holds for any $\boldsymbol{\omega}$

$$\left[\hat{J}^i, \hat{V}^k\right] = -M^i_{kl}\hat{V}^l \tag{171}$$

$$\left[\hat{J}^i, \hat{V}^k\right] = i\epsilon_{ikl}\hat{V}^l \tag{172}$$

These commutation relations define a vector operator.

Exercise 4.

We have shown that Eq.(168) implies Eq.(172). The converse is also true. To prove it start with

$$\hat{A}(\theta) := e^{-i\theta n_i J^i}\hat{V}^k e^{i\theta n_i J^i} \tag{173}$$

Differentiate this expression with respect θ and integrate the corresponding differential equation to show

$$\hat{A}(\theta) = \left[e^{i\theta n_i M^i}\right]_{kl}\hat{V}^l = R^T_{kl}(\boldsymbol{\omega})\hat{V}^l$$

Comparing Eqs.(172) and (166), we see that angular momentum is a specific instance of a vector operator.

6. Irreducible representations of SO(3)

The importance of the algebra of the generators is better appreciated by showing that they allow the complete classification of the irreducible representations of the group.

1. The first point to note is that a space which is invariant under the unitary transformations of SO(3) is also invariant under the action of the generators and vice-versa.

2. A operator which is invariant under rotations (called a scalar operator) has a constant value in any space which is irreducible under group operations.

   Let $|\psi\rangle$ be an eigenstate of $\hat{O}$ with eigenvalue o

   $$\hat{O}\,|\psi\rangle = o\,|\psi\rangle \tag{174}$$

   Since is $\hat{O}$ commuteswith all the unitary transformations of the group

   $$\hat{O}\hat{U}(\boldsymbol{\omega})\,|\psi\rangle = \hat{U}(\boldsymbol{\omega})\hat{O}\,|\psi\rangle = o\hat{U}(\boldsymbol{\omega})\,|\psi\rangle \tag{175}$$

   The eigenvalue of $\hat{O}$ is unchanged by any symmetry operation. As varying $\hat{U}(\boldsymbol{\omega})$ we generate the entire irreducible space, we conclude that all states of the same irreducible representation have the same eigenvalue of any invariant observable: irreducible representations are characterized by the eigenvalues of invariant operators.

3. Since $\hat{J}^k$ is a vector operator, it is clear that $\hat{\mathbf{J}}\cdot\hat{\mathbf{J}} = J^2$ is an invariant operator and we can specify irreducible representations of SO(3) by its eigenvalue.

4. Any component of the angular momentum, commutes with $\hat{J}^2$, and it is customary to construct basis of irreducible representations with simultaneous eigenstates of $\hat{J}^2$ and $\hat{J}^z$

$$\hat{J}^2 |\lambda, m\rangle = \lambda |\lambda, m\rangle \tag{176}$$

$$\hat{J}^z |\lambda, m\rangle = m |\lambda, m\rangle \tag{177}$$

In elementary courses in QM (see appendix), one then uses commutation relations of angular momentum to show that

$$\lambda = j(j+1), \qquad j \text{ positive integer of half-integer,} \tag{178}$$

$$m = -j, -j+1, \ldots, j \tag{179}$$

gives a basis for an irreducible representation of SO(3)

$$\mathcal{B}_j = \{|j, m\rangle : m = -j, \ldots, j\}. \tag{180}$$

on which

$$\hat{J}^2 |j, m\rangle = j(j+1) |j, m\rangle \tag{181}$$

and for the generators

$$J^z |j, m\rangle = m |j, m\rangle \tag{182}$$

$$J^{\pm} |j, m\rangle = \sqrt{j(j+1-m(m\pm 1)}\, |j, m\pm 1\rangle \tag{183}$$

You may question whether this is a basis for an irreducible representation. By construction, it generates a space invariant under group transformations. But how do we know there is no smaller invariant subspace? Well, imagine $|\psi\rangle$ is a vector is such a space. By acting with J^+ repeatedly, we eventually kill the state, since $|\psi\rangle = \sum_{m=-j}^{j} a_m |j, m\rangle$. Just before that

$$\left(J^+\right)^p |\psi\rangle \propto |j, j\rangle \tag{184}$$

Then, by applying J^- we generate all the states $\mathcal{B}_j$. This means *all* the states of the original representation can be generated as linear combinations of states obtained by applying rotation generators to *any state of the representation.* We conclude that there is no smaller invariant subspace and the representation generated by $\mathcal{B}_j$ is irreducible.

We thus obtain a complete characterization of all possible irreducible representations of SO(3):

- $j = 0, \dim = 1$;
- $j = 1/2$, $\dim = 2$;
- $j = 1$, $\dim = 3$;
- $j = 3/2$, $\dim = 4$;
- ..... .

6.1. Finite Rotation Matrices

As $\mathcal{B}_j = \{|j,m\rangle : m = -j,\ldots,j\}$ is a basis for an $SO(3)$ representation we can state, for any rotation

$$\hat{U}(\boldsymbol{\omega})\,|j,m\rangle = \sum_{m'} D^J_{m'm}(\boldsymbol{\omega})\,\big|j,m'\big\rangle \tag{185}$$

The representation matrices may be hard to compute, but is is important to note that they are completely determined by the j quantum number. They do not depend on any eigenvalue of other scalar operators. For an infinitesimal transformation, Eq.(185) becomes

$$(\mathsf{1} - i\boldsymbol{\omega}\cdot\mathbf{J})\,|j,m\rangle = \sum_{m'} (\delta_{m'm} - i\boldsymbol{\omega}\cdot\mathbf{N}_{m'm})\,\big|j,m'\big\rangle \tag{186}$$

and the set of matrices $N^r_{m'm}$ are very easy to compute; since

$$J^r\,|j,m\rangle = \sum_{m'} N^r_{m'm}\,\big|j,m'\big\rangle \qquad r = x,y,z \tag{187}$$

one can use Eqs.(182) and (183)

$$J^z\,|j,m\rangle = m\,|j,m\rangle \tag{188}$$

$$J^\pm\,|j,m\rangle = \sqrt{j(j+1-m(m\pm1)}\,|j,m\pm1\rangle \tag{189}$$

to compute them. Formally

$$D^J(\boldsymbol{\omega}) = e^{-i\boldsymbol{\omega}\cdot\mathbf{N}}$$

which shows that $D^J(\boldsymbol{\omega})$, as $\mathbf{N}$, is entirely determined by the angular momentum relations (Eqs. (182) and (183)).

Exercise 5.
Determine the matrix N^k that represents J^k $(k = x,y,z)$ in the basis $\{|j,m\rangle\,;\, m = -j,\ldots,j\}$.

The most important point of this section is to note that Eqs.(182) and (183) and (185) are essentially equivalent statements: one implies the other.

7. Spin and Orbital Angular momentum

If we apply the preceding discussion to the case of a particle described by a wave function in position space, $\psi(\mathbf{r})$,

$$\hat{U}(\boldsymbol{\omega})\psi(\mathbf{r}) = \psi(\mathbf{R}^T\cdot\mathbf{r}) \tag{190}$$

We have seen that $\mathbf{R}(\boldsymbol{\omega}) = 1 - i\omega_k\mathbf{M}^k$, so that to linear order in $\boldsymbol{\omega}$

$$\begin{aligned}\left(\mathsf{1} - i\omega_k\hat{J}^k\right)\psi(\mathbf{r}) &= \psi(x_j + i\omega_k M^k_{jl}x_l)\\ &= \psi(\mathbf{r}) + i\omega_k M^k_{jl}x_l\partial_j\psi(\mathbf{r})\\ &= [\mathsf{1} + \omega_k\epsilon_{kjl}x_l\partial_j]\,\psi(\mathbf{r})\\ &[1 - \boldsymbol{\omega}\cdot(\mathbf{r}\times\nabla)]\,\psi(\mathbf{r})\end{aligned} \tag{191}$$

The rotation generator is

$$\mathbf{J} = \boldsymbol{\ell} = (\mathbf{r} \times \frac{\nabla}{i}) \tag{192}$$

i.e., the usual orbital angular momentum in units of $\hbar$. It follows, without the need to check explicitly, that

$$\left[\hat{l}^k, \hat{l}^l\right] = i\epsilon_{klm}\hat{l}^m$$

The transformation of Eq.(190) applies to any classical scalar field such as a temperature of hydrostatic pressure. But not to a vector field such as a velocity. In that case, the components of the field also mix. Using the active viewpoint they transform exactly as $\mathbf{r}$

$$v_i(\mathbf{r}) \to v_i'(\mathbf{r}) = R_{ij}(\boldsymbol{\omega})v_j\left(\mathbf{R}^T(\boldsymbol{\omega})\cdot\mathbf{r}\right) \tag{193}$$

This states that the vector $\mathbf{v}'$ at $\mathbf{r}$ is obtained by rotating $\mathbf{v}$ at the point that maps to $\mathbf{r}$. If the transformation is infinitesimal

$$v_j\left(\mathbf{R}^T(\boldsymbol{\omega})\cdot\mathbf{r}\right) = \left(1 - i\boldsymbol{\omega}\cdot\boldsymbol{\ell}\right)v_j\left(\mathbf{r}\right)$$

and

$$\begin{aligned} v_i'(\mathbf{r}) &= \left(\delta_{ij} - i\omega_k M_{ij}^k\right)\left(1 - i\boldsymbol{\omega}\cdot\boldsymbol{\ell}\right)v_j\left(\mathbf{r}\right) \\ &= \left(\delta_{ij} - \delta_{ij}i\boldsymbol{\omega}\cdot\boldsymbol{\ell} - i\omega_k M_{ij}^k\right)v_j\left(\mathbf{r}\right) \end{aligned}$$

or

$$\mathbf{J} = \hat{\boldsymbol{\ell}} + \hat{\mathbf{s}}$$

where

$$\begin{aligned} \hat{s}^k v_i\left(\mathbf{r}\right) &= M_{ij}^k v_j\left(\mathbf{r}\right) \\ \hat{\boldsymbol{\ell}} v_i\left(\mathbf{r}\right) &= \left(\mathbf{r}\times\frac{\nabla}{i}\right)v_i\left(\mathbf{r}\right) \end{aligned}$$

The commutation relations of the $\hat{\mathbf{s}}$ operators is clearly that of the generators of rotation (the matrices M)

$$\left[\hat{s}^i, \hat{s}^j\right] = i\epsilon_{ijk}\hat{s}^k$$

and, furthermore they commute, with the orbital angular momentum (the matrices M do not depend on $\mathbf{r}$). We see that a vector field, such as a velocity has intrinsic angular momentum, or *spin*. From the quantum mechanical point of view, one can say that the orbital angular momentum commutation relations do not imply that $\boldsymbol{\ell}$ is the generator of rotations. One can always add to $\boldsymbol{\ell}$ and operator $\hat{\mathbf{s}}$ that commutes with the former and satisfies the same algebra as $\boldsymbol{\ell}$. The sum $\hat{\boldsymbol{\ell}} + \hat{\mathbf{s}}$ has the commutation relations of rotation generators.

In a situation analogous the the classical velocity field, the wave function would have three components $\Psi(\mathbf{r}) = [\psi_1(\mathbf{r}), \psi_2(\mathbf{r}), \psi_3(\mathbf{r})]^T$ and

$$\hat{J}^k \Psi(\mathbf{r}) = \left(\mathbf{r} \times \frac{\nabla}{i}\right) \mathbf{M}^k \cdot \begin{bmatrix} \psi_1(\mathbf{r}) \\ \psi_2(\mathbf{r}) \\ \psi_3(\mathbf{r}) \end{bmatrix}$$

Such a particle is called a vector particle and has spin quantum number $s = 1$ because its components transform as the components of the $j = 1$ representation.

In summary, as long as

$$\left[\hat{s}^k, \hat{s}^l\right] = i\epsilon_{klm}\hat{s}^m \tag{194}$$

$$\left[\hat{l}^k, \hat{l}^l\right] = i\epsilon_{klm}\hat{l}^m \tag{195}$$

and

$$\left[\hat{s}^k, \hat{l}^l\right] = 0 \tag{196}$$

the operator $\hat{\mathbf{j}} := \hat{\mathbf{s}} + \hat{\mathbf{l}}$ obeys

$$\left[\hat{j}^k, \hat{j}^l\right] = i\epsilon_{klm}\hat{j}^m \tag{197}$$

and is the rotation generator.

In quantum mechanics, in addition to the scalar, vector and tensor fields of classical physics, we also have spinor fields, of half-integer spin, as follows from the existence of such irreducible representations of the rotation group.

7.1. Rotation matrices for spin 1/2.

A spin 1/2 particle will have a wave-function of the form

$$\Psi(\mathbf{r}) = \begin{bmatrix} \psi_1(\mathbf{r}) \\ \psi_2(\mathbf{r}) \end{bmatrix}$$

and

$$\hat{J}^k \Psi(\mathbf{r}) = \left(\mathbf{r} \times \frac{\nabla}{i}\right) \boldsymbol{S}^k \begin{bmatrix} \psi_1(\mathbf{r}) \\ \psi_2(\mathbf{r}) \end{bmatrix}$$

where the $\mathbf{S}^k$, $k = x, y, x$ are 2×2 matrices that obey the angular momentum relations[4]

$$\left[\mathbf{S}^k, \mathbf{S}^l\right] = i\epsilon_{klm}\mathbf{S}^m \tag{198}$$

Since we know there eigenvalues to be $\pm 1/2$ is is customary to define $\sigma^k = 2\mathbf{S}^k$ so that the eigenvalues of the σ^k are ± 1 and therefore $\left(\sigma^k\right)^2 = 1$. We know, of course that these are the famed Pauli matrices, from any quantum mechanics beginner course, but is is still instructive to derive them in general terms.

[4]We are keeping our notation of representing matrices by bold capitals. So $\mathbf{S}^k$ is the kth component of a vector of Matrices

Exercise 6.
Determine the Pauli matrices with the following suggested steps: (a) Choose to determine the matrices σ^k in the basis where σ^z is diagonal. (b) Use the commutation relations to prove that in any eigenstate of σ^z, $\langle\sigma^x\rangle = \langle\sigma^y\rangle = 0$;(c) write general expressions of $\sigma^{x,y}$ compatible with these results. Use the commutation relations to fix the form of σ^x and σ^y.

We recall them, built in the basis of eigenstates of σ^z

$$\sigma^z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \tag{199}$$

$$\sigma^x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \tag{200}$$

$$\sigma^y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \tag{201}$$

It is a simple exercise to check to prove that $\sigma^k/2$ satisfy Eqs. (198). Furthemore since $\left(\sigma^k\right)^2 = 1$ the finite rotation matrices can be calculated in a straightforward manner (α the rotation angle) :

$$\begin{aligned} \hat{U}_{1/2}(\boldsymbol{\omega}) = e^{-i\alpha(\mathbf{n}\cdot\boldsymbol{\sigma})/2} &= \sum_{r=0}^{\infty} \frac{(-i\alpha/2)^r}{r!}(\mathbf{n}\cdot\boldsymbol{\sigma})^r \\ &= \sum_{p=0}^{\infty} \frac{(-i\alpha/2)^{2p}}{(2p)!}\mathbf{1} + (\mathbf{n}\cdot\boldsymbol{\sigma})\sum_{p=0}^{\infty} \frac{(-i\alpha/2)^{2p+1}}{(2p+1)!} \end{aligned} \tag{202}$$

And

$$\begin{aligned} e^{-i\alpha/2} = \sum_{r=0}^{\infty} \frac{(-i\alpha/2)^r}{r!} &= \sum_{r=0}^{\infty} \frac{(-i\alpha/2)^{2p}}{2p!} + \sum_{p=0}^{\infty} \frac{(-i\alpha/2)^{2p+1}}{(2p+1)!} \\ \cos(\alpha/2) - i\sin(\alpha/2) & \end{aligned} \tag{203}$$

Equating real and imaginary parts

$$\cos(\alpha/2) = \sum_{r=0}^{\infty} \frac{(-i\alpha/2)^{2p}}{2p!} \tag{204}$$

$$-i\sin(\alpha/2) = \sum_{p=0}^{\infty} \frac{(-i\alpha/2)^{2p+1}}{(2p+1)!} \tag{205}$$

e

$$\hat{U}_{1/2}(\boldsymbol{\omega}) = \cos(\alpha/2)\mathbf{1} - i\sin(\alpha/2)(\mathbf{n}\cdot\boldsymbol{\sigma}) \tag{206}$$

The matrix

$$\hat{U}_{1/2}(\boldsymbol{\omega})\,|1/2,m\rangle = \sum_{m'} D^{1/2}_{m'm}\,|1/2,m'\rangle$$

$$D^{1/2}_{m'm}(\boldsymbol{\omega}) = \langle 1/2,m'|\,\hat{U}_{1/2}(\boldsymbol{\omega})\,|1/2\,m\rangle = \cos(\alpha/2)\delta_{mm'} - i\sin(\alpha/2)(\mathbf{n}\cdot\boldsymbol{\sigma}_{m'm})$$

$$\begin{aligned} D^{1/2}(\boldsymbol{\omega}) &= \cos(\alpha/2)\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} - i\sin(\alpha/2)\begin{bmatrix} n_z & n_x - in_y \\ n_x + in_y & -n_z \end{bmatrix} \\ &= \cos(\alpha/2)\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} - i\sin(\alpha/2)\begin{bmatrix} n_z & n_x - in_y \\ n_x + in_y & -n_z \end{bmatrix} \\ &= \cos(\alpha/2)\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} - i\sin(\alpha/2)\begin{bmatrix} \cos\theta & e^{-i\phi}\sin\theta \\ e^{i\phi}\sin\theta & -\cos\theta \end{bmatrix} \end{aligned} \tag{207}$$

2π rotation

$$D^{1/2}(\boldsymbol{\omega}) = \cos(\pi)\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} = \begin{bmatrix} -1 & 0 \\ 0 & -1 \end{bmatrix} \tag{208}$$

So for $\alpha = \sqrt{\boldsymbol{\omega}\cdot\boldsymbol{\omega}} = 2\pi$

$$\hat{U}_{1/2}(\boldsymbol{\omega})\,|\psi\rangle = -\,|\psi\rangle\,; \tag{209}$$

This result could have been obtained more simply. For a rotation about Oz (and any axis can be chose to be Oz)

$$\hat{U}_J(0,0,\alpha) = e^{-i\alpha\hat{J}^z}$$

So in the $\hat{J}^z$ basis

$$\hat{U}_J(0,0,\alpha)\,|j,m\rangle = e^{-i\alpha m}\,|j,m\rangle$$

If j is half-integer so is any m and

$$\hat{U}_J(0,0,2\pi)\,|j,m\rangle = e^{-i2\pi m}\,|j,m\rangle = -\,|j,m\rangle$$

This means $\hat{U}_J(0,0,2\pi) = -\hat{\mathbf{1}}$, since this is a basis. Hence, under a 2π rotation any system with half-integer spin undergoes a phase change of π. Note that is is still the same physical state, so no observable properties change.

8. $SO(3)$ and $SU(2)$

The matrix $D^{1/2}(\boldsymbol{\omega})$, was parametrized by the 3 components of $\boldsymbol{\omega} = \theta\hat{\boldsymbol{\omega}}$. A unit vector can be specified by a point on a unit sphere, *i.e.,* by two angles, a latitude $\beta \in [0,\pi]$ and a longitude $\phi \in [0,2\pi[$. A different choice of three angles, the Euler angles, proves to be more convenient for calculations. It is illustrated in Fig.1. One starts by rotating about Oz by the angle between Ox and $\mathbf{N}$, the normal to the YZ plane; rotating about $\mathbf{N}$ by β, maps $Oz \to OZ$; a final rotation by γ about OZ, maps $\mathbf{N} \to OX$. We can write the sequence of these three rotations as

$$\mathbf{R}(\alpha,\beta,\gamma) = \mathbf{R}(\gamma\hat{\mathbf{e}}_Z)\cdot\mathbf{R}(\beta\mathbf{N})\cdot\mathbf{R}(\alpha\hat{\mathbf{e}}_z) \tag{210}$$

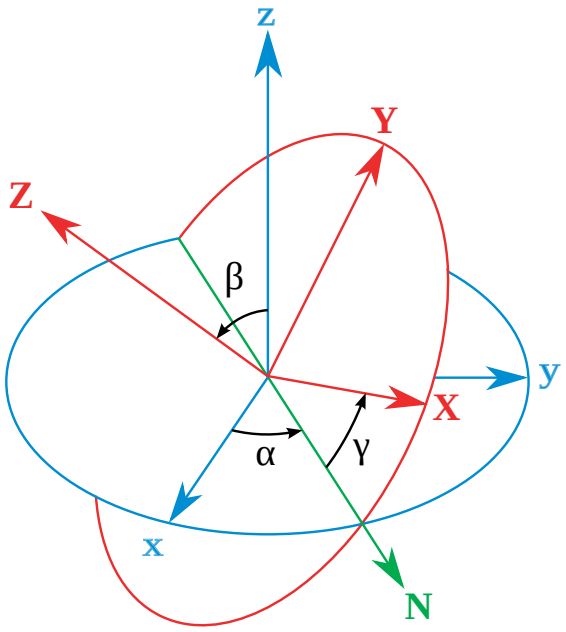

Figure 1: Euler angles parametrization of the rotation from $(x, y, x) \rightarrow (X, Y, Z)$ (source: Wikipedia, by Lionel Brits.

As before the range of these angles is $\alpha \in [0, 2\pi[$, $\beta \in [0, \pi]$ and $\gamma \in [0, 2\pi[$. Remarkably, it is possible to write this as a sequence of three rotations about the three original axis Ox, Oy and Oz. All one has to do is to relate rotations about different axis using

$$\mathbf{R}(\boldsymbol{\omega}') = \mathbf{R}(\alpha) \cdot \mathbf{R}(\boldsymbol{\omega}) \cdot \mathbf{R}^T(\alpha) \tag{211}$$

if the rotation $\mathbf{R}(\alpha)$ maps $\boldsymbol{\omega} \rightarrow \boldsymbol{\omega}$'; in plain English, we can rotate about $\boldsymbol{\omega}'$ by first rotating $\boldsymbol{\omega}' \rightarrow \boldsymbol{\omega}$, rotate about $\boldsymbol{\omega}$ and then rotate back $\boldsymbol{\omega} \rightarrow \boldsymbol{\omega}'$.

Exercise 7.
If you require formal proof of intuitive results, you can try to prove Eq.211 as follows. Define

$$\mathbf{N}(\theta) = \mathbf{R}(\alpha) \cdot \mathbf{R}(\theta\boldsymbol{\omega}) \cdot \mathbf{R}^T(\alpha)$$

Differentiate with respect to to θ, and use the fact that the generator matrices transform as vectors, to prove that $\mathbf{N}(\theta) = \mathbf{R}(\theta\hat{\boldsymbol{\omega}}')$, where $\mathbf{R}(\alpha)$ maps $\boldsymbol{\omega} \rightarrow \boldsymbol{\omega}'$.

Using Eq.(211), we write

$$\mathbf{R}(\gamma\hat{\mathbf{e}}_Z) = \mathbf{R}(\beta\mathbf{N}) \cdot \mathbf{R}(\gamma\hat{\mathbf{e}}_z) \cdot \mathbf{R}^T(\beta\mathbf{N})$$
$$\mathbf{R}(\beta\mathbf{N}) = \mathbf{R}(\alpha\hat{\mathbf{e}}_z) \cdot \mathbf{R}(\beta\hat{\mathbf{e}}_x) \cdot \mathbf{R}^T(\alpha\hat{\mathbf{e}}_z)$$

leads to

$$\mathbf{R}(\alpha, \beta, \gamma) = \mathbf{R}(\alpha\hat{\mathbf{e}}_z) \cdot \mathbf{R}(\beta\hat{\mathbf{e}}_x) \cdot \mathbf{R}(\gamma\hat{\mathbf{e}}_z) \tag{212}$$

In quantum mechanics textbooks (and tables) you will generally find a different version

$$\mathbf{R}(\alpha,\beta,\gamma) = \mathbf{R}(\alpha\hat{\mathbf{e}}_z)\cdot\mathbf{R}(\beta\hat{\mathbf{e}}_y)\cdot\mathbf{R}(\gamma\hat{\mathbf{e}}_z) \tag{213}$$

This is obtained if α is the rotation that maps Oy to $\mathbf{N}$, the normal to the OzZ plane, and so

$$\mathbf{R}(\beta\mathbf{N}) = \mathbf{R}(\alpha\hat{\mathbf{e}}_z)\cdot\mathbf{R}(\beta\hat{\mathbf{e}}_y)\cdot\mathbf{R}^T(\alpha\hat{\mathbf{e}}_z)$$

In the $\hat{J}^z$ basis the rotation about Oz is a diagonal matrix

$$\hat{U}(\gamma\hat{\mathbf{e}}_z)\left|j,m\right\rangle = e^{-i\gamma\hat{J}^z}\left|j,m\right\rangle = e^{-im\gamma}\left|j,m\right\rangle$$

and so

$$D^J_{mm'}(\alpha,\beta,\gamma) = e^{-i(m\alpha+m'\gamma)}D^J_{mm'}(0,\beta,0)$$

with

$$D^J_{mm'}(0,\beta,0) = \left\langle jm\right| e^{-i\beta\hat{J}^y}\left|j,m'\right\rangle$$

For $j=1/2$ this is easily calculated

$$\begin{aligned} D^{1/2}_{mm'}(0,\beta,0) &= \left\langle \frac{1}{2},m\right| e^{-i(\beta/2)\sigma^y}\left|\frac{1}{2},m'\right\rangle \\ &= \cos(\beta/2)\,\delta_{mm'} - i\sin(\beta/2)\left\langle \frac{1}{2},m\right|\sigma^y\left|\frac{1}{2},m'\right\rangle \end{aligned}$$

or

$$\mathbf{D}^{1/2}(0,\beta,0) = \begin{bmatrix} \cos(\beta/2) & -\sin(\beta/2) \\ \sin(\beta/2) & \cos(\beta/2) \end{bmatrix}$$

and

$$\mathbf{D}^{1/2}(\alpha,\beta,\gamma) = \begin{bmatrix} e^{-i(\alpha+\gamma)/2}\cos(\beta/2) & -e^{-i(\alpha-\gamma)/2}\sin(\beta/2) \\ e^{i(\alpha-\gamma)/2}\sin(\beta/2) & e^{i(\alpha+\gamma)/2}\cos(\beta/2) \end{bmatrix} \tag{214}$$

One of the advantages of this parametrization is that it shows more naturally a very important result. This is the *most general* 2×2 unitary matrix with determinant 1, the $SU(2)$ group. Any element of $SU(2)$ uniquely defines a rotation in $SO(3)$. The reverse is not true because the the rotation by 0 and 2π are the same element in $SO(3)$ and correspond to two different matrices in $SU(2)$, the identity and minus the identity. Nevertheless, the algebra of generators is the same.

Exercise 8.
A general 2×2 matrix has the form

$$\begin{bmatrix} a & b \\ c & d \end{bmatrix}$$

where the entries are, in general, complex. If it is unitary, the column vectors $[a,c]^T$ and $[b,d]$ have to be orthonormal. The determinant is $ad-cb$.Hence for an matrix of $SU(2)$

$$\begin{aligned} |a|^2 + |c|^2 &= 1 \\ |b|^2 + |d|^2 &= 1 \\ a^*b + c^*d &= 0 \\ ad - cb &= 1 \end{aligned}$$

Show that these conditions allow you to parametrize the entries by 3 real angles, and the matrix can be reduced to the form of Eq.(214)

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9. Irreducible tensor operators

It is not just states that transform under rotations. The same happens with observables.

$$\hat{A} \to \hat{A}_g = \hat{U}(g)\hat{A}\hat{U}^\dagger(g) \tag{215}$$

This map is linear in $\hat{A}$. This begs the question of whether we can find operator sets transforming according to the irreducible representations of $SO(3)$. Since we derived the representations exclusively from the commutation relations of the generators, they do not depend on the nature of the objects which we are transforming. We know that

$$U(\boldsymbol{\omega})\,|j,m\rangle = \sum_{m'} D^J_{m'm}(\boldsymbol{\omega})\,\left|j,m'\right\rangle \tag{216}$$

where the matrices $D^J_{m'm}(\boldsymbol{\omega})$ can, in principle, be obtained from the angular momentum relations of Eqs. (182) and (183). For an infinitesimal transformation we derived

$$\hat{J}^r\,|j,m\rangle = \sum_{m'} N^r_{m'm}\left|j,m'\right\rangle; \qquad r = x,y,z \tag{217}$$

These equations, and the matrices $N^r_{m'm}$ are determined by the usual relations

$$J^z\,|j,m\rangle = m\,|j,m\rangle \tag{218}$$

$$J^\pm\,|j,m\rangle = \sqrt{j(j+1-m(m\pm1)}\,|j,m\pm1\rangle \tag{219}$$

A set of $2k+1$ operators $\hat{T}^k_q$, k integer or semi-integer[5], and $q=-k,\ldots,k$ will define the $j=k$ representation if

$$U(\boldsymbol{\omega})\hat{T}^k_q\hat{U}^\dagger(g) = \sum_{q'} D^k_{q'q}(\boldsymbol{\omega})\hat{T}^k_{q'} \tag{220}$$

Of course, this must hold also for infinitesimal transformations. For states this means

$$\hat{J}^r\,|j,m\rangle = \sum_{m'} N^r_{m'm}\left|j,m'\right\rangle, \tag{221}$$

whereas for operators

$$(1-i\boldsymbol{\omega}\cdot\mathbf{J})\,\hat{T}^k_q\,(1-i\boldsymbol{\omega}\cdot\mathbf{J}) = \hat{T}^k_q - i\omega^r\left[\hat{J}^r,\hat{T}^k_q\right] \tag{222}$$

[5] I am not aware of any examples of operator sets with k semi-integer.

and so to get the same representation

$$\left[\hat{J}^r, \hat{T}^k_q\right] = \sum_{m'} N^r_{q'q} T^k_{q'} \tag{223}$$

with the same matrix as in Eq.(217). This is only possible if

$$\left[\hat{J}^z, \hat{T}^k_q\right] = q\hat{T}^k_q \tag{224}$$

$$\left[\hat{J}^\pm, \hat{T}^k_q\right] = \sqrt{k(k+1) - q(q\pm 1)}\hat{T}^k_{q\pm 1} \tag{225}$$

There equations define the set of operators as a *irreducible tensor operator* (ITO), *i.e.* a basis for an irreducible representation of $SO(3)$with $j = k$.

9.1. Examples: scalar and vector operators

If $k = 0$, one must have $q = 0$ and the definition of ITO becomes

$$\left[\hat{J}^z, \hat{T}^0_0\right] = 0 \tag{226}$$

$$\left[\hat{J}^\pm, \hat{T}^0_0\right] = 0 \tag{227}$$

This precisely how we defined a scalar operator. This is not surprising: a scalar operator being invariant under rotation generates the 1D identity representation.

A less trivial example is a vector operator. For the cartesian components,

$$\left[\hat{J}^r, \hat{V}^s\right] = i\epsilon_{rst}\hat{V}^t \tag{228}$$

There is no doubt that this is a dim = 3 representation. But is it the $j = 1$ irreducible one? Th answer is yes, first by the fact that there is no linear combination of vector components invariant under rotations. But we can also show this explicitly by writing linear combinations of the cartesian components that transform according to the definition of ITO. These are the so-called spherical components of a vector

$$\hat{T}^1_0 = \hat{V}^z \tag{229}$$

$$\hat{T}^1_1 = -\frac{1}{\sqrt{2}}\left(\hat{V}^x + i\hat{V}^y\right) \tag{230}$$

$$\hat{T}^1_{-1} = \frac{1}{\sqrt{2}}\left(\hat{V}^x - i\hat{V}^y\right) \tag{231}$$

Exercise 9.

Show that the spherical components of a vector operator satisfy the commutation relations of Eqs.(224) and (225) for $k = 1$.

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10. Product of representations

10.1. Two spin 1/2 systems

Take a atom with filled shell and add an electron in s ($l = 0$) orbital state. This could be, for instance the Na atom with configuration $11s^2 2s^2 2p^6 3s^1$. Discarding all the quantum numbers which are fixed, we can denote its basis as states as $\{|\sigma_1\rangle ; \sigma_i = \uparrow, \downarrow\}$. But if we have two such atoms our space of states will be a product space with dimension 4 and a basis

$$\mathcal{B} = \{|\sigma_1\rangle \otimes |\sigma_2\rangle = |\sigma_1, \sigma_2\rangle ; \sigma_i = \uparrow, \downarrow\}$$

A spin rotation will rotate each spin accordind to the $j = 1/2$ representation

$$\hat{U}(\boldsymbol{\omega}) |\sigma_1, \sigma_2\rangle = \hat{U}^{(1)}(\boldsymbol{\omega}) |\sigma_1\rangle \otimes \hat{U}^{(2)}(\boldsymbol{\omega}) |\sigma_2\rangle = D^{1/2}_{\sigma_1' \sigma_1'} D^{1/2}_{\sigma_2' \sigma_2} \left|\sigma_1', \sigma_2'\right\rangle$$

It is clear that this product space $\mathcal{E}_1 \otimes \mathcal{E}_2$ generates another, 4 dimensional, representation of $SO(3)$, with matrices

$$\left\langle \sigma_1', \sigma_2' \right| \hat{U}(\boldsymbol{\omega}) |\sigma_1, \sigma_2\rangle = D^{1/2}_{\sigma_1' \sigma_1'} D^{1/2}_{\sigma_2' \sigma_2}$$

This is called a product representation of the ones generated by each of the two invariant spaces, $\mathcal{E}_1$ and $\mathcal{E}_2$.

This is a rather general way of building representations. The most common way to build the space of states of a physical system is by taking tensor products of states of simpler sub-systems. Each subsystem comes with its vector space of states $\mathcal{E}_1$ and $\mathcal{E}_2$ and its sets of observables $\hat{A}^{(1)}, \hat{B}^{(1)}, \ldots$ and $\hat{P}^{(2)}, \hat{Q}^{(2)}, \ldots$ and a basis for the product space $\mathcal{E}_1 \otimes \mathcal{E}_2$ is

$$|i, j\rangle = \left|\phi_i^{(1)}\right\rangle \otimes \left|\psi_j^{(2)}\right\rangle$$

where $\left|\phi_i^{(1)}\right\rangle$, $\left|\psi_j^{(2)}\right\rangle$, $i, j = 1, 2, \ldots$ are basis of $\mathcal{E}_1$ and $\mathcal{E}_2$. The operators defined in $\mathcal{E}_1$ and $\mathcal{E}_2$ naturally extend to the product space by

$$\begin{aligned} \hat{A}^{(1)} \to \hat{A}; \qquad & \hat{A} |i, j\rangle = \left(\hat{A}^{(1)} \left|\phi_i^{(1)}\right\rangle\right) \otimes \left|\psi_j^{(2)}\right\rangle \\ \hat{P}^{(2)} \to \hat{P}; \qquad & \hat{P} |i, j\rangle = \left|\phi_i^{(1)}\right\rangle \otimes \left(\hat{P}^{(2)} \left|\psi_j^{(2)}\right\rangle\right) \end{aligned}$$

Imagine now that $\mathcal{E}_1$ and $\mathcal{E}_2$ are invariant spaces under a symmetry group like $SO(3)$ so that

$$\begin{aligned} \hat{U}^{(1)}(\boldsymbol{\omega}) \left|\phi_i^{(1)}\right\rangle &= M_{ij}^{(1)}(\boldsymbol{\omega}) \left|\phi_j^{(1)}\right\rangle \\ \hat{U}^{(2)}(\boldsymbol{\omega}) \left|\psi_i^{(2)}\right\rangle &= N_{ij}^{(2)}(\boldsymbol{\omega}) \left|\psi_j^{(2)}\right\rangle \end{aligned}$$

In the composite system, of space of states $\mathcal{E}_1 \otimes \mathcal{E}_2$ the symmetry transformation is $\hat{U}(\boldsymbol{\omega}) = \hat{U}^{(1)}(\boldsymbol{\omega}) \otimes \hat{U}^{(2)}(\boldsymbol{\omega})$ and

$$\begin{aligned} \hat{U}(\boldsymbol{\omega}) |i, j\rangle &= \hat{U}^{(1)}(\boldsymbol{\omega}) \left|\phi_i^{(1)}\right\rangle \otimes \hat{U}^{(2)}(\boldsymbol{\omega}) \left|\psi_i^{(2)}\right\rangle \\ &= M_{ik}^{(1)}(\boldsymbol{\omega}) N_{jl}^{(2)}(\boldsymbol{\omega}) |k, l\rangle \end{aligned}$$

s_1^z	s_2^z	$m = \sigma_1 + \sigma_2$
1/2	1/2	1
1/2	-1/2	0
-1/2	1/2	0
-1/2	-1/2	-1

Table 2: Total S^z eigenvalues for two spin 1/2 particles

This shows that the basis $\{|i,j\rangle, i = 1,\dots; j = 1,\dots\}$ generates a representation with the matrices

$$Q_{(ij),(kl)}(\boldsymbol{\omega}) := \langle i,j|\hat{U}(\boldsymbol{\omega})|k,l\rangle := M^{(1)}_{ik}(\boldsymbol{\omega}) N^{(2)}_{jl}(\boldsymbol{\omega}).$$

This is called the *product of* the representations corresponding to the matrices $\mathbf{M}^{(1)}(\boldsymbol{\omega})$ and $\mathbf{N}^{(2)}(\boldsymbol{\omega})$. In terms of infinitesimal generators

$$\begin{aligned}\hat{U}(\boldsymbol{\omega}) &= \left(1 - i\omega_k \hat{M}^k\right) \otimes \left(1 - i\omega_k \hat{N}^k\right) \\ &= 1 - i\omega_k \left(\hat{M}^k + \hat{N}^k\right) + \mathcal{O}\left(\omega^2\right)\end{aligned}$$

which shows the the generator of the product representation is the *sum* of the generators. In the case of $SO(3)$, the problem of product of representations is, therefore, the problem of *addition* of angular momenta.

Let us step back to the problem of two spins 1/2. The 4-dimensional product representation is either irreducible, or a sum of irreducible representations. In the first case that would mean the the spin of the composite system would be $S = 3/2$. That would imply the existence of 4 states with eigenvalues of $S^z = s_1^z + s_2^z$, $m_s = \pm 3/2, \pm 1/2$. But we know that the basis states, $|\sigma_1, \sigma_2\rangle$ are eigenstates of s_1^z and s_2^z and these operators commute. So we can list immediately the eigenvalues of S^2, shown in Table 2

By simple inspection we notice that this can only be a direct sum of $S = 1$ and $S = 0$ representations. For one, the maximum value of S^z is 1, so there is no representation with $S > 1$ and there must therefore be one with $S = 1$. The corresponding basis must contain the states with $S^z = \pm 1$, ($|\uparrow,\uparrow\rangle$ and $|\downarrow,\downarrow\rangle$) and a linear combination of the two states states of $S^z = 0$. Removing these 3 states of the $S = 1$ representation, leaves only one state with $S^z = 0$, which must therefore define a $S = 0$ representation. We conclude that this is a direct sum of $S = 1$ and $S = 0$ representations.

$$1/2 \otimes 1/2 = 1 \oplus 0$$

This is an example of the celebrated *theorem of addition of angular momenta.* A similar counting argument leads easily to the statement that

$$j_1 \otimes j_2 = (j_1 + j_2) \oplus (j_1 + j_2 - 1) \oplus \cdots \oplus |j_1 - j_2| \tag{232}$$

This still begs an important question. How do we *reduce the representation?* In other words, how do we determine the states that form the basis of the irreducible representations?

The state of the representation J with eigenstate M of $\hat{J}^z$ is linear combination of the product basis

$$|J,M\rangle = \sum_{m_1,m_2} C^{j_1 j_2 J}_{m_1 m_2 M} |j_1,m_1\rangle \otimes |j_2,m_2\rangle$$

where

$$C^{j_1 j_2 J}_{m_1 m_2 M} := \langle j_1,m_1;j_2,m_2|J.M\rangle$$

Both states in this product are eigenstates of S^z with eigenvalues m_1+m_2 and M,so

$$C^{j_1 j_2 J}_{m_1 m_2 M} = 0 \qquad \text{if } M \neq m_1+m_2$$

and by Eq.(232).

$$J \in \{j_1+j_2, j_1+j_2-1, \ldots, |j_1-j_2|\}$$

The amplitudes $C^{j_1 j_2 J}_{m_1 m_2 M}$ are the *Clebsh-Gordan* (CG) coefficients. As implied by the notation, they are independent of any any quantum numbers characterizing the states, other than the angular momentum ones. It is irrelevant whether we are speaking of one or many particle states, of spin or orbital angular momentum, etc.

Exercise 10.

You can determine the CG coefficients for $j_1 = j_2 = 1/2$ and $J = 0,1$ in the following way: (a) The $J = 1, M = 1$ is $|\uparrow,\uparrow\rangle$. Why? (b) use the J^- operator to determine the state of the same representation with $M = 0$. (c) Apply again J^- to obtain the $J = 1, M = -1$, state. Is it what you expected? (d) The $J = 0$, state must be orthogonal to the the one with $J = 1$,$M = 0$. If you further require that $C^{1/2,1/2,0}_{1/2,-1/2,0}$ be real and positive, you should be able to complete the determination of all $C^{1/2,1/2,J}_{m_1,m_2 M}$.

The CG coefficients can be determined systematically from two recursion relations derived in Appendix B

$$C^{j_1 j_2;J}_{m,m',J} = -\frac{c_-(j_2,m')}{c_+(j_1,m)} C^{j_1 j_2;J}_{m+1,m'-1,J} \tag{233}$$

$$C^{j_1,j_2;J}_{m,m';M-1} == \frac{c_-(j_1,m+1)}{c_-(J,M)} C^{j_1 j_2;J}_{m+1 m';M} + \frac{c_-(j_2,m'+1)}{c_-(J,M)} C^{j_1 j_2;J}_{m,m'+1;M} \tag{234}$$

With no loss of generality we can assume $j_1 \geq j_2$. Using Eq.256 we can express all $C^{j_1 j_2;J}_{m,J-m,J}$ in terms of $C^{j_1 j_2;J}_{j_1,J-j_1,J}$; we choose this coefficient to be positive and determine its value by the normalization of the state

$$|J,J\rangle = \sum_m C^{j_1 j_2;J}_{m,J-m,J} |j_1,m;j_2,J-M\rangle$$

$$\sum_m \left(C^{j_1 j_2;J}_{m,J-m,J}\right)^2 = 1$$

Once these coefficients are determined for $M = J$, one uses the relation of Eq.(257) to find the remaining coefficients.

Exercise 11.
Use the recursion relations to find all CG coefficients and reduce the $1 \otimes 1/2$ product representation to the corresponding irreducible ones.

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11. Applications

11.1. Atomic Spectroscopy

Our basic understanding of spectra of multi-electron atoms is based on approximations whereby electrons are assumed to move in effective one-electron potentials, assumed to have rotational invariance. The one electron solutions are angular momentum eigenstates, characterized by the usual quantum numbers l,and m, and many body states are built by occupying some of these orbitals. For partially filled shells, these *electronic configurations* actually refer to a degenerate subspace and interactions and perturbations like spin-orbit coupling lift these degeneracies. Unsurprisingly, spin-independent interactions give rise to eigenstates characterized by total orbital angular momentum and spin quantum numbers

$$\hat{\mathbf{L}} = \sum_i \hat{l}_i$$
$$\hat{\mathbf{S}} = \sum_i \hat{\mathbf{s}}_i$$

since invariance under rotations is preserved by interactions, and in the absence of spin-orbit coupling, the Hamiltonian commutes with $\hat{\mathbf{S}}$ and therefore with $\hat{\mathbf{L}}$ (since it commutes with $\hat{\mathbf{J}} = \hat{\mathbf{L}} + \hat{\mathbf{S}}$). The famous Hund's rules, are semi-empirical statements that predict the values of S and L of the levels with lower energy, using angular momentum addition rules for each configuration.

First Hund rule: The value of S is the largest possible of the configuration manifold;

Second Hund rule: The value of L is the largest possible of the configuration manifold, compatible with the first rule.

As an example a $1s^2 2s^2 2p^2$ configuration would have $S = 1$,and $L = 1$, as follows from the enumeration of the two electron states in p orbitals. It is already obvious from this partial enumeration of Table 3 that the are terms with $L = 1$ and $S = 0$ and $S = 1$.

Spin-orbit coupling is a relativistic correction that expresses the fact that in the electron reference frame the electric field of the nucleus is seen as a magnetic filed that interacts with the spin

$$\mathcal{H}_{so} = \alpha_{so} \sum_i \hat{\mathbf{s}}_i \cdot \hat{\mathbf{l}}_i$$

m_l	m_s	n_l	n_l	M_s	M_l
1	1/2	0	1/2	1	1
1	1/2	0	-1/2	0	1
1	-1/2	0	1/2	0	1
1	-1/2	0	-1/2	-1	1
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$

Table 3: Multiplets in a $2p^2$ configuration

The nuclear charge, in the reference frame of the electron, has an angular velocity parallel to $\hat{\mathbf{l}}_i$ and creates a magnetic field also parallel to $\hat{\mathbf{l}}_i$; as the electron magnetic moment is opposite to $\hat{\mathbf{s}}_i$, the constant α_{so} is positive and favors anti-parallel alignment of spin and orbital angular momentum.

When the shell is less than half-filled, the state with spin projection $M_s = S$ and $S = n_e/2$, the ground state, by the first Hund rule, is obviously symmetric under exchange of electrons. It is just the product state

$$|\psi\rangle = \left| \overbrace{\uparrow, \uparrow \ldots \uparrow}^{n_e} \right\rangle \otimes |\text{orbital state}\rangle$$

The states with the same S and different M_s are obtained by applying the $\hat{S}^- = \sum_i \hat{s}_i^-$ and remain symmetrical. In this manifold, when doing first order degenerate perturbation theory we can replace

$$\mathbf{s}_i \to \frac{\mathbf{S}}{n_e}$$

and

$$\mathcal{H}_{so} = \alpha_{so} \sum_i \hat{\mathbf{s}}_i \cdot \hat{\mathbf{l}}_i \to \frac{\alpha_{so}}{n_e} \sum_i \hat{\mathbf{S}} \cdot \hat{\mathbf{l}}_i = \frac{\alpha_{so}}{n_e} \hat{\mathbf{S}} \cdot \hat{\mathbf{L}}$$

On the other hand, a shell that is more than half–filled can be seen as a completely filled shell ($L = 0, S = 0$) with holes, $n_h = 2\,(2l+1) - n_e$. The maximum spin multiplet has $S = n_h/2$. But holes are positively charged and the spin orbital coupling α_{so} changes sign. So, for more than a half filled shell, the spin orbit coupling term, in the ground multiplet is

$$\mathcal{H}_{so} = -\frac{\alpha_{so}}{n_h} \hat{\mathbf{S}} \cdot \hat{\mathbf{L}}$$

In either case, degenerate perturbation theory, if one uses angular momentum addition to determine the J possible values in the sub-space of states,

$$\{|S, M_s\rangle \otimes |L, M_L\rangle : \; M_s = -S, \ldots, S; M_L = -L, \ldots, L\}$$

becomes trivial, since

$$A\hat{\mathbf{S}} \cdot \hat{\mathbf{L}} = \frac{A}{2}\left(\hat{J}^2 - \hat{S}^2 - \hat{L}^2\right) \to \frac{A}{2}\left(\hat{J}^2 - S(S+1) - L(L+1)\right)$$

and the energy levels separate according to the value of J, as expected from full rotational symmetry. In spectroscopy one usually denotes a set of levels with given values of L , S and J as

$$^{2S+1}X_J$$

where $X = S, P, D, F$ is the usual letter notation for values of L.

The form of the spin orbit coupling accounts for the third Hund's rule:

Third Hund rule: the lowest energy level of an L, S multiplet has the smallest possible value of J if the shell is less than half-filled and the highest possible J if more than half-filled.

11.2. Selection Rules

Interaction Hamiltonian

$$\hat{V}(t) = (-e) \int d^3 r \hat{n}(r) v(\mathbf{r}, t)$$

dipole approximation

$$\begin{aligned} \hat{V}_0(t) &= (-e) \int d^3 r \hat{n}(r) v(0, t) \\ &= (-e)\, \hat{N}_e v(0, t) \end{aligned}$$

$$\begin{aligned} \hat{V}_{dip}(t) &= e\mathbf{E} \cdot \int d^3 r \hat{n}(r) \mathbf{r} \\ &= e\mathbf{E} \cdot \hat{\mathbf{p}} \end{aligned}$$

$\hat{\mathbf{p}}$ is the atomic dipole operator, and is a vector operator

$$\left\langle \beta, J', M' \right| \hat{V}_{dip}(t) \left| \alpha, J, M \right\rangle = e\mathbf{E}(t) \cdot \left\langle \beta, J', M' \right| \hat{\mathbf{p}} \left| \alpha, J, M \right\rangle$$

$\hat{\mathbf{p}} \left| \alpha, J, M \right\rangle$ belongs to the product representation $1 \otimes J = J+1 \oplus J \oplus J-1$ (unless $J = 0$). This gives the first selection rule for *electric dipole* transitions, $\Delta J = 0, \pm 1$. To obtain the other selection rules we resort to writing the scalar product of $\mathbf{p}$ and $\mathbf{E}$ in spherical components. We write

$$\mathbf{E} = (E_x, E_y, E_z)\, e^{-i\omega t} + h.c.$$

and consider complex amplitudes to encode the phase differences between the various components. Note, however, that $\mathbf{E} \cdot \mathbf{k} = 0$ where $\mathbf{k}$ is the direction of propagation of the electric field. So the three components of the radiation field cannot be specified independently.

$$\begin{aligned} (E_x \hat{p}_x + E_y \hat{p}_y + E_z \hat{p}_z) &= E_x \left(-\frac{\hat{p}_1 - \hat{p}_{-1}}{\sqrt{2}} \right) + E_y \left(\frac{\hat{p}_1 + \hat{p}_{-1}}{i\sqrt{2}} \right) + E_z \hat{p}_0 \\ &= -\frac{1}{\sqrt{2}} (E_x - iE_y)\, \hat{p}_1 - \frac{1}{\sqrt{2}} (E_x + iE_y)\, \hat{p}_{-1} + E_z \hat{p}_0 \\ &= E_z \hat{p}_0 - E^{(-)} \hat{p}_1 - E^{(+)} \hat{p}_{-1} \end{aligned}$$

we can now consider several situations, when a magnetic field $\mathbf{B} = H\hat{\mathbf{e}}_z$ splits each multiplet by the Zeeman effect

$$E(\alpha, J, M) = E_0(\alpha, J) + g_J \mu_B H M$$

1. The radiation field is linearly polarized along Oz (possible only for incidence normal to the magnetic field.

   $$\left\langle \beta, J', M' \right| \hat{V}_{dip}(t) \left| \alpha, J, M \right\rangle = eE_z(t) \left\langle \beta, J', M' \right| \hat{p}_0 \left| \alpha, J, M \right\rangle$$

   Since $\hat{p}_0 \left| \alpha, J, M \right\rangle$ has the angular momentum quantum number of the product state $\left| 1, 0 \right\rangle \otimes \left| \alpha, J, M \right\rangle$, using CG coefficients

   $$\hat{p}_0 \left| \alpha, J, M \right\rangle = \sum_{J'=J, J\pm 1} C^{1JJ'}_{0,M,M} \left| \gamma, J', M \right\rangle$$

   and

   $$\left\langle \beta, J', M' \right| \hat{p}_0 \left| \alpha, J, M \right\rangle = 0,$$

   unless

   $$\Delta M = 0 \tag{235}$$
   $$\Delta J = 0, \pm 1 \tag{236}$$

   If $J = J' = 0$, however, the matrix element is also zero, because $\hat{p}_0 \left| \alpha, 0, 0 \right\rangle$ has angular Momentum $J = 1$

2. In this case the transitions between levels J, M and J', M' have the frequencies

   $$\hbar\omega = E_0(\beta, J') - E_0(\alpha, J) + (g_{J'} - g_J)\, \mu_B H M$$

   an we have as many lines as values of M, unless $J = J'$, in which case there is no splitting of spectral lines with magnetic field.

3. The radiation field is linearly polarized along a direction orthogonal to Oz, that we choose as Ox (possible for incidence normal or parallel to the magnetic field)

   $$\begin{aligned} \left\langle \beta, J', M' \right| \hat{V}_{dip}(t) \left| \alpha, J, M \right\rangle = & -eE^{(+)}(t) \left\langle \beta, J', M' \right| \hat{p}_{-1} \left| \alpha, J, M \right\rangle \\ & - -eE^{(-)}(t) \left\langle \beta, J', M' \right| \hat{p}_1 \left| \alpha, J, M \right\rangle \end{aligned}$$

   In this case non-zero values of the transition matrix element require

   $$\begin{aligned} M' &= M \pm 1 \\ \Delta J &= 0, \pm 1 \end{aligned} \tag{237}$$

   and

   $$\hbar\omega = E_0(\beta, J') - E_0(\alpha, J) + \mu_B H \left(g_{J'} - g_J\right) M \pm \mu_B H g_{J'}$$

   Even when $J = J'$ the spectral line is split into two. Note that circularly polarized light can be obtained by choosing $E^{(+)} = 0$ or $E^{(-)} = 0$ in which case one of the lines disappears.

It should be stressed tat while these results for the matrix elements are exact, it does not mean that optical transitions cannot occur between states which violate these selection rules. Higher order expansions of the potential $v(\mathbf{r}, t)$ about $\mathbf{r} = 0$ give rise to tensor operators of higher order, which, by Wigner-Eckart theorem, have non-zero matrix elements for higher values of ΔM or ΔJ. The expansion parameter is $ka_0 \sim 2\pi a_0/\lambda$ where a_0 is of order of the Bohr radius (atom size) and λ the transition frequency. Because transitions involve the square of the matrix element the intensity ratio between, say quadrupole transitions and dipole one is expected to be of order $4\pi^2 a_0^2/\lambda^2$. Estimating

$$\hbar\omega = \frac{2\pi\hbar c}{\lambda} = \frac{\hbar^2}{2m_e a_0^2}$$

leads to

$$\begin{aligned} 2\pi\frac{a_0}{\lambda} &= \frac{\hbar}{cm_e a_0} = \frac{\hbar}{cm_e\left(\hbar/m_e c\alpha\right)} \\ &= \alpha \end{aligned}$$

where $\alpha \approx 1/137$ in the fine structure constant

$$\alpha = \frac{1}{4\pi\epsilon_0}\frac{e^2}{\hbar c}$$

12. I-spin

(...)

A. Irreducible representations from generator Algebra

$$\hat{J}_\pm := \hat{J}^x \pm i\hat{J}^y \tag{238}$$

$$\left[\hat{J}^z, \hat{J}_\pm\right] = i\hat{J}^y \pm \hat{J}^x = \pm\hat{J}_\pm \tag{239}$$

$$\left[\hat{J}_+, \hat{J}_-\right] = 2J^z \tag{240}$$

$$\begin{aligned} \hat{J}^2 &= \hat{J}_z^2 + \frac{1}{2}\left(\hat{J}_+\hat{J}_- + J_-\hat{J}_+\right) \\ &= \hat{J}_z^2 - \hat{J}_z + \hat{J}_+\hat{J}_- \end{aligned} \tag{241}$$

The commutation relations establish $\hat{J}_\pm$ as ladder operator for J_z

$$\begin{aligned} J_z J_\pm |\lambda, m\rangle &= \left(\left[\hat{J}^z, \hat{J}_\pm\right] + J_\pm J_z\right)|\lambda, m\rangle \\ &= \left(\pm\hat{J}_\pm + mJ_\pm\right)|\lambda, m\rangle \\ &= (m \pm 1)\hat{J}_\pm |\lambda, m\rangle \end{aligned} \tag{242}$$

and

$$\hat{J}_+\hat{J}_- |\lambda, m\rangle = \left(\lambda - m^2 + m\right) |\lambda, m\rangle \tag{243}$$

So

$$\langle\lambda, m| \hat{J}_+\hat{J}_- |\lambda, m\rangle = \left(\lambda - m^2 + m\right) \geq 0 \tag{244}$$

because the LHS is the norm of $\hat{J}_- |\lambda, m\rangle$ .By the same token

$$\langle\lambda, m| \hat{J}_-\hat{J}_+ |\lambda, m\rangle = \left(\lambda - m^2 - m\right) \geq 0 \tag{245}$$

To satisfy these inequalities the series of values of m must terminate at a maximum m_1 and a minimum m_2

$$\lambda - m_1(m_1 + 1) = 0 \tag{246}$$
$$\lambda - m_2(m_2 - 1) = 0 \tag{247}$$

and

$$m_1^2 - m_2^2 - (m_1 + m_2) = 0 \tag{248}$$
$$(m_1 - m_2 + 1)(m_1 + m_2) = 0 \tag{249}$$

the first factor in non zero, so

$$m_2 = -m_1 \tag{250}$$

and since values of m change by integers,

$$m_1 = j; \quad m_2 = -j \tag{251}$$

with $2j$ and integer and

$$\lambda = j(j + 1) \tag{252}$$

In summary:

- Irreducible representations of SO(3) are generated by basis of eigenvectors of $\hat{J}^2$,$\hat{J}_z$

  $$\hat{J}^2 |j, m\rangle = j(j + 1) |j, m\rangle \tag{253}$$
  $$\hat{J}_z |j, m\rangle = m |j, m\rangle ; \qquad m = -j, -j + 1, \ldots, j \tag{254}$$

  with J a positive integer of half-integer;

- The action of the ladder operators in this basis

  $$J_\pm |j, m\rangle = \sqrt{j(j + 1) - m(m \pm 1)}\, |j, m \pm 1\rangle \tag{255}$$

  showing that the basis has $2j + 1$ states.

B. Clebsh-Gordan Coefficients

The Clebsh-Gordan are build by applying systematically recursion relations. Let us sketch the procedure

1. We know that
$$|j_1 + j_1; j_1 + j_2\rangle = C^{j_1 j_2; j_1+j_2}_{j_1 j_2; j_1+j_2} |j_1, j_1; j_2, j_1\rangle$$
and we choose
$$C^{j_1 j_2 j_1+j_2}_{j_1 j_2 j_1+j_2} = 1$$

2. Using $\hat{J}^- = \hat{j}_1^- + \hat{j}_2^-$ and defining
$$\begin{aligned}\hat{J}^{\pm} |J, M\rangle &= \sqrt{J(J+1) - M(M \pm 1)}\, |J, M \pm 1\rangle \\ &= c_{\pm}(J, M) |J, M \pm 1\rangle\end{aligned}$$
we derive a recursion relation
$$\begin{aligned}c_-(J, M) |J, M-1\rangle = \sum_{m_1, m_2} C^{j_1 j_2; J}_{m_1 m_2; M} [&c_-(j_1, m_1) |j_1 m_1 - 1; j_2 m_2\rangle \\ &+ c_-(j_2, m_2) |j_1 m_1; j_2 m_2 - 1\rangle]\end{aligned}$$
Taking the inner product with $|j_1, m; j_2, m'\rangle$
$$C^{j_1, j_2; J}_{m, m'; M-1} = \frac{c_-(j_1, m+1)}{c_-(J, M)} C^{j_1 j_2; J}_{m+1 m'; M} + \frac{c_-(j_2, m'+1)}{c_-(J, M)} C^{j_1 j_2; J}_{m, m'+1; M}$$
equivalent to
$$C^{j_1 j_2; J}_{m, m'; M-1} = \frac{c_+(j_1, m)}{c_-(J, M)} C^{j_1 j_2; J}_{m+1 m; M} + \frac{c_+(j_2, m')}{c_-(J, M)} C^{j_1 j_2; J}_{m, m'+1; M} \tag{256}$$
This relation allows to move from the coefficients at M to the ones at $M-1$ (see Fig.(2)).

3. The other recursion relation is obtained by using $J^+ |J, J\rangle = 0$.
$$\begin{aligned}0 = \sum_{m, m'} C^{j_1 j_2; J}_{m, m', J} \big[&c_+(j_1, m) \big|j_1, m+1; j_2, m'\big\rangle \\ &+ c_+(j_2, m') \big|j_1, m; j_2, , m'+1\big\rangle\end{aligned}$$
giving
$$c_+(j_1, m) C^{j_1 j_2; J}_{m, m', J} + c_+(j_2, m'-1) C^{j_1 j_2; J}_{m+1, m'-1} = 0$$
which we rewrite as
$$C^{j_1 j_2; J}_{m, m', J} = -\frac{c_+(j_2, m'-1)}{c_+(j_1, m)} C^{j_1 j_2; J}_{m+1, m'-1, J}$$
and, with no loss of generality
$$C^{j_1 j_2; J}_{m, m', J} = -\frac{c_-(j_2, m')}{c_+(j_1, m)} C^{j_1 j_2; J}_{m+1, m'-1} \tag{257}$$

4.

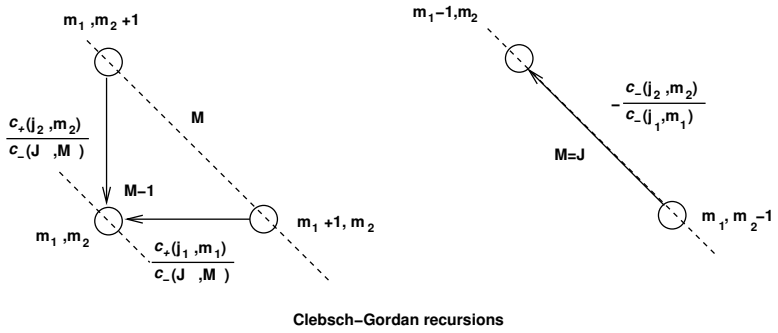

Figure 2: Clebsh- Gordan Recursion relations