3. Quantum Theory in Space-Time I-frames

Why do we need space-time descriptions? Well, quantum states are basic elements of abstract Hilbert space and as such they do not have space-time localization. Abstract quantum mechanics provides a general framework that would cover all possibilities a system may show up; it is a foundational construct but one does not get hints to construct actual models for most operators. The only thing one can require in abstract space is existence that is ensured by endowing the framework with a definite mathematical structure. But the world of laboratory experiments imposes space-time frameworks.

Real space descriptions require concepts of spatiality and temporality lying down foundational elements supporting space and time approaches construction. But its mathematical structure cannot be induced from experiments reflecting quantum phenomena in laboratory (real) space. While these levels are incommensurate mappings bridging both would do the job.

Because abstract Hilbert space is a pure mathematical structure, the task (problem) is to relate the abstract level to the laboratory world via a quantum theory incorporating aspects of space-time physics. To delineate these mappings the concept of Fence helps "interfacing" pure mathematics to real space representations; they point to selected measurable responses in laboratory world.

Laboratory benches are placed in real world space; experiments are performed at particular moments and locations; electromagnetic energy (photons) serves communication purposes; interaction outcomes have a character of events that can be recorded, read and/or used to set up further experiments; all these elements use a space-time framework. In the space separating/relating these realms (Fence) the formalism is cast in terms of elements allowing for a bridge linking real to quantum levels. Inertial frames play such a role.

In Chapter 1, abstract quantum states $|\Psi\rangle$ were projected in (mathematical) time space: the mapping $\langle t|\Psi\rangle$ corresponds to a complex function $\Psi(t)$ with argument on a real time axis. This mapping plays the role of image in time space of the abstract state $|\Psi\rangle$. The time variable is just a mathematical construct until concepts of processes are used to help introduce physical (measurable) time. Inertial frames play a double role. Firstly, they locate a given material 1-system with respect to another I-frame that may serve as a laboratory frame. Secondly, internal degrees of freedom for the 1-system permit defining the dimension of a

coordinate space that are used as labels identifying base vectors in a configuration space: $\{|x_1,x_2,x_3>\}$ as wel as reciprocal space base vectors: $\{|k_1,k_2,k_3>\}$. In Section 3.1 these spaces are examined in more detail.

At a Fence material systems are present. For electromagnetic matter, the number of electrons and nuclei defines the material system. Masses, spin and electric charge are fixed parameters for each of the n-electrons and m-nuclei defining a 1-system; electrons and protons, for instance, are endowed spin state S=1/2 each.

Axiom 5. *Configuration space projected base vectors defined via inertial coordinate systems provide labels to identify base states in Hilbert-like spaces*.

Let **x** be a vector belonging to $R^{3(n+m)}$, then $|\mathbf{x}>$ is a base vector label by this set of real numbers (coordinates). The reciprocal space, $|\mathbf{k}>$ is label with reciprocal space coordinates. Introduction of an inertial frame, I-frame, is one step towards landing the study of quantum physics (mechanics) in configuration space.

Abstract quantum states are projected in configuration space. The frames can be submitted to changes of origin and rotated with respect to another I-frame. The abstract quantum states are fully invariant towards the way we tinker with I-frames. This property is used later on to construct appropriate bases sets.

I-frames of interest are closely related to special relativity spacetime. The reason for such a choice is simple: we know how to transform events from one I-frame to another moving with relative speed **v**. The speed of light (c) is independent from the state of motion of the I-frame sustaining an internal quantum state change leading to light emission. The subtlety here is that c equals the product of wavelength (λ) and frequency (ω) and these factors do depend upon the state of motion taken independently while the product does not.

Note, the origin of its space part is located in real space with three orthogonal unit vectors: $\mathbf{i}_1$, $\mathbf{i}_2$, $\mathbf{i}_3$; this real space is located with respect to a second frame the unit orthogonal vectors are indicated by $\mathbf{i'}_1$, $\mathbf{i'}_2$, $\mathbf{i'}_3$ (laboratory frame). Inside an I-frame, there is no way to realize if it is displacing with a uniform velocity, say $\mathbf{v} \rightarrow (v_1\mathbf{i'}_1, v_2\ \mathbf{i'}_2, v_3\ \mathbf{i'}_3)$; the I-frame is hence seen in motion when sensed from another I-frame. Motion always relates at least two I-frames; for an observer it is always another I-frame that is in motion; of course one is considering a non-accelerated dynamic state.

3.1. Configuration space projected Hilbert space

Given a configuration space, the symbol **q** is used as a label to identify a quantum base state $|\mathbf{q} > = | q_1, q_2, q_3> = | q_1> |q_2> |q_3>$. A position operator $\hat{q}$ is defined in such a way that eq.(3.1.1) holds:

$$\hat{q} \mid \mathbf{q} > = \mathbf{q} \mid \mathbf{q} > \qquad (3.1.1)$$

The position operator is taken to be Hermitian; the coordinates are real numbers.

Consider a commutative geometric space, meaning by this sentence that the operators products $\hat{q}_i \hat{q}_j$ commute for all index pairs i, j, i.e. $\left[\hat{q}_i, \hat{q}_j\right] = \hat{q}_i\hat{q}_j - \hat{q}_j\hat{q}_i$ is equal to nihl operator, $\hat{0}$. Thus **q** represents a vector with well-defined coordinate labels. This makes **q** to stand as a point in the Euclidean configuration space R^{3N}; but remember that it is the distance between the origin and the configuration point that what really matters; thus, keep in mind that **q** is a label. For the time being the material system is reflected in the dimension of the configuration space; we are in the kinematics business. The point now is to show that a quantum state, be it in abstract space or in configuration space must be invariant under rotations of the I-frame and translations of the origin.

E&E.3.1-2 On Dirac Bra-Ket formalism

Dirac formulation of quantum mechanics according to von Neumann "is scarcely be surpassed in brevity and elegance", but that "in no way satisfies the requirements of mathematical rigor". The situation has dramatically changed with the introduction of the so-called rigged Hilbert space. The reader desiring an appropriate description is referred to the papers by: J.E.Roberts, J.Math.Phys.,7(1966)1097-1104; and O. Melsheimer, J.Math.Phys. 15 (1974) 902-916. We retain that Dirac's formalism is mathematically sound when defined in appropriate function spaces.

The set of base states $\{|\mathbf{q}>\}$ is orthonormal in a generalized function sense, namely:

$$<\mathbf{q}'|\mathbf{q}> = \delta(\mathbf{q} - \mathbf{q}') \qquad (3.1.2)$$

The symbol $\delta(\mathbf{q}-\mathbf{q}')$ stands for a measure, Dirac's generalized function; in short, it acts inside integration symbol:

$$\int d\mathbf{q}'\ f(\mathbf{q}')\ \delta(\mathbf{q} - \mathbf{q}') = f(\mathbf{q});$$
$$\int d\mathbf{q}'\ \delta(\mathbf{q} - \mathbf{q}') = 1 \qquad (3.1.3)$$

It is not difficult to see that a unit operator can be defined as:

$$\hat{1} = \int d\mathbf{q}'\ |\mathbf{q}'><\mathbf{q}'| \qquad (3.1.4)$$

The complex "function" $<\mathbf{q}'|\mathbf{q}>$ is actually a generalized function with properties given above. It is for this generalization among others that people talk about "rigged" Hilbert space.

E&E.3.1-3 Prove eq.(3.1.4)

First, we test whether or not the equation (3.1.4) functions as a unit vector. Consider the abstract quantum state $|\Psi>$ and multiply it by $\hat{1}$ which trivially means: $\hat{1}|\Psi>=|\Psi>$. Now:

$$|\Psi\rangle = \hat{1}\,|\Psi\rangle \rightarrow \int d\mathbf{q}'\ |\mathbf{q}'\rangle\langle\mathbf{q}'|\Psi\rangle = \int d\mathbf{q}'\ |\mathbf{q}'\rangle\,\Psi(\mathbf{q}')$$

Multiplying now from the left by $\langle\mathbf{q}''|$ and integrating over $d\mathbf{q}''$ one finds:

$$\begin{aligned}
&\hat{1}\ (\int d\mathbf{q}'\ |\mathbf{q}'\rangle\,\Psi(\mathbf{q}')) = \\
&\int d\mathbf{q}''\ |\mathbf{q}''\rangle\langle\mathbf{q}''|\ (\int d\mathbf{q}'\ |\mathbf{q}'\rangle\,\Psi(\mathbf{q}')) = \\
&\int d\mathbf{q}' \int d\mathbf{q}''\ |\mathbf{q}''\rangle\langle\mathbf{q}''|\mathbf{q}'\rangle\,\Psi(\mathbf{q}') = \\
&\int d\mathbf{q}' \int d\mathbf{q}''\ |\mathbf{q}''\rangle\,\delta(\mathbf{q}' - \mathbf{q}'')\Psi(\mathbf{q}') = \int d\mathbf{q}'|\mathbf{q}'\rangle\Psi(\mathbf{q}')
\end{aligned}$$

The operator given by eq.(3.1.4) actually function as the identity operator. The procedure is tautologic.
Second, you have to show that the unit operator actually has the form given in (3.1.4).
Pick up now from above

$$\begin{aligned}
&\int d\mathbf{q}' \int d\mathbf{q}''\ |\mathbf{q}''\rangle\langle\mathbf{q}''|\mathbf{q}'\rangle\,\Psi(\mathbf{q}') = \\
&\int d\mathbf{q}'\ (\int d\mathbf{q}''\ |\mathbf{q}''\rangle\langle\mathbf{q}''|)|\mathbf{q}'\rangle\,\Psi(\mathbf{q}')
\end{aligned}$$

This must be equal to $\int d\mathbf{q}'|\mathbf{q}'\rangle\Psi(\mathbf{q}')$.
Therefore one has to write:

$$(\int d\mathbf{q}''\ |\mathbf{q}''\rangle\langle\mathbf{q}''|) = \hat{1}$$

Consider the (abstract) quantum state $|\Psi\rangle$ of a 1-system given as a linear superposition using eq.(3.1.4):

$$\begin{aligned}
|\Psi\rangle = \hat{1}\ |\Psi\rangle \rightarrow \\
\int d\mathbf{q}'\ |\mathbf{q}'\rangle\langle\mathbf{q}'|\Psi\rangle = \int d\mathbf{q}'\ |\mathbf{q}'\rangle\,\Psi(\mathbf{q}') \qquad (3.1.5)
\end{aligned}$$

The quantum state $|\Psi\rangle$ projected in the inertial frame is a *linear superposition* with amplitudes given by its wave function $\Psi(\mathbf{q}') \leftrightarrow \langle\mathbf{q}'|\Psi\rangle$.

Note that the symbol Ψ is used for two different situations: 1) as a label (name); 2) as a mathematical function (mapping).

From eq.(3.1.4) it is clear that we have to have the wave function defined in a neighborhood $d\mathbf{q}'$ of the point $\mathbf{q}'$. *Reconstruction* of a quantum state implies knowledge of its wave function at all points in configuration space.

The wave function is first of all the amplitude calculated at a point of Euclidean space containing information about the abstract quantum state $|\Psi\rangle$. It is a complex function of a real variable, namely $\Psi(\mathbf{q}') \leftrightarrow \langle\mathbf{q}'|\Psi\rangle$; a phase is always implicit.

Note that in any neighborhood to a point $\mathbf{q}'$, the projection $\langle\mathbf{q}'|\Psi\rangle$ embodies full information about the quantum state $|\Psi\rangle$. In function space, $\Psi(\mathbf{q}')$ stands for a quantum state from abstract rigged Hilbert space. This mapping permits shifting the study towards mathematical constructs, e.g. partial differential equations,

familiar in mathematical physics. Of course, the reciprocal statement is not always valid, namely, a complex function on a real domain does not necessarily represent a quantum state; keep this caveat always in mind.

Quantum states are sustained by an invariant material system. Two different quantum states of the same material system have different wave functions; they do not need be orthogonal; only the base functions must be orthogonal as they are eigenfunctions derived from self-adjoint operators. From eq. (1.3.1.1), the particularities of the material system are incorporated in the Hamiltonian, while general symmetry properties would appear in the base set elements; the reason for this is simple: base states are fixed, quantum states can be variable. Make always the distinction between base function and wave function.

There are two classes of base functions. One relates to denumerable base states the other to continuum base states to be defined below starting from eq.(3.1.5).

Consider now a quantum system for which we know a complete, denumerable base set. Then the following relation can easily be proved right starting from eq.(2.2):

$$<\mathbf{q}|\Psi> \leftrightarrow \Psi(\mathbf{q}) = \Sigma_i <\mathbf{q}|a_i><a_i|\Psi> = \Sigma_i \phi_i(\mathbf{q})\, C_i(\Psi) \qquad (3.1.6)$$

The wave function contains now information on all those base states showing a non-zero $C_i(\Psi)$.

Observe that, once we get the base set, all what is necessary to construct the quantum state is in the set of amplitudes, $\{C_i(\Psi)\}$; these are numbers *independent* from the configuration point $\mathbf{q}$ selected by any reason. The base set $\{\phi_i(\mathbf{q})\}$ is totally independent of the quantum state $\Psi(\mathbf{q})$; in fact base functions are determined by complete sets of commuting operators (Cf. Axioms 1 to 4).

Because the base functions have definite and fixed quantum numbers, the configuration vector has been given a sequence order totally arbitrary that is kept fix. For a 1-system, lets order the configuration vectors for electron states first, namely, an R^{3n} object; for nuclei use R^{3m} space. The electronic space component shows new symmetry properties related to the ordering assigned: $\mathbf{q}_1,\mathbf{q}_2,\ldots\mathbf{q}_n$ in the argument of the base function. But one may take for instance $\mathbf{q}_2,\mathbf{q}_1,\ldots\mathbf{q}_n$ that would do as argument because the underlying material system consists of identical elements. Define a permutation operator P_{ij} that move the *label* j to the position i and vice versa:

$$\hat{P}_{ij}\, \phi_k(\mathbf{q}_1,\ldots, \mathbf{q}_i,\ldots, \mathbf{q}_j,\ldots,\mathbf{q}_n) = \phi_k(\mathbf{q}_1,\ldots, \mathbf{q}_j,\ldots, \mathbf{q}_i,\ldots,\mathbf{q}_n)$$

This relationship must be read as follows: the effect of the operator $\hat{P}_{ij}$ substitutes the *labels* found at position i by those found at position j, the implicit initial order is conserved. Just to give a hint: take base configurations $n_i\, d(\mathbf{q}_i)$

$n_j f(\mathbf{q}_j)$ the permuted ones reads as: $n_j f(\mathbf{q}_i)\, n_i d(\mathbf{q}_j)$ you do not swap "particles" as they are identical by hypothesis. Here, n_i and n_j are principal quantum numbers.

By applying $\hat{P}_{ij}$ again, one gets the operator equation $\hat{P}_{ij}^2=1$, its eigen values are +1 or –1. Thus, the base function $\phi_k(\mathbf{q}_1,\ldots, \mathbf{q}_j,\ldots, \mathbf{q}_i,\ldots,\mathbf{q}_n)$ is either symmetric or antisymmetric under permutation $\hat{P}_{ij}$.

If the spin base function is arranged as $\sigma(1,2,\ldots n)$ where the argument only indicates spin labels, then, under permutation of these labels the function can be either symmetric or anti symmetric. For electron states, assume that $\sigma_k(1,2,\ldots n)$ is the adequate spin basis to be combined with the space one. The total space-spin base function is given as direct product: $\phi_k(\mathbf{q}_1,\ldots,\mathbf{q}_j,\ldots,\mathbf{q}_i,\ldots,\mathbf{q}_n) \otimes \sigma_k(1,2,\ldots n)$. This product must be antisymmetric to permutations. Electron states are said to stand for *fermions*. But the anti-symmetry property can be attained in two different manners:

a) Space component antisymmetric and spin part is symmetric;
b) Spin part is antisymmetric, the space part symmetric.

Whatever the picture we would like to hang on the base set, provided global symmetry properties are respected, it would have no effect on the determination of the quantum state. Provided the base set is complete, eq.(3.1.6) shows the amplitudes to be the place where the quantum state is disclosed. Note that we assume the base states are implicitly multiplied by the appropriate spin base function. Integration over spin degrees of freedom is implicit.

In Hilbert space, quantum states normalized to one that can be projected in configuration space are represented by square integrable functions. Quantum states in the continuum are included in an expanded space, rigged Hilbert space where mathematical objects such as $\langle\mathbf{q}|\mathbf{q}'\rangle$ are defined in the space of generalized functions. Note that the problem resides at the pure mathematical level. Existence of quantum states in the continuum is taken for granted; this has to do with Physics.

The measure $\langle\mathbf{q}|\mathbf{q}'\rangle$ and eq.(3.1.5) are used to formally calculate the norm of $\langle\Psi|\Psi\rangle$:

$$
\begin{aligned}
&(\langle\Psi|\hat{1})(\hat{1}\Psi\rangle) = \int d\mathbf{q}\, \langle\mathbf{q}|\, \Psi^*(\mathbf{q}) \int d\mathbf{q}'\, |\mathbf{q}'\rangle\, \Psi(\mathbf{q}') = \\
&\int d\mathbf{q} \int d\mathbf{q}'\, \langle\mathbf{q}|\mathbf{q}'\rangle\, \Psi^*(\mathbf{q})\, \Psi(\mathbf{q}') = \\
&\int d\mathbf{q} \int d\mathbf{q}'\, \delta(\mathbf{q}-\mathbf{q}')\, \Psi^*(\mathbf{q})\, \Psi(\mathbf{q}') = \\
&\int d\mathbf{q}\, \Psi^*(\mathbf{q})\, \Psi(\mathbf{q}) = 1 \qquad\qquad (3.1.7)
\end{aligned}
$$

The two ends of eq.(3.1.7) are numbers. The maps connect elements from abstract to the projected Hilbert space using a configuration space with respect to an I-frame with origin in real space. Moving from left to the right will show up that square integrable functions relate to states in abstract Hilbert space, namely it provides a sufficient condition. Note that an arbitrary square integrable function does not necessarily represents a quantum state.

In what follows, we retain the hypothesis: Hilbert space is the physical states space while the mathematical mappings to a Fence are defined in a rigged Hilbert space including an I-frame.

3.2. Translation operator

Hilbert space states do not depend upon configuration coordinates. This is apparent from the amplitudes $C_i(\Psi)$ discussed above. The question now is to study the behavior of space eigenkets ($|\mathbf{q}'\rangle$) towards an origin translation. While the quantum state is frame independent, the projections given by $\langle\mathbf{q}|\Psi\rangle$ may show specific properties under origin translation; we study now some issues.

3.2.1. Infinitesimal translations

Let us define $\hat{T}(d\mathbf{q}')$ as the operator accomplishing an infinitesimal translation:

$$\hat{T}(d\mathbf{q}')\,|\mathbf{q}'\rangle = |\mathbf{q}'+d\mathbf{q}'\rangle \qquad (3.2.1.1)$$

What effect would produce the translation operator of the quantum state represented in eq.(3.1.5)? Let us operate that equation with the help of eq(3.1.5):

$$\begin{aligned}&\hat{T}(d\mathbf{q}')\,|\Psi\rangle \rightarrow \hat{T}(d\mathbf{q}')\,|\mathbf{q}'\rangle\langle\mathbf{q}'|\Psi\rangle = \\ &\hat{T}(d\mathbf{q}')\,|\mathbf{q}'\rangle\,\Psi(\mathbf{q}') = |\mathbf{q}'+d\mathbf{q}'\rangle\langle\mathbf{q}'|\Psi\rangle = \\ &|\mathbf{q}'\rangle\,\Psi(\mathbf{q}'-d\mathbf{q}') \qquad (3.2.1.2)\end{aligned}$$

The last equality follows from a change of variables, $\mathbf{q}' \rightarrow \mathbf{q}'-d\mathbf{q}'$, the integral of (3.2.1.2) can be written as:

$$\begin{aligned}&\int d\mathbf{q}'\,|\mathbf{q}'+d\mathbf{q}'\rangle\langle\mathbf{q}'|\Psi\rangle = \int d\mathbf{q}'\,|\mathbf{q}'\rangle\langle\mathbf{q}'-d\mathbf{q}'|\Psi\rangle = \\ &\int d\mathbf{q}'\,|\mathbf{q}'\rangle\,\Psi(\mathbf{q}'-d\mathbf{q}') \qquad (3.2.1.3)\end{aligned}$$

Thus, a *displacement in a given direction of a position ket label corresponds to a translation of the wave function argument in the opposite direction*. The change in the ket label amounts to an origin shift in laboratory space.

As it was done in Chapter 1 for a time displacement operator, norm invariance is imposed. Therefore, $\hat{T}(d\mathbf{q}')$ is a unitary operator such that: $\hat{T}^{\dagger}(d\mathbf{q}')\hat{T}(d\mathbf{q}')=\hat{1}$. The group property under composition of two displacements is given as: $\hat{T}(d\mathbf{q}')\hat{T}(d\mathbf{q}'')=\hat{T}(d\mathbf{q}'+d\mathbf{q}'')$. There is an inverse operation: $\hat{T}(-d\mathbf{q}')=\hat{T}^{-1}(d\mathbf{q}')$; and continuity,

$$\lim_{d\mathbf{q}'\to 0}\hat{T}(d\mathbf{q}')=\hat{1} \qquad (3.2.1.4)$$

For the operator fulfilling the above properties it can be shown that

$$\hat{T}(d\mathbf{q}')=\hat{1}-i\,\hat{k}\cdot d\mathbf{q}' \qquad (3.2.1.5)$$

The reciprocal space enters into the handling of translation operators; the reason for this result is located in a dimensional analysis, the translation operator is dimensionless, so must be for the product $\hat{k}\cdot d\mathbf{q}'$.

3.2.2. Reciprocal (momentum) space

The vector operator $\hat{k}$ must hence be Hermitian in order to be norm conserving; with inverse of length as the appropriate dimension: $\hat{k}$ is the *generator* of displacement in configuration space. The direct and inverse spaces share the origin.

Eigen vectors for the wave operator $\hat{k}$ are labeled as $|k_1,k_2,k_3\rangle$ in the understanding that operator components commute among themselves. Thus,

$$\hat{k}\,|k_1,k_2,k_3\rangle=\hat{k}\,|\mathbf{k}\rangle=\mathbf{k}\,|\mathbf{k}\rangle \qquad (3.2.2.1)$$

The eigen values of $\hat{k}$ are real numbers as they should. Furthermore, in **k**-space the scalar product is a generalized function (distribution) that only makes sense inside an integral:

$$\langle\mathbf{k}|\mathbf{k}'\rangle=\delta(\mathbf{k}-\mathbf{k}') \qquad (3.2.2.2)$$

With these properties, it is easy to show a resolution of the identity in **k**-space:

$$\hat{1}=\int d\mathbf{k}'\,|\mathbf{k}'\rangle\langle\mathbf{k}'| \qquad (3.2.2.3)$$

An arbitrary quantum state $|\Psi\rangle$ can be expanded in k-space with eq.(3.2.1.9) as:

$$|\Psi\rangle=\hat{1}|\Psi\rangle=\int d\mathbf{k}'\,|\mathbf{k}'\rangle\langle\mathbf{k}'|\Psi\rangle \qquad (3.2.2.4)$$

$<\mathbf{k}'|\Psi>$ is the wave function standing for the quantum state $|\Psi>$ in reciprocal space, $\Psi(\mathbf{k}')$.

E&E.3.2-1. Find a relation between **k**- and **q**-space wave functions
Multiplying eq.(3.2.1.10) from the left with $<\mathbf{q}'|$:

$$<\mathbf{q}'|\Psi> = \int d\mathbf{k}' <\mathbf{q}'|\mathbf{k}'><\mathbf{k}'|\Psi>$$

This equality leads to the definition of the transformation function: $<\mathbf{q}'|\mathbf{k}'>$. The set of plane waves $\exp(i\,\mathbf{k}'\bullet\mathbf{q}')$ can be equated to $<\mathbf{q}'|\mathbf{k}'>$. Thus, $<\mathbf{q}'|\mathbf{k}'>$ provides a complete set of base functions relating these two spaces. The relationship is thence proportional to a Fourier transform: $<\mathbf{q}'|\Psi> = \int d\mathbf{k}' \exp(i\,\mathbf{k}'\bullet\mathbf{q}') <\mathbf{k}'|\Psi>$. The reverse relationship reads:

$$<\mathbf{k}|\Psi> = (1/2\pi) \int d\mathbf{q}' \exp(-i\,\mathbf{k}\bullet\mathbf{q}') <\mathbf{q}'|\Psi>.$$

Let us examine the bra obtained from $<\mathbf{q}'|\hat{k}$. The result when multiplying from the right with $|\mathbf{k}>$ from eq. (3.2.2.1) is $\mathbf{k}<\mathbf{q}'|\mathbf{k}>$. This suggests that $<\mathbf{q}'|\mathbf{k}>$ may be proportional to $\exp(i\mathbf{k}\bullet\mathbf{q}')$. The operator $\hat{k}$ is proportional to $-i\,(\partial/\partial\mathbf{q}')$.

Consider the relation $<\mathbf{q}'|\hat{k} = -i\,(\partial/\partial\mathbf{q}')<\mathbf{q}'|$ that gives the form of the k-operator in coordinate space. It follows the matrix elements of this operator are:

$$<\mathbf{q}'|\hat{k}|\mathbf{q}''> = -i\,(\partial/\partial\mathbf{q}')\,\delta(\mathbf{q}'-\mathbf{q}'') \qquad (3.2.2.5)$$

Let us use eq.(3.1.2) in conjunction with (3.2.2.5) to get the effect of the reciprocal space operator:

$$<\mathbf{q}'|\hat{k}|\Psi> = \int d\mathbf{q}'' <\mathbf{q}'|\hat{k}|\mathbf{q}''>\Psi(\mathbf{q}'') =$$
$$\int d\mathbf{q}'' -i\,(\partial/\partial\mathbf{q}')\,\delta(\mathbf{q}'-\mathbf{q}'')\Psi(\mathbf{q}'') = -i\,(\partial\Psi(\mathbf{q}')/\partial\mathbf{q}') =$$
$$-i\,(\partial/\partial\mathbf{q}')<\mathbf{q}'|\Psi> \qquad (3.2.2.6)$$

The rule commonly used replacing operator $\hat{k}$ by $-i\,(\partial/\partial\mathbf{q}')$ in configuration space appears here in a natural way. Note that $<\mathbf{q}'|\hat{k}$ is symbolically replaced by $-i\,(\partial/\partial\mathbf{q}')<\mathbf{q}'|$ to get eq.(3.2.2.6).

The transformation function connecting **q**- to **k**- representations obtains when $|\Psi>\rightarrow|k'>$ in (3.2.2.6). Bearing in mind that $\hat{k}\,|\,\mathbf{k}'>=\mathbf{k}'|\mathbf{k}'>$:

$$\mathbf{k}'<\mathbf{q}'|\,\mathbf{k}'> = -i\,(\partial<\mathbf{q}'|\,\mathbf{k}'>/\partial\mathbf{q}') \qquad (3.2.2.7)$$

The solution to this differential equation is the transformation function

$$<\mathbf{q}'|\ \mathbf{k}'> = A\ \exp(i\mathbf{k}'.\mathbf{q}') \qquad (3.2.2.8)$$

$A=1/\sqrt{2\pi}$. Thus, the projected base function of a reciprocal space eigen vector is a plane wave. Note that it is common to use the symbol ∇ for $\partial/\partial\mathbf{q}' = \mathbf{i}_1\partial/\partial q_1' + \mathbf{i}_2\partial/\partial q_2' + \mathbf{i}_3\partial/\partial q_3'$.

All the discussion above concerns "kinematic" elements of the theory. There is no dynamic element yet.

3.2.3 Finite real space translations

Here, one should consider displacements and rotations of the whole I-frame. Internal quantum systems can be seen as determining properties of the associated total mass, charge and spin. To the extent that no couplings between internal and "external" degrees of freedom are let in, there is now a possibility to treat the global I-frame as a "particle" in a way to be determined in later chapters. Now, let us take for granted such separation.

A finite displacement obtains by successively applying infinitesimal translations given by eq.(3.2.1.5). Consider the unit vector $\mathbf{i}_j$ and a finite segment $\Delta q_j'$, divided it in N parts, so that $\Delta q_j'/N$ when $N\to\infty$ approaches dq_j'. Thus, one gets

$$\hat{T}(\Delta q_j'\ \mathbf{i}_j) = \lim_{N\to\infty}(\hat{1} - i\ \hat{k}_j\cdot(\Delta q_j'/N))^N = \exp(-i\,\hat{k}_j\cdot\Delta q_j') \qquad (3.2.3.1)$$

E&E-3.2-2. Show that successive translations in different directions commute. Show also that this result implies that the commutator $[\hat{k}_j,\hat{k}_i]=\delta_{jk}\hat{1}$.

A finite displacement of a base state in **k**-space obtains when summed over repeated indexes:

$$\hat{T}(\Delta\mathbf{q}')|\mathbf{k}> = \exp(-i\,\hat{k}_j\cdot\Delta q_j')|\mathbf{k}> = \exp(-i\,\mathbf{k}\cdot\Delta\mathbf{q}')\ |\mathbf{k}> \qquad (3.2.3.2)$$

Thus, a displacement of the origin for the inertial frame puts a phase onto the base kets in reciprocal space. The change of origin is reminded by the phase factor $\exp(-i\mathbf{k}\cdot\Delta\mathbf{q}')$ that is the eigen value of the operator $\hat{T}(\Delta\mathbf{q}')=\exp(-i\,\hat{k}_j\cdot\Delta q_j')$. The operator $\hat{T}(\Delta\mathbf{q}')$ is unitary but not Hermitian.

Observe on the other hand that $\hat{k}=-i(\partial/\partial\mathbf{q}')$ is Hermitian; its base states $\{|\mathbf{k}>\}$ fulfill: $\hat{k}\,|\mathbf{k}>=\mathbf{k}\,|\mathbf{k}>$. The vector **k** signals (label) a direction in reciprocal space.

Note that for one value |**k**| there are infinite number of directions. The mathematical functions standing for <**q**|**k**> are not square-integrable functions; this is one of the reasons explaining the expansion of Hilbert space to a rigged Hilbert space.

One easy way to introduce dynamical elements in this scheme obtains by multiplying the operator $\hat{k}$ by Planck's constant a linear momentum operator $\hat{p}$ obtains:

$$\hat{p} = \hbar\ \hat{k} = -\mathrm{i}\ \hbar\ (\partial/\partial \mathbf{q}') = -\mathrm{i}\ \hbar\ \nabla \qquad (3.2.3.3)$$

Multiplying eq. (3.2.1.6) by Planck constant we get standard commutation rules for position-momentum operators:

$$\left[\hat{q}_i, \hat{p}_j\right] = \mathrm{i}\hbar\ \delta_{ij}\ \hat{1} \qquad (3.2.3.4)$$

These are fundamental equations that would to quantum mechanics. You do not need to postulate them as they result from general invariance properties. What do you have to postulate is that the operator $\hat{p}$ is the momentum operator for a particle if you want to introduce a classical particle view.

Note that one only has an operator form: $\hat{p} = \hbar\ \hat{k}$. The position, the reciprocal space and momentum operator components commute among themselves, which implies that their average values ($<\hat{q}> = \mathbf{q}$, $<\hat{k}> = \mathbf{k}$ and $<\hat{p}> = \mathbf{p}$) can be taken as full vectors at variance with angular momentum that we start to analyze below. Finally, invariance to translations of the base states generates the most important relation between operators in abstract space and their projection in configuration space; the dimensions are fixed by Planck constant.

E&E.3.2.3. Calculate the linear momentum of a given quantum state |ϕ>

First name the projection in **k**-space: <**k**|ϕ> = ϕ(**k**). Calculate the representation in **k**-space:

$$|\phi> = \int d\mathbf{k}'\ |\mathbf{k}'><\mathbf{k}'|\phi>$$

This is a linear superposition where the information on the quantum state is collected in the continuum set {<**k**'|ϕ>}. The momentum is the average value of $\hat{p}$: $<\phi \mid \hat{p} \mid \phi>$. Thus,

$$<\phi \mid \hat{p} \mid \phi> = \int d\mathbf{k}''\ <\phi|\mathbf{k}''><\mathbf{k}''|\ \hat{p}\ \int d\mathbf{k}'\ |\mathbf{k}'><\mathbf{k}'|\phi> =$$
$$\int d\mathbf{k}'\ \int d\mathbf{k}''\ <\phi|\mathbf{k}''><\mathbf{k}''|\ \hat{p}\ |\mathbf{k}'><\mathbf{k}'|\phi> =$$
$$\int d\mathbf{k}'\ \int d\mathbf{k}''\ <\phi|\mathbf{k}''><\mathbf{k}''|\ \hbar\ \hat{k}\ |\mathbf{k}'><\mathbf{k}'|\phi> =$$
$$\hbar\ \int d\mathbf{k}'\ \int d\mathbf{k}''\ <\phi|\mathbf{k}''><\mathbf{k}''|\ \hat{k}\ |\mathbf{k}'><\mathbf{k}'|\phi> =$$
$$\hbar\ \int d\mathbf{k}'\ \int d\mathbf{k}''\ \mathbf{k}'<\phi|\mathbf{k}''><\mathbf{k}''|\mathbf{k}'><\mathbf{k}'|\phi> =$$

$$\hbar \int d\mathbf{k'} \int d\mathbf{k''}\ \mathbf{k'} \langle \phi|\mathbf{k''}\rangle\ \delta(\mathbf{k''}-\mathbf{k'})\langle \mathbf{k'}|\phi\rangle =$$
$$\hbar \int d\mathbf{k'}\ \mathbf{k'}\ \langle \phi|\mathbf{k'}\rangle\ \langle \mathbf{k'}|\phi\rangle = \mathbf{0}$$

Reflect about the fact that for any quantum state the momentum in the inertial frame is zero. From mathematics the last equality follows from the fact that $\langle \phi|\mathbf{k'}\rangle\ \langle \mathbf{k'}|\phi\rangle$ is positive and **k'** is an odd function (positive and negative parts add up to zero.
Hint: $|\phi\rangle$ becomes a stationary state.

3.2.4. Direct-Reciprocal Spaces: Fourier transforms

Translation symmetry generates two types of base states, namely, position coordinate and reciprocal space coordinate. The range accorded to configuration space coordinates goes from -∞ to +∞; in reciprocal space the k-coordinates have also the range:]-∞,+∞[. The transformation function Aexp(i**k**.**q**) forms a complete basis set serving to express a given quantum state in k-space in **q**-space:

$$\phi(\mathbf{q}) = 1/\sqrt{2\pi} \int_{-\infty}^{+\infty} dk\ \exp(i\mathbf{k}.\mathbf{q})\ \phi(\mathbf{k}) \qquad (3.2.4.1)$$

What is projected here is the quantum state $|\phi\rangle$ first in **k**-space and then multiplied by $\langle \mathbf{q}|$ from the left. In the theory of Fourier transformations, $\phi(\mathbf{q})$ is the Fourier transform of $\phi(\mathbf{k})$.

From the structure of the equation above it is clear that exp(i**k**.**q**) plays the role of a base function. The inverse relation reads as:

$$\phi(\mathbf{k}) = 1/\sqrt{2\pi} \int_{-\infty}^{+\infty} dq\ \exp(-i\mathbf{k}.\mathbf{q})\ \phi(\mathbf{q}) \qquad (3.2.4.2)$$

Because the actual mathematical forms of $\phi(\mathbf{q})$ and $\phi(\mathbf{k})$ are different, albeit they represent the same abstract quantum state, different symbols are commonly used to identify them; here, maintain the same symbol (label) to stress the connection with a quantum state.

Consider a time dependent quantum state $|\phi,t\rangle$ and project it in **k**-space first; then take a system separable in space-time as we have already done in the preceding chapter:

$$\langle \mathbf{q}|\phi,t\rangle = \int_{-\infty}^{+\infty} dk\ \langle \mathbf{q}\ |\mathbf{k}\rangle\langle \mathbf{k}|\phi,t\rangle = \int_{-\infty}^{+\infty} dk\ \langle \mathbf{q}\ |\mathbf{k}\rangle\langle \mathbf{k}|\phi\rangle|t\rangle =$$
$$\int_{-\infty}^{+\infty} dk\ \langle \mathbf{q}\ |\mathbf{k}\rangle\ \langle \mathbf{k}|\phi\rangle\ \exp(-i\omega t).$$

Using eq. (3.2.4.1) one gets:

$$\phi(\mathbf{q},t) = 1/\sqrt{2\pi} \int_{-\infty}^{+\infty} dk \ \exp(i(\mathbf{k}.\mathbf{q}-\omega t)\ \phi(\mathbf{k}) \qquad (3.2.4.3)$$

In the case that **k** and ω were independent, the separation leading to $\phi(\mathbf{q},t)$ starting from a quantum state prepared in **k**-space would just be an apparent time evolution: the wave packet would come back to $\phi(\mathbf{q},t=0)$ and start up again a new cycle; the amplitudes in absolute value are invariant.

The situation showing physical interest corresponds to

$$<\mathbf{k}|\phi,t> = <\mathbf{k}|\phi>\exp(-i\omega(\mathbf{k})t);$$

the frequency would appear as a function of **k**. In other words, space and time become mingled. The function $\omega(\mathbf{k})$ is known as a dispersion relationship. Examples come up in solid-state physics and many other branches of physics.

Equations (3.2.4.1-2) are expressions of the linear superposition principle. As they stand no physical representation is required: they are mathematical entities in configuration (abstract) space. It is a formalism that covers all possibilities a system may show. The formalism includes all frequency (polychromatic) combinations that may stand for particular quantum states we might be capable of constructing. This is what $\phi(\mathbf{k})$ means, i.e. everything until specific sets of amplitudes are introduced.

At this point it is appropriate to part pure mathematical from physical elements. To the former belongs Fourier transforms theory. The latter relates to the mapping $|\alpha> \rightarrow <\mathbf{q}|\alpha>$ meaning with this arrow a projection of a quantum state on a configuration space the labels of which are real numbers but the elements $<\mathbf{q}|\alpha>$ are complex numbers. These types of complex numbers are those that can be manipulated leading to representations of different quantum state representations at a Fence. Remember that real numbers are a subset of the complex numbers.

In pure mathematics one study functions $\alpha(\mathbf{q})$ without a necessary relation to possible projected $<\mathbf{q}|\alpha>$ quantum states. We have to bear in mind the difference: not every mathematical function stands for a projected quantum state; in the early days these functions belonged to the so-called square integrable functions. A large set of projected quantum states did not belong to this class. Mathematics was hence enlarged with generalized (distributions) functions to which Fourier analysis was extended. Because we use mathematical analysis to construct solutions for a number of physical problems, how do we know correct physical answers obtain? In science, it is experiment and the experimental results that help solving such a type of questions. Those experiments belong to our Fence domain.

3.2.5. Quantum states prepared at a Fence (laboratory)

Two examples are introduced that illustrate a host of experimental situations.

A) Gaussian states
A first practical example corresponds to a Gaussian quantum state:

$$\phi_G(\mathbf{q}) = (2/\pi\ \alpha^2)^{3/4} \exp(-|\mathbf{q}|^2/\ \alpha^2) \qquad (3.2.5.1)$$

The representation of this quantum state in reciprocal space **k** can be calculated to be:

$$\phi_G(\mathbf{k}) = (2\pi\ \alpha^2)^{3/4} \exp(-|\mathbf{k}|^2\ \alpha^2/4) \qquad (3.2.5.2)$$

The Fourier transform of a Gaussian quantum state in configuration space is also a Gaussian in reciprocal space. The widths at half-maximum, $\Delta\mathbf{q}$ and $\Delta\mathbf{k}$, are controlled by the parameter α, they are roughly inverse to each other so that:

$$\Delta\mathbf{q}\ \Delta\mathbf{k} \approx 1 \qquad (3.2.5.3)$$

Observe that the magnitudes $\Delta\mathbf{q}$ and $\Delta\mathbf{k}$ refer to a property of the quantum state $\phi_G(\mathbf{q})$ or to $\phi_G(\mathbf{k})$. The axis **q** and **k** cover real number systems while $\Delta\mathbf{q}$ and $\Delta\mathbf{k}$ are a different type of number. This distinction is important to bear in mind. It is at this level that physical situations enter. To talk of particular $\Delta\mathbf{q}$ and $\Delta\mathbf{k}$ one must know that a particular quantum state is involved. In other words, the amplitudes intervening in the representation of the quantum state are well defined.

Now, it is a common practice to multiply **k** by Planck's constant and using the prescription $\mathbf{p}=\hbar\mathbf{k}$ to get an expression like:

$$\Delta\mathbf{q}\ \Delta\mathbf{p} \approx \hbar \qquad (3.2.5.4)$$

The widths are associated to a preparation of the quantum state and have nothing to do with measurements as these latter belong to real space situations. This issue asks for a little more discussion. Of course, design of a measuring device leading to a particular quantum state of the system after interaction will generate a relationship like eq.(3.2.5.4), namely, the famous Heisenberg uncertainty

relationship that would appear as result derived from the quantum state prepared and expressed as linear superpositions.

B) Box-states

Construct a quantum state in momentum space ($<k|\phi>$) when the space dependent function shows zero amplitudes outside a range about the origin of length L; this is related to the common case of a particle in a box; the material system at the Fence is trapped inside $-L/2 \leq x \leq L/2$ so that $\phi(x) = 0$ for $x \leq -L$ and $x \geq L$. Remember that $\phi(x)$ are the amplitudes of the quantum state in the configuration base set: $<x|\phi>$.

The result concerning the basis set required to represent $\phi(x)$ in this range is amazing. From the continuous range shown by eq(3.2.4.1) one gets a Fourier series:

$$\phi(x)=a_o+\sum_{n=1}^{n=\infty} \{a_n\cos(2n\pi x/L)+b_n\sin(2n\pi x/L)\} \quad (3.2.5.5)$$

This form given to $\phi(x)$ cannot represent a quantum state as the trigonometric functions (cos and sin) do not have the properties to function as a basis set appropriate for the task; to get there one uses equality below:

$$e^{(i(2n\pi\, x/L))} = \cos(2n\pi x/L) + i\, \sin(2n\pi x/L).$$

Then after some mathematical contortions the quantum state is represented as:

$$\phi(x) = \sum_{n=-\infty}^{n=+\infty} c_n\, e^{(i(2n\,\pi\, x/L))} = \sum_{j=-\infty}^{j=+\infty} c_{nj}\, e^{ix\ kj} \qquad (3.2.5.6)$$

From the boundary condition imposed one gets the allowed momenta:

$$2n_j\pi/L = k_j \text{ and } n_j=0, \pm1,\pm2,\ldots \qquad (3.2.5.7)$$

In the latter sum only values allowed for (3.2.5.7) contribute.

The introduction of a configuration space domain constraint changes the nature of the basis functions. The quantum state is given as a function of basis functions over discrete momenta given by eq. (3.2.5.7).

A discrete series of energy values, energy levels, replace the continuum distribution. This is an important result. The constraint instead of being trapping the system in a finite region of space can also be thought as a periodicity constraint.

C) Discrete-continuum connections

A common relation between discrete and continuum pictures obtains if one takes L to be the period in each of the three space directions q_1,q_2,q_3 defining vector **q**. The Fourier series reads

$$\phi(\mathbf{q}) = (1/L)^{3/2} \sum_{k} c_{\mathbf{k}}(t)\, e^{i(\mathbf{k}\cdot\mathbf{q} - \omega t)} ;$$
$$\omega = (\hbar/2m)\, \mathbf{k}\cdot\mathbf{k} = (\hbar/2m)\, k^2 \qquad (3.2.5.8)$$

The sum includes terms only with components k_j given by eq.(3.2.5.7) of each vector **k**.

In **k**-space for large L a volume element d^3k includes a number of states with k's different: $d^3k\ (L^3/2\pi)$. The normalization of series (3.2.5.8) is to be chosen by selecting the coefficients $c_{\mathbf{k}}$. The square integral over the periodicity cube is then:

$$\int_{(L^3)} d^3q\ |\phi(\mathbf{q})|^2 = L^{-3} \sum_{k,k'} c_{\mathbf{k}}^*\, c_{\mathbf{k}'}\, e^{i(\omega-\omega')\,t} \int d^3k\, e^{(\mathbf{k}'-\mathbf{k})\cdot\mathbf{q}} \qquad (3.2.5.9)$$

At the right-hand-side the space integral is zero for $\mathbf{k}' \neq \mathbf{k}$ and for the equality the result is $V=L^3$ to finally get a fundamental theorem:

$$\int_{(L^3)} d^3q\ |\phi(\mathbf{q})|^2 = \sum_{k} c_{\mathbf{k}}^*\, c_{\mathbf{k}} \qquad (3.2.5.10)$$

The key result concerning the quantum state in the periodicity cube is the connection with the set of amplitudes signaling the relative intensity response of the associated eigen states. For zero amplitude no response is expected; if some response is to be found it will correspond to the allowed k-values indicated by the periodic boundary conditions eq.(3.2.5.8).

It is apparent that in the limit $L\to\infty$ the continuum representation should emerge. By using the rule

$$\sum_{k} \to (L/2\pi)^3\, d^3k \qquad (3.2.5.11)$$

Eq.(3.2.5.8) yields

$$\phi(\mathbf{q},t) \to$$
$$(L^{1/2}/2\pi)^3 \int d^3k\, c(\mathbf{k},t)\, \exp(i(\mathbf{k}\cdot\mathbf{q} - \omega t)) \qquad (3.2.5.12)$$

Consider the limit now, the function $(L^{1/2}/2\pi)^3\ c(\mathbf{k})$ must correspond to $\phi(\mathbf{q})$ in our notation.

If only a few $c(\mathbf{k})$-values define the quantum state we do not need to do this conversion. But if the quantum state is defined by some dense set of values, eq.(3.2.5.12) would represent the Fourier transform of $\phi(\mathbf{q})$ in the limit $L\to\infty$ only if

$$\phi(\mathbf{k}) = \lim_{L\to\infty} (L^{1/2}/2\pi)^3\ c(\mathbf{k}) \qquad (3.2.5.13)$$

Provided this limit holds for each $\mathbf{k}$, the continuum representation can be homologated to the discrete one.

The connection between $c(\mathbf{k})$ and $\phi(\mathbf{k})$ ensures the contention that quantum states can be expressed by the amplitudes of linear superpositions. These numbers represent the quantum state. The basis functions inform us about the nature of the energy levels a material system has; we have to calculate them with a well-defined procedure: Schrödinger equation seen in Chapter 1. More about this is to be found in the following chapters and section 3.10 where the material system is electromagnetic energy trapped in cavities or propagating in free space.

But before examining EM systems we need to study the invariance of quantum states to rotations of I-frames.

3.3. Rotation invariance: Angular Momentum

Quantum states cannot depend upon the way an I-frame is oriented while origin is kept fixed. Furthermore, in quantum mechanics there is no such a thing as the direction of the angular momentum; there is its magnitude (J) and a projection along a given direction; this is related to the commutation relationships, as we will see below.

Still, the way experimental apparatuses are oriented with respect to a fixed I-frame does matter to the extent they enter under controlled interactions with the material system sustaining the quantum states. This is to remind that one does not measure a material physical system as if were an object but one measure varied changes in their quantum states expressed as response functions. The same material system sustains infinity of quantum states referred to a fixed base set. Here, our aim is the construction of relevant base sets that can elicit space isotropy.

Quantum states are abstract concepts. If you are studying quantum states for an elephant for sure the states must be invariant to rotations of I-frames. Do not try to move a real elephant, just the frames. If you can sense the difference between a material system and associated quantum states, then we are in business.

In real space there are arbitrary proper rotations of a I-frame with respect to a second fixed one denoted as $\mathbf{R}_1,\mathbf{R}_2,\ldots$ Proper rotations do not change the hand of a frame. Two rotations carried out in the sequence $\mathbf{R}_1$ first and then $\mathbf{R}_2$ are written as a product $\mathbf{R}_2\,\mathbf{R}_1$. The product *is not commutative* if $\mathbf{R}_2$ is a rotation away from the orientation achieved with $\mathbf{R}_1$; i.e. rotation axes are different. Let **E** stand for no-rotation, the inverse rotation to **R**, designated by $\mathbf{R}^{-1}$, is defined by $\mathbf{R}^{-1}\mathbf{R}=\mathbf{R}\mathbf{R}^{-1} = \mathbf{E}$. The rotation group is the set of all proper rotations; this excludes reflection operations that change the hand of the I-frame (left-handed into right-handed and vive versa).

We have already met examples of invariance to changes of origin in time and space; there, an unitary operator relates to a displacement generator operator $\hat{O}$ in a simple manner as shown by eqs.(1.3.1.3) and (3.2.2.2): $\hat{U}_z = \hat{1}\text{-i}\,\hat{O}\varepsilon$.

For $\varepsilon = \delta t$ operator $\hat{O}$ takes on the form $\hat{H}/\hbar$ while for translations $\varepsilon = d\mathbf{q}$ and operator $\hat{O}$ gets the form $\hat{p}/\hbar$.

Planck constant can be expressed in three different ways: in units of energy by time; or linear momentum by length; and finally it has the dimension of angular momentum. The latter relates to rotations in 3-space.

Let $\hat{J}$ be the angular momentum operator and **n**, a unit vector, around which an infinitesimal rotation $\delta\phi$ is carried out; this is a one-parameter rotation. By analogy to the preceding cases define the rotation operator $\hat{D}(\mathbf{n},\delta\phi)$ as:

$$\hat{D}(\mathbf{n}, \delta\,\phi) = \hat{1} - \text{i}\,(\hat{J}.\mathbf{n}/\hbar)\,\delta\,\phi \qquad (3.3.1)$$

The angular momentum operator $\hat{J}=(\hat{J}_1, \hat{J}_2, \hat{J}_3)$ fulfils the commutation rules:

$$\hat{J}_\text{i}\,\hat{J}_\text{j} - \hat{J}_\text{j}\,\hat{J}_\text{i} = [\,\hat{J}_\text{i}, \hat{J}_\text{j}] = \text{i}\,\hbar\;\varepsilon_{\text{ijk}}\,\hat{J}_\text{k} \qquad (3.3.2)$$

The symbol $\varepsilon_{ijk} = 0$ if there are two equal indexes; $\varepsilon_{ijk} = 1$ if the indexes are a cyclic permutation of (1,2,3); $\varepsilon_{ijk} = -1$ for non-cyclic ordering.

For $\hat{D}(\mathbf{n}, \delta\,\phi)$ to be unitary, $\hat{J}$ must be Hermitian and consequently, the eigenvalues must be real numbers. The relationship with rotation matrices and operators will be examined later on. Here, eq.(3.3.2) defines angular momentum in terms of commutation relations.

The subsections ahead are rather painful. For readers having a more operational view by only browsing, if at all, would do. Another possibility is to simply jump to the last section where the linear superposition principle is illustrated by using the complete basis sets for translation and rotation invariance. Again, I-frames are objects in real space that can be used to identify the mass related dynamics determining the nature of internal quantum states. Configuration

space is a mathematical construct used to project abstract quantum states. Keep this in mind if you decide to move to the last section of this chapter.

3.3.1.Base states and eigen values

The rotation operator $\hat{D}(\mathbf{R}_\Theta)$ commutes with $\hat{H}$, namely,

$$[\hat{D}(\mathbf{R}_\Theta), \hat{H}] = \hat{D}(\mathbf{R}_\Theta)\hat{H} - \hat{H}\hat{D}(\mathbf{R}_\Theta) = \hat{0}.$$

This means that base states and their eigen values will serve to classify (label) energy quantum base states.

The commutation relations eq.(3.3.2) are the key to construct base states. First, note angular momentum components do not commute among themselves. A quantum base state cannot be label simultaneously with the three of them. Only one component, usually taken to be $\hat{J}_3$, is selected to generate quantum numbers (label), that are named here as M_J; i.e. the quantizing direction **n**= (0,0,1). The rotation matrix mixes components 1 and 2.

E&E.3.3.1. Calculate the commutator of $\hat{J}^2$ and $\hat{J}_3$
Use the definition of commutator:

$$\begin{aligned}
&[\hat{J}^2, \hat{J}_3] = [(\hat{J}_1{}^2 + \hat{J}_2{}^2 + \hat{J}_3{}^2), \hat{J}_3] = \\
&[\hat{J}_1{}^2, \hat{J}_3] + [\hat{J}_2{}^2, \hat{J}_3] + [\hat{J}_3{}^2, \hat{J}_3] = \\
&\hat{J}_1[\hat{J}_1, \hat{J}_3] + [\hat{J}_1, \hat{J}_3]\hat{J}_1 + \hat{J}_2[\hat{J}_2, \hat{J}_3] + [\hat{J}_2, \hat{J}_3]\hat{J}_2 = \\
&-\hat{J}_1\hat{J}_2 - \hat{J}_2\hat{J}_1 + \hat{J}_1\hat{J}_2 + \hat{J}_2\hat{J}_1 + \hat{J} = \hat{0} \qquad (3.3.1.1)
\end{aligned}$$

We have given some of the algebraic properties in an implicit manner. Record them for future use.

The final result is that $\hat{J}^2$ commute with all components of $\hat{J}$:

$$[\hat{J}^2, \hat{J}] = \hat{0} \qquad (3.3.1.2)$$

The construction of a complete base set employs $\hat{J}^2$ and one component $\hat{J}_k$ as a complete set of commuting operators; they provide appropriate labels: $|J, M_J\rangle$. The operators fulfill the eigen value equations:

$$\hat{J}^2 |J, M_J\rangle = \hbar^2 a_J |J, M_J\rangle \qquad (3.3.1.3)$$
$$\hat{J}_3 |J, M_J\rangle = \hbar M_J |J, M_J\rangle \qquad (3.3.1.4)$$

Let us find expressions for a_J and the range of M_J as a function of J. From now on $\hbar$=1.

We have shown that $\hat{J}^2$ commutes with $\hat{J}$, but used only one projection $\hat{J}_3$ to define the eigen value above. The operators $\hat{J}_1$ and $\hat{J}_2$ can be used to construct two non-Hermitian operators $\hat{J}_+$ and $\hat{J}_-$ called ladder operators.

3.3.2. Ladder operators

The ladder operators are defined as:

$$\hat{J}_+ = (\hat{J}_1 + i\,\hat{J}_2)$$
$$\hat{J}_- = (\hat{J}_1 - i\,\hat{J}_2) \qquad (3.3.2.1)$$

Note that the components of the angular momentum $\hat{J}_1$ and $\hat{J}_2$ do not commute; Cf. eq.(3.3.2). Instead, calculate now the commutation relations for the set $\hat{J}_+, \hat{J}_2$ and $\hat{J}_3$. The results are:

$$[\hat{J}_3,\ \hat{J}_+] = \hat{J}_+ \qquad (3.3.2a)$$
$$[\hat{J}_3,\ \hat{J}_-] = -\hat{J}_- \qquad (3.3.2b)$$
$$[\hat{J}_+,\ \hat{J}_-] = 2\,\hat{J}_3 \qquad (3.3.2c)$$

Vectors obtained from $\hat{J}_+|JM_J\rangle$ and $\hat{J}_-|JM_J\rangle$ can be worked out if we apply $\hat{J}_3$ from the left: $\hat{J}_3(\hat{J}_+ |J,M_J\rangle)$, and use of the commutation relations (3.3.2.2a) and (3.3.1.4) to get:

$$\hat{J}_3(\hat{J}_+ |J,M_J\rangle) = (\hat{J}_+\hat{J}_3)\,|J,M_J\rangle + (\hat{J}_+|J,M_J\rangle) =$$
$$(M_J+1)\,(\hat{J}_+|J,M_J\rangle) \qquad (3.3.2.3)$$

Thus, the vector $\hat{J}_+|J,M_J\rangle$ is proportional to $|J,M_J+1\rangle$. Now, apply $\hat{J}_+$ to vector $|J,M_J+1\rangle$ to gets a vector proportional to $|J,M_J+2\rangle$ and so on, until attaining the value J.

Taking operator $\hat{J}_-$ and successively apply to $|J,M_J\rangle$, the procedure leads from M_J-1, M_J-2 down to -J; below we cannot go. Given J, the projection may have a minimal and a maximum value, -J and J, respectively. The dimension (multiplicity) of this subspace is 2J+1.

Eq. (3.3.2c) is obtained once the products of ladder operators are constructed from the commutation relations:

$$\hat{J}_+\hat{J}_- = \hat{J}^2 - \hat{J}^2_3 + \hat{J}_3 \qquad (3.3.2.4a)$$
$$\hat{J}_-\hat{J}_+ = \hat{J}^2 - \hat{J}^2_3 - \hat{J}_3 \qquad (3.3.2.4b)$$

It is clear that the commutator $[\hat{J}_+\hat{J}_-, \hat{J}_-\hat{J}_+] = 2\hat{J}_3$.

Also, $\hat{J}_+\hat{J}_- + \hat{J}_-\hat{J}_+ = 2(\hat{J}^2 - \hat{J}_3^2)$ to get:

$$\hat{J}^2 = (1/2)(\hat{J}_+\hat{J}_- + \hat{J}_-\hat{J}_+) + \hat{J}_3^2 \qquad (3.3.2.5)$$

E&E.3.3.2-1. Calculate a_J

To get an answer take first the action of $\hat{J}_+\hat{J}_-$ because from eq. (3.3.3.4a) the calculation can be performed with the help of the eigen value equations for the angular momentum, (3.3.1.3) and (3.3.1.4). The results are:

$$\hat{J}_+\hat{J}_-|J,-J\rangle = (\hat{J}^2 - \hat{J}_3^2 + \hat{J}_3)\,|J,M_J=-J\rangle = (a_J - J^2 - J)\,|J,-J\rangle \qquad (3.3.2.6a)$$
$$\hat{J}_-\hat{J}_+|J,J\rangle = (\hat{J}^2 - \hat{J}^2_3 - \hat{J}_3)\,|J,M_J=J\rangle = (a_J - J^2 - J)\,|J,J\rangle \qquad (3.3.2.6b)$$

From the second equation, $\hat{J}_+|J,J\rangle$ must be equal zero thereby implying $(a_J - J^2 - J)=0$ and the result is

$$a_J = J^2 + J = J(J+1).$$

Now, $\hat{J}_-|J,-J\rangle$ must be zero, and eq. (3.3.3.6a) shows that again $a_J = J^2 + J = J(J+1)$. Thus, $a_J = J(J+1)$.

The value for a_J obtained above permits writing down the eigen value relations for the product operators $\hat{J}_+\hat{J}_-$ and $\hat{J}_-\hat{J}_+$:

$$\hat{J}_+\hat{J}_-|JM_J\rangle = (\hat{J}^2 - \hat{J}^2_3 + \hat{J}_3)\,|JM_J\rangle = (J(J+1) - M_J^2 + M_J)\,|JM_J\rangle \qquad (3.3.2.7a)$$
$$\hat{J}_-\hat{J}_+|JM_J\rangle = (\hat{J}^2 - \hat{J}^2_3 - \hat{J}_3)\,|JM_J\rangle = (J(J+1) - M_J^2 - M_J)\,|JM_J\rangle \qquad (3.3.2.7b)$$

Again, for a given J, the system shows a subspace of dimension 2J+1 covered by the projections M_J. Because the Hamiltonian commutes with $\hat{J}_3$ all these values label the same energy level: they are "degenerate". The base set |J,–J>, |J, -J+1>,…,|J,J-1>, |J,J> is complete for a given J.

For a given J, the projections M_J cover the range from –J, -J+1,…,J-1,J. The space has a multiplicity of 2J+1.

Total angular momentum quantum number J can have integer and half-integer values:

-Angular momentum: J = 0, 1/2, 1, 3/2, 2,…(3.3.2.8)
-Multiplicity: 2J+1 = 1, 2, 3, 4, 5,.. (3.3.2.9)

Singlet, doublet, triplet, quadruplet, quintuplet,… To close this section, let us give the expression for the ladder operators. From eq. (3.3.2.3) one can write

$$\hat{J}_+ |J,M_J\rangle = C(M_J+1)\, |J,M_J+1\rangle$$
$$\hat{J}_- |J,M_J\rangle = C(M_J-1)\, |J,M_J-1\rangle \quad (3.3.2.10)$$

Consider the maximum M_J =+J. Thus $\hat{J}_+ |J,J\rangle = C(J,J+1)\, |J, J+1\rangle$ must necessarily be zero. Thus, C(J,J +1)=0.

For the minimum value of the projection, M_J =-J. Thus $\hat{J}_- |J,-J\rangle = C(J,-J-1)\, |J, -J-1\rangle$ and again C(J,-J -1)=0. It can be shown that:

$$\hat{J}_+ |J,M_J\rangle = \sqrt{(J-M_J)(J+M_J+1)}\, |J,M_J+1\rangle \quad (3.3.2.11a)$$
$$\hat{J}_- |J,M_J\rangle = \sqrt{(J+M_J)(J-M_J+1)}\, |J,M_J-1\rangle \quad (3.3.2.11b)$$

E&E-3.3.2-2. Prove eqn(3.3.2.11a)
Observe that eq. (3.3.2.7a) can be multiplied by the bra $\langle JM_J|$ to get:

$$\langle JM_J| \hat{J}_- \hat{J}_+ |JM_J\rangle = (J(J+1) - M_J^2 - M_J) \langle JM_J| JM_J\rangle$$

By definition, $\langle JM_J| \hat{J}_- \hat{J}_+ |JM_J\rangle = |\hat{J}_+ |JM_J\rangle|^2$. Using the definition $\hat{J}_+ |J,J\rangle = C(J,J+1)\, |J, J+1\rangle$ one gets:

$$|C(J,J+1)|^2 = (J(J+1) - M_J^2 - M_J) =$$
$$(J-M_J)(J+M_J+1) \quad (3.3.2.13)$$

Retaining the positive sign in the square root one obtains eq. (3.3.2.11a).

3.3.3. Matrix representations

In general, given a base set such as the one for angular momenta or any other, Cf. eq.(2.1.1), a quantum state is represented by amplitudes obtained after projecting the state in that base set, eq.(2.1.2). An operator $\hat{O}$ acting on specific base set elements, say $|a_j\rangle$, generates a function in Hilbert space; this is a linear superposition. Use eq.(2.2.1) from the left to get:

$$\hat{O} |a_j\rangle = \hat{I}\, \hat{O} |a_j\rangle = \Sigma_i |a_i\rangle \langle a_i| \hat{O} |a_j\rangle =$$
$$\Sigma_i |a_i\rangle O_{ij} \quad (3.3.3.1)$$

The numbers O_{ij} arranged in a tableau of infinite rows and columns stands for the matrix representation of operator $\hat{O}$. The base set is understood. For finite dimension (m) base sets, the matrix is a square array of dimension m x m.

Some matrix representations of angular momentum operators in the base $\{|JM_J>\}$ follow from the eigen value equations and operator relationships. For each J-value there is a complete set of base function of dimension 2J+1.

$$1)\ <J'M'_{J'}|\ \hat{J}^2\ |J\ M_J> = \delta_{JJ'}\delta_{M'J'MJ}\ J(J+1) \qquad (3.3.3.2)$$

$$2)\ <J'M_{J'}|\ \hat{J}_3\ |J\ M_J> = \delta_{JJ'}\delta_{M'J'MJ}\ M_J \qquad (3.3.3.3)$$

$$3)\ <J'M'_{J'}|\ \hat{J}_1\ |J\ M_J> = (1/2)\ <J'M'_{J'}|\ (\hat{J}_+ + \hat{J}_-)|J\ M_J>\ \delta_{JJ'} \qquad (3.3.3.4)$$

$$4)\ <J'M'_{J'}|\ \hat{J}_2\ |J\ M_J> = (-i/2)\ <J'M'_{J'}|\ (\hat{J}_+ - \hat{J}_-)|J\ M_J>\ \delta_{JJ'} \qquad (3.3.3.5)$$

The operators of angular momentum in the base are block diagonal matrices. The case J=0 is a scalar base state.

E&E-3.3.3-1. Calculate the matrices corresponding to eqs.(.3.3.2)-(3.3.3.5) above for the case J=2

Once the J-value is fixed, the subspace has dimension 2J+1 corresponding to M_J that can change as –2,-1,0,1,2. The matrices will have 5x5 dimension.

-The matrix elements $<J'M'_{J'}|\ \hat{J}^2|JM_J> = \delta_{JJ'}\delta_{M'J'MJ}\ J(J+1)$ are independent from M_J thereby leading to a constant (diagonal) matrix: J(J+1) = 2(2+1)=6.

-The matrix elements $<J'M_{J'}|\ \hat{J}_3\ |J\ M_J> = \delta_{JJ'}\delta_{M'J'MJ}\ M_J$ with J=J' can be assembled in the diagonal matrix:

$$J_3=\begin{bmatrix}2&0&0&0&0\\0&1&0&0&0\\0&0&0&0&0\\0&0&0&-1&0\\0&0&0&0&-2\end{bmatrix}\quad J_1=\begin{bmatrix}0&1&0&0&0\\1&0&\sqrt{3/2}&0&0\\0&\sqrt{3/2}&0&\sqrt{3/2}&0\\0&0&\sqrt{3/2}&0&1\\0&0&0&1&0\end{bmatrix}\quad J_2=\begin{bmatrix}0&-i&0&0&0\\i&0&-\sqrt{3/2}i&0&0\\0&\sqrt{3/2}i&0&-\sqrt{3/2}i&0\\0&0&\sqrt{3/2}i&0&-i\\0&0&0&i&0\end{bmatrix}$$

Give an explicit calculation of matrices J_+ and J_-.

Using these matrices calculate explicitly the commutator: $J_1\ J_2 - J_2\ J_1$. Show that it is equal to iJ_3.

E&E-3.3.3-2 Calculate the matrices corresponding to eqs.(.3.3.2)-(3.3.3.5) above for the case J=1

3.3.4. Angular momentum and rotations

So far, there has been no mention on rotation matrices in real space and their connection with angular momentum. Quantum states in Hilbert space are totally independent on the way we put an inertial frame including any type of rotation. In standard approaches, a rotation is described either by causing the axes of the system of coordinates (I-frame) to rotate while holding the physical objects fixed or by holding the axis fixed and causing the inverse rotation of the physical system. In the quantum state view the "object" is replaced by the coordinates base states $|\mathbf{q}>$; there is a subtle shift from place (object location) to coordinate space where base state take central stage. There will always be (at least) two inertial frames involved to describe rotations. Thus either the I-frame rotate with base vector remains fixed or the base state vectors rotate with a fixed I-frame; in short, this is the reason for needing two frames as there are no objects; one describes the changes of quantum states of a material system, not the system itself.

The infinitesimal rotation operator in eq.(3.3.1) was suggested in analogy to time and space displacement operators. Angular momentum was defined via the commutation relations eq.(3.3.2). The real space labels, **n** and $d\phi$ enter as numeric factors affecting $\hat{J}$. It is apparent that taken $|\alpha>$ as a quantum state in Hilbert space, $\hat{D}(\mathbf{n},d\phi)|\alpha>$ does not make sense because the state $|\alpha>$ bear no connection to the parameters in real space. The ambiguity is eliminated if we work with this quantum state projected in configuration space:$<\mathbf{q}|\alpha> = \Psi_\alpha(\mathbf{q})$. A rotation cannot change the label α but it can change the argument of the wave function. Thus, bearing in mind that **R** is the rotation matrix associated to the operator one gets,

$$<\mathbf{q}|\hat{D}(\mathbf{n},d\phi) = <\mathbf{R}^{\dagger}(\mathbf{n},d\phi)\,\mathbf{q}| = <\mathbf{R}^{-1}(\mathbf{n},d\phi)\,\mathbf{q}| \quad (3.3.4.1)$$

and by right-multiplying with the quantum state $|\alpha>$:

$$<\mathbf{q}|\hat{D}(\mathbf{n},d\phi)|\alpha> = <\mathbf{R}^{-1}(\mathbf{n},d\phi)\mathbf{q}\,|\,\alpha> = \Psi_\alpha(\mathbf{R}^{-1}(\mathbf{n},d\phi)\,\mathbf{q}) \quad (3.3.4.2)$$

The state label remains invariant while the wave function depends upon rotation parameters.

Euler angles are customary used to define rotations. Take the I-frame as fixed with the unit vectors. $\mathbf{i}_1$, $\mathbf{i}_2$, $\mathbf{i}_3$ and the rotated frame : $\mathbf{i'}_1$, $\mathbf{i'}_2$, $\mathbf{i'}_3$. To find the rotation axis allowing for a rotation from $\mathbf{i}_3$ to $\mathbf{i'}_3$ consider the $(\mathbf{i}_1, \mathbf{i}_2)$-plane intersecting the $(\mathbf{i'}_1, \mathbf{i'}_2)$-plane. The intersection line defines a vector from the common origin in the direction of the wedge product $\mathbf{i}_3 \wedge \mathbf{i'}_3$. This is called **n**-axis in what follows. The angles $\angle(\mathbf{i}_2,\mathbf{n}) = \alpha$; $\angle(\mathbf{i}_3,\mathbf{i'}_3) = \beta$ and $\angle(\mathbf{n}, \mathbf{i'}_2) = \gamma$ are known as

Euler angles. The rotation matrix $\mathbf{R}(\alpha,\beta,\gamma)$ can be written after some manipulations starting from the original one, $\mathbf{R}_{i'1}(\gamma)\mathbf{R}_{n}(\beta)\ \mathbf{R}_{i1}(\alpha)$ as:

$$\mathbf{R}(\alpha,\beta,\gamma) = \mathbf{R}_{i1}(\alpha)\ \mathbf{R}_{n}(\beta)\ \mathbf{R}_{i'1}(\gamma) \qquad (3.3.4.3)$$

Using a series of properties, the rotation matrices can be expressed in terms of the original axis. The corresponding operator form is given by :

$$\hat{D}(\alpha,\beta,\gamma) = \exp(-i\,\hat{J}_{i3}\,\alpha/\hbar)\exp(-i\,\hat{J}_{i2}\,\beta/\hbar)\exp(-i\,\hat{J}_{i3}\,\gamma/\hbar) \qquad (3.3.4.4)$$

Rotation functions $D_{MM'}^{(J)}(\alpha,\beta,\gamma)$ are defined as:

$$D_{MM'}^{(J)}(\alpha,\beta,\gamma) = \langle JM|\,\hat{D}(\alpha,\beta,\gamma)|JM'\rangle \qquad (3.3.4.5)$$

Note that even if the rotations referred to one frame, a second fame there is always involved.

3.4. Addition of angular momenta

This is a key theme helping in the construction of base states for complex systems. Only some basic elements are presented here. Again, at this stage focus is on the construction of base set labels characterizing the invariance of a quantum state towards the way we have oriented the I-frame; only one I-frame is involved, unless specific indications on the contrary.

3.4.1. Addition of two angular momenta

Let consider the addition of two angular momentum operators for generic systems 1 and 2, $\hat{j}_1$ and $\hat{j}_2$ leading to a total angular momentum $\hat{j}$:

$$\hat{j} = \hat{j}_1 + \hat{j}_2 \qquad (3.4.1.1)$$

In their respective domains the eigen equations are:

$$(\hat{j}_1)^2\,|j_1m_1\rangle = j_1(j_1+1)\,|j_1m_1\rangle \text{ and}$$
$$(\hat{j}_1)_3\,|j_1m_1\rangle = m_1|j_1m_1\rangle \qquad (3.4.1.2)$$

$$(\hat{j}_2)^2 |j_2 m_2\rangle = j_2(j_2+1) |j_2 m_2\rangle \text{ and}$$
$$(\hat{j}_2)_3 |j_2 m_2\rangle = m_2 |j_2 m_2\rangle \qquad (3.4.1.3)$$

Now, $(\hat{j})^2 |j\ m\rangle = j(j+1) |j\ m\rangle$ and $(\hat{j})_3 |j\ m\rangle = m |j\ m\rangle$.

The dimension of j-space must equal that of the direct product $(2j_1+1)(2j_2+1)$ if subsystems are independent. The commutator $[(\hat{j})_1,(\hat{j})_2] = \hat{0}_{12}$ because the operators act on different subspaces. There are two sets of commuting operators:

$$\{(\hat{j}_1)^2, (\hat{j}_1)_3, (\hat{j}_2)^2, (\hat{j}_2)_3\} \text{ and}$$
$$\{(\hat{j})^2, (\hat{j})_3, (\hat{j}_1)^2, (\hat{j}_2)^2\} \qquad (3.4.1.5)$$

The quantum labels are:

$$\{j_1, j_2, m_1, m_2\} \text{ and}$$
$$\{j, m, j_1, j_2\} \qquad (3.4.1.6)$$

The joint base sets are:

$$\{|j_1, j_2, m_1, m_2\rangle\} \text{ and}$$
$$\{|j, m, j_1, j_2\rangle\} \qquad (3.4.1.7)$$

The problem is to find all possible values for $\hat{j}$ knowing those of $\hat{j}_1$ and $\hat{j}_2$. The direct product set $\{|j_1 m_1\rangle|j_2 m_2\rangle\}$ provides a complete base set. We know that $\{|jm\rangle\}$, the eigen vectors of the total angular momentum provides a complete base set of dimension 2j+1. The dimension $(2j_1+1)(2j_2+1)$ of the direct product space is then 2j+1. The problem is to find the matrix elements of the unitary transformation between both, equivalent, base sets. They are the Clebsch-Gordan coefficients.

First we give the relationship between j_1, j_2 and j. The maximum value of j is just j_1+j_2; j will decrease by one unit until getting at $|j_1-j_2|$. That's it.

$$|j_1 - j_2| \le j \le j_1 + j_2 \qquad (3.4.1.8)$$

Thus, if we combine two systems, $j_1 = 8$ and $j_2=3$, the allowed values of j are: 11,10,….4,5. The projections fulfill the rule: $m=m_1+m_2$; and $-j \le m \le j$. There is no more to it. Now, go for the base functions.

The dimension covered by both base sets of eq.(3.4.7) are then equal to the numeric value 2j+1 that by construction equals the product $(2j_1+1)(2j_2+1)$. The base set elements of one set can be expanded on the other, the amplitudes are called Clebsch-Gordan coefficients.

3.4.2. Clebsch-Gordan coefficients

The unit operators in the direct product space and in j-space are:

$$\hat{I} = \Sigma_{m1m2} \{|j_1m_1>|j_2m_2>\}\{< j_1m_1|< j_2m_2|\} = \Sigma_{m1m2} |j_1m_1,j_2m_2>< j_1m_1, j_2m_2| \quad (3.4.2.2)$$

The index m_1 varies from - j_1 up to +j_1; m_2 range from – j_2 up to +j_2.

$$\hat{I} = \Sigma_m|jm><j\ m| \quad (3.4.2.3)$$

The index m varies from –j up to +j.

Let us calculate the base state |jm> in the direct product base set:

$$|jm> = \hat{I}\ |jm> = \Sigma_{m1m2} |j_1m_1,j_2m_2>< j_1m_1, j_2m_2|jm> \quad (3.4.2.4)$$

The corresponding Clebsch-Gordan amplitude (coefficient) is then:

$$C(j_1j_2m_1m_2;jm) = < j_1m_1, j_2m_2|jm> \quad (3.4.2.5)$$

Calculate the amplitudes the other way round:

$$|j_1m_1,j_2m_2> = \hat{I}\ |j_1m_1,j_2m_2> = \Sigma_m|jm><j\ m|j_1m_1,j_2m_2> \quad (3.4.2.6)$$

We can see that the amplitudes taken as a transpose and complex conjugating leads to:

$$<j\ m|j_1m_1,j_2m_2> = (< j_1m_1, j_2m_2|jm>)^{\dagger} = C(j_1j_2m_1m_2;jm) \quad (3.4.2.7)$$

It is common practice to have real amplitudes; thus, complex conjugation is superfluous, only transposition survives.

3.4.3. Wigner coefficients: 3j symbols

Any field of scientific research develops historically. This means that people in different societies come up with related discoveries. Without entering in more detail about history, let us introduce some symbols that are presently used in connection with angular momentum. Note that there is no rational explanation to the question why they look the way they do.

An example of these coefficients is known as 3j symbols defined as:

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} = (-1)^{j1-j2-m3}(2j_3+1)^{-1/2}\, C(j_1j_2m_1m_2;jm) \quad (3.4.3.1)$$

Where we substitute j_3=j and m_3=m.

There are a number of symmetry rules verified by these 3j symbols:

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} = \begin{pmatrix} j_2 & j_3 & j_1 \\ m_2 & m_3 & m_1 \end{pmatrix} = \begin{pmatrix} j_3 & j_1 & j_2 \\ m_3 & m_1 & m_2 \end{pmatrix} \qquad (3.4.3.2)$$

These correspond to cyclic permutation of indexes. To break cyclic ordering once and the 3j symbol must be multiplied by $(-1)^{j1+j2+j3}$; also, if we substitute m_1,m_2,m_3 by $-m_1,-m_2,-m_3$, e.g.

$$(-1)^{j1+j2+j3}\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} = \begin{pmatrix} j_3 & j_2 & j_1 \\ m_3 & m_2 & m_1 \end{pmatrix} = \begin{pmatrix} j_1 & j_2 & j_3 \\ -m_1 & -m_2 & -m_3 \end{pmatrix} \qquad (3.4.3.3)$$

3.4.4. Addition of three angular momenta

By definition, there are three different angular momentum operators and the resultant vector operator is sought: $\hat{J} = \hat{j}_1 + \hat{j}_2 + \hat{j}_3$. There is no unique procedure to get a result. The problem can be reduced to addition of two angular momenta, $\hat{J}_{ij} = \hat{j}_i + \hat{j}_j$, the result is combined with the remaining operator again as a sum of two angular momenta: $\hat{J}_{ij} + \hat{j}_k$.

Select two complete sets of commuting operators:

i) $\{(\hat{j}_1)^2, (\hat{j}_1)_3, (\hat{j}_2)^2, (\hat{j}_2)_3, (\hat{j}_3)^2, (\hat{j}_3)_3\}$ with base set:
$\{|j_1m_1j_2m_2j_3m_3>\}$

ii) $\{(\hat{j}_1)^2, (\hat{j}_2)^2, (\hat{j}_3)^2, (\hat{j}_{ij})^2, (\hat{j})^2, (\hat{j})_3\}$ with base set:
$\{|j_1j_2j_3j_{ij}jm>\}$

$j_{ij} = (j_i + j_j), (j_i + j_j)-1,\ldots,|(j_i - j_j)|$
$j = (j_{ij} + j_k), (j_{ij} + j_k)-1,\ldots,|(j_{ij} - j_k)|$
$m_{ij} = m_i+m_j$, $m = m_{ij} + m_k = m_1 + m_2 + m_3$
$m_i = j_i, j_i -1,\ldots,- j_i$

3.4.5. 6j-symbols

Consider the linear superposition using the base set $|j_1m_1j_2m_2j_3m_3\rangle$ to represent the base vectors $|j_1j_2j_3j_{ij}jm\rangle$:

$$|j_1j_2j_3j_{ij}jm\rangle = \Sigma \langle j_im_ij_jm_j|j_1j_2j_3j_{ij}m_{ij}\rangle \langle j_{ij}m_{ij}j_km_k|j_1j_2j_3j_{ij}jm\rangle \; |j_1m_1j_2m_2j_3m_3\rangle \qquad (3.4.5.1)$$

The sum covers all possible values for m_1, m_2, m_3 and m_{ij} with the corresponding Clebsh-Gordan coefficients.

The inverse transformation is given by:

$$|j_1j_2j_3j_{ij}jm\rangle = \Sigma\,(j_{jk}) \langle j_1j_2j_3j_{jk}jm|\, j_1j_2j_3j_{ij}jm\rangle \,|\, j_1j_2j_3j_{jk}jm\,\rangle \qquad (3.4.5.2)$$

The amplitudes $\langle j_1j_2j_3j_{jk}jm|\, j_1j_2j_3j_{ij}jm\rangle$ will be given in terms of 6j coefficients $\begin{pmatrix} j_1 & j_2 & j_{jk} \\ j_3 & j & j_{ij} \end{pmatrix}$ that are defined by:

$$\langle j_1j_2j_3j_{jk}jm|\, j_1j_2j_3j_{ij}jm\rangle = (-1)^{j1+j2+j3+j}\,[(2j_{ij}+1)(2j_{jk}+1)]^{1/2} \begin{pmatrix} j_1 & j_2 & j_{jk} \\ j_3 & j & j_{ij} \end{pmatrix} = [(2j_{ij}+1)(2j_{jk}+1)]^{1/2}\, W(j_1j_2jj_3;j_{jk}\, j_{ij}) \qquad (3.4.5.3)$$

$W(j_1j_2jj_3;j_{jk}\, j_{ij})$ is known as Racah coefficient; its definition follows by combining the last two lines above.

The base sets label with so related quantum numbers is actually fixed. You can then go to special tables to read the actual values. Usually, a given problem can be formulated in one base set but the physics may require another one. Then, it is useful to know al least the way the connections are defined and the meaning of the symbols. More on this will be found in the following sections.

3.5. Orbital and spin base functions

The number of electrons and number and types of nuclei define the material system at hand, in analytical chemistry terms. The quantum states in Hilbert space and in the fence domain correspond to spin 1/2 for 1-electron states and a variety of nuclear spins, I ranging from half odd integers to integers. A general theory can be done for electron states; they show a peculiar relationship between spin and permutation properties of the n-electron space base functions. The spin/space base functions are anti-symmetric under odd permutation of the labels.

3.5.1. Orbital angular momentum; Spherical harmonics

The orbital angular momentum operator $\hat{L}$ takes on the form from the classical expression:

$$\hat{L} = \hat{q} \wedge \hat{p} \qquad (3.5.1.1)$$

Equation (3.2.2.3) besides Planck constant introduces the gradient operator such that the components read:

$$\begin{aligned} \hat{L}_1 &= -i\hbar\,(\hat{q} \wedge \nabla)_1 = -i\hbar\,(\hat{q}_2 \nabla_3 - \hat{q}_3 \nabla_2) \\ \hat{L}_2 &= -i\hbar\,(\hat{q} \wedge \nabla)_2 = -i\hbar\,(\hat{q}_3 \nabla_1 - \hat{q}_1 \nabla_3) \\ \hat{L}_3 &= -i\hbar\,(\hat{q} \wedge \nabla)_3 = -i\hbar\,(\hat{q}_1 \nabla_2 - \hat{q}_2 \nabla_1) \end{aligned} \qquad (3.5.1.2)$$

With the help of relationships eq.(3.2.2.4) it is easy to show the commutation relations for the components of $\hat{L}$ actually define an angular momentum. Spherical polar coordinates are used to transform the operator equations (3.5.1.2):

$$\begin{aligned} &q_1 = |\mathbf{q}|\sin\theta\cos\phi;\ q_2 = |\mathbf{q}|\sin\theta\sin\phi;\ q_1 = |\mathbf{q}|\cos\theta \\ &\mathbf{q}^2 = q_1^2 + q_2^2 + q_3^2; \\ &\cos\theta = q_3/|\mathbf{q}|\ ;\ \tan\phi = q_2/q_1 \end{aligned} \qquad (3.5.1.3)$$

Equations (3.5.1.2) become

$$\begin{aligned} \hat{L}_1 &= i\,(\sin\phi\,\partial/\partial\theta + \cot\theta\cos\phi\,\partial/\partial\phi) \\ \hat{L}_2 &= i\,(-\cos\phi\,\partial/\partial\theta + \cot\theta\sin\phi\,\partial/\partial\phi) \\ \hat{L}_3 &= -i\,(\partial/\partial\phi) \end{aligned} \qquad (3.5.1.4)$$

A spinless base state besides the base ket $|L,M_L>$, there is a radial quantum number (n) with a radial function $F_{nL}(r)$ that contains dynamic information. Consider the vector **q'** in spherical coordinates so that **n'** is a unit vector in the direction θ,ϕ of **q'**, then

$$<\mathbf{n}'|L,M_L> = Y_L^{ML}(\theta,\phi) \qquad (3.5.1.1)$$

$Y_L^{ML}(\theta,\phi)$ is a spherical harmonic. The spinless base set function remains useful for any system state invariant to frame rotations; a fortiori, it is valid whenever a system retains spherical symmetry. Because the base set is complete, the angular part of any quantum state can be expressed as a linear superposition in this base. Again, we are about to treat quantum states not material systems as objects. The eigen value equations are:

$$\hat{L}^2\, Y_L^{ML}(\theta,\phi) = \hbar^2\, L(L+1)\, Y_L^{ML}(\theta,\phi), \qquad (3.5.1.2)$$

$$\hat{L}_3\, Y_L^{ML}(\theta,\phi) = \hbar\, M_L\, Y_L^{ML}(\theta,\phi)\ ;\ -L \le M_L \le L \qquad (3.5.1.3)$$

L=0,1,2,3…The operators $\hat{L}^2$ and $\hat{L}_3$ must be taken as projected in the I-frame space. We give their form:

$$\hat{L}^2 \rightarrow \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2} \qquad (3.5.1.4)$$

Spherical harmonics are eigenfunctions of this operator that appears as the angular part of $\nabla\cdot\nabla = \nabla^2$ (nabla square) that is the operator characterizing kinetic energy in an inertial Cartesian frame. Bearing in mind that the spherical harmonic can be written as a product: $Y_L^{ML}(\theta,\phi) = \Phi^{ML}(\phi)\,\Theta_L^{ML}(\theta)$, where $(\partial^2/\partial\phi^2)\,\Phi^{ML}(\phi) = -M_L^2\,\Phi^{ML}(\phi)$ then the theta part fulfils the differential equation:

$$\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + L(L+1) - M_L^2/\sin^2\theta\right)\Theta_L^{ML}(\theta) = 0 \qquad (3.5.1.5)$$

Rotation matrices and spherical harmonics are closely related. Assign $\ell \rightarrow L$, $m \rightarrow M_L$ Matrix elements of a rotation operator with the angular momentum base set define the matrix: $\langle \ell\, m'|\hat{D}(\mathbf{R})|\,\ell\, m\rangle = \mathcal{D}_{mm'}^{(\ell)}(\alpha,\beta,\gamma)$. The operator should transform the base ket $|\mathbf{i}_3\rangle$ into a ket associated to the rotation unit vector $|\mathbf{n}'\rangle$ identified with Euler angles (α,β,γ): $|\mathbf{n}\rangle = \hat{D}(\mathbf{R})\,|\mathbf{i}_3\rangle$. Take the simple case where first rotate around 2-axis by θ, and by φ around the 3-axis, then $\beta\rightarrow\theta$ and $\alpha\rightarrow\phi$ and $\gamma=0$, the operator $\hat{D}(\mathbf{R}) = \hat{D}(\alpha,\beta,\gamma)$, and for the present case $\hat{D}(R) = \hat{D}(\alpha=\phi,\beta=\theta,\gamma=0)$, to finally get

$$|\mathbf{n}\rangle = \hat{D}(R)\,|\mathbf{i}_3\rangle = \Sigma_\ell\,\Sigma_m\,\hat{D}(R)\,|\,\ell\, m\rangle\langle\ell\, m|\mathbf{i}_3\rangle \qquad (3.5.1.6)$$

Calculate now $\langle\ell\, m'|\,\mathbf{n}\rangle$ to get

$$\langle\ell\, m'|\,\mathbf{n}\rangle = \Sigma_m\,\mathcal{D}_{mm'}^{(\ell)}(\alpha=\phi,\beta=\theta,\gamma=0)\,\langle\ell\, m|\mathbf{i}_3\rangle \qquad (3.5.1.7)$$

The function $\langle\ell\, m|\mathbf{i}_3\rangle$ correspond to the spherical harmonic $Y_\ell^{m*}(\theta,\phi)$ evaluated at $\theta=0$ at an undetermined φ and

$$\langle\ell\, m|\mathbf{i}_3\rangle = Y_\ell^{m*}(\theta=0,\phi) = \sqrt{((2\ell+1)/4\pi)}\,\delta_m \qquad (3.5.1.8)$$

The rotation operator matrix elements read $\beta\rightarrow\theta$

$$\mathcal{D}_{mm'}^{(\ell)}(\alpha=\phi,\beta=\theta,\gamma=0) = \left(\sqrt{((2\ell+1)/4\pi)}\right)^{-1}\,Y_\ell^{m*}(\theta,\phi)\,\big|_{\theta=\beta,\phi=\alpha} \qquad (3.5.1.9)$$

The actual derivation of this result is not as important as the relationship expressed in eq. (3.5.1.9) relating spherical harmonics to rotation functions.

Take one I-frame as fixed with the unit vectors. $\mathbf{i}_1$, $\mathbf{i}_2$, $\mathbf{i}_3$ and the rotated frame : $\mathbf{i'}_1$, $\mathbf{i'}_2$, $\mathbf{i'}_3$. You have above the way to set up the appropriate base set to represent rotated quantum states. If the symmetry of the material system is lower, the quantum states will reflect that situation.

3.5.2. Spin 1/2 angular momentum

Angular momentum with odd half integer is named as spin. For electron states, with 1, 2, 3,… base states, the total spin changes from 1/2 up to an integer if the number of base states is even and half integer if that number is odd:

$$\hat{S}^2 |S,M_S\rangle = \hbar^2 S(S+1) |S,M_S\rangle$$
$$S=1/2,1,3/2,2,5/2,3,\ldots \qquad (3.5.2.1)$$
$$\hat{S}_3 |S,M_S\rangle = \hbar M_S |S,M_S\rangle; \; -S \leq M_S \leq S \qquad (3.5.2.2)$$

Combined with the symbols for orbital angular momentum L=0 → S, L=1 → P, L=2 → D, L=3 → E, L=4 → F, etc., the spin multiplicity appears as a left supra index and total angular momentum as right sub index: $^{2S+1}L_J$. Rules for addition of angular momenta are examined below (Sect.3.5.3).

For a one-electron spin base J=1/2=s; low case letters are used to indicate single electron base configurations. The multiplicity is 2s+1=2, the operators are given by sets of 2x2 matrices known as Pauli matrices that we construct below.

Particle-states of spin 1/2 have three basic properties:

-1) The vector operator $\hat{S}$ does not depend upon space coordinates.

-2) The addition of $\hat{L}$ and $\hat{S}$ leads to the total angular momentum operator $\hat{J}$.

-3) A spin quantum state |s> is a linear superposition in the base set with elements:

$$|S=1/2,M_S=+1/2\rangle \text{ and } |S=1/2,M_S=-1/2\rangle.$$

It is common practice to alleviate this nomenclature to write |1/2> and |-1/2> or |+> and |-> or in some other cases |0> and |1>. Thus, using the symbol [<+1/2|s> <-1/2|s>] as a column vector where its elements are the amplitudes of the linear superposition and the row vector (|+1/2> |-1/2>) the element of which are the base vectors the quantum state |s> can be cast in two complementary ways as:

$$|s\rangle = \langle 1/2|s\rangle |1/2\rangle + \langle -1/2|s\rangle |-1/2\rangle =$$
$$(|+1/2\rangle \; |-1/2\rangle) \cdot [\langle +1/2|s\rangle \; \langle -1/2|s\rangle] \qquad (3.5.2.3)$$

If the system is in the state [1 0] we see that |s> maps directly onto |+1/2> according to the first line in this equation while the second line emphasizes the fact that the basis functions actually do not "disappear". The state [1 0] is known as a pure state. Also, [0 1] is another pure state.

The direction 3 is taken to carry out a measurement of $\hat{S}$, the result can be only one of its two eigen values, $+\hbar/2$ or $-\hbar/2$. Notation has been simplified. The case where the measurement direction differs from the standard one is examined below.

Pauli spin operators $\{\hat{\sigma}_j\}_{j=1,2,3}$ are simply defined as:

$$\hat{s}_j = (\hbar/2)\ \hat{\sigma}_j ;\ j=1,2,3 \qquad (3.5.2.4)$$

The commutation relations permit writing down the matrices in the base set [|+1/2> |-1/2>]:

$$\hat{\sigma}_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}; \qquad \hat{\sigma}_2 = \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix};$$
$$\hat{\sigma}_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \qquad (3.5.2.5)$$

1-electron spin space. There are subtle relationships between rotations in real space and spinorial quantities. Whatever the direction of spin quantization you may choose, the base states will always be [|+1/2> |-1/2>]; but if you look at the projections from the original frame things look differently.

In terms of Pauli 2x2 matrices spin vector operator $\hat{s}=(\hat{s}_1, \hat{s}_2, \hat{s}_3)$ is similar to those found in eq.(3.5.1.4). The base set in quantum chemical pictorial labeling is column vector [|↑> |↓>] for so-called spin up and down states;

$$\hat{s}_3|\uparrow> = (1/2)\,|\uparrow>,\ \hat{s}_3|\downarrow> = -(1/2)\,|\downarrow>$$
$$\hat{s}^2|\downarrow> = (1/2)\,(1/2+1)\,|\downarrow> = 3/4\,|\downarrow>;$$
$$\hat{s}^2|\uparrow> = (1/2)\,(1/2+1)\,|\uparrow> = 3/4\,|\uparrow>.$$

With a transpose conjugate of the base row vector defining a column base vector in bra-space, a 2x2 unit matrix operator is given as:

$$\underline{\underline{\mathbf{1}}} = (<\uparrow| \ <\downarrow|) \otimes [|\uparrow> \ |\downarrow>]$$

The unit operator $\hat{1} = |\uparrow><\uparrow| + |\downarrow><\downarrow|$ completes the mathematical objects used in this context.

For a one-electron system, an arbitrary quantum spin state (|Z>) is a linear superposition:

$$|Z> = \hat{1}\,|Z> = (|\uparrow><\uparrow| + |\downarrow><\downarrow|\,)\,|Z> =$$
$$|\uparrow>\,\alpha(Z) + |\downarrow>\,\beta(Z) =$$
$$(|\uparrow> \ \ |\downarrow>) \bullet [\alpha(Z) \ \ \beta(Z)] \qquad (3.5.2.6)$$

The amplitudes $\alpha(Z) = <\uparrow|\ Z>$ and $\beta(Z) = <\downarrow|\ Z>$ define the quantum state and are represented by a column vector.

The states |Z=0> and |Z=1> relate to standard spin representation used in molecular physics; these states are defined by $\alpha(Z=0)=1, \beta(Z=0) = 0$ and $\alpha(Z=1)= 0, \beta(Z=1) = 1$. The α and β spin functions commonly used in chemistry must be mapped to the row vectors (1 0) for α and (0 1) for β ; $< Z'=1| Z=0> = 0$. Thus the correct representation of quantum state |Z> is given by the second line of eq.(3.5.2.6). The spin space is two dimensional; this is the aspect that must be emphasized and one should understand the first line in the above equation as a short hand notation. Thus the base is just: (α β) $\Leftrightarrow$($|\uparrow>$ $|\downarrow>$) while the *quantum state* is given as a column spinor, [C_α C_β]. To this column vector corresponds a quantum state $|\psi> = [C_\alpha \; C_\beta]$. As usual, the amplitudes are a function of the quantum state, namely, $C_\alpha(\psi) = <\uparrow|\psi>$ and $C_\beta(\psi) = <\downarrow|\psi>$.

The apparatuses designed to measure spin-related responses are local. Let $\mathbf{e}_1$, $\mathbf{e}_2$, $\mathbf{e}_3$ be orthonormal unit vectors and found the direction of the spinor [C_α C_β] with respect to the unit vector $\mathbf{e}_3$. For the quantum state $|\psi>$ the set of numbers $\{<\psi| \underline{\boldsymbol{\sigma}}_i |\psi> = n_i\}$ form the components of a unit vector **n**:

$$n_1= C_\alpha C_\beta^* + C_\alpha^* C_\beta;\; n_2= i(C_\alpha C_\beta^* - C_\alpha^* C_\beta);$$
$$n_3= C_\alpha C_\alpha^* - C_\beta^* C_\beta. \qquad (3.5.2.7)$$

These components are real numbers. Calculating $|\mathbf{n}|^2$ from the components we check that it is a unit vector in 3-space. Introducing polar coordinates one gets for a unit vector **n**: $n_1= \sin(\theta)\cos(\phi)$; $n_2= \sin(\theta)\sin(\phi)$; $n_3= \cos(\theta)$ where θ is the angle between **n** and the frame 3-axis, ϕ is the angle between 1-axis and the projection of **n** on the (1,2)-plane, i.e. $|\mathbf{n}|\sin(\theta)$.

In Hilbert space, $C_\alpha = \cos(\theta/2)\exp(i\gamma)$ and $C_\beta = \sin(\theta/2)\exp(i\delta)$. Using the definition $\phi = (\gamma-\delta)/2$ the quantum state in spinorial form is given as:

$$|\psi> \rightarrow$$
$$[\cos(\theta/2)\exp(-i\phi/2) \quad \sin(\theta/2)\exp(i\phi/2)]\exp(i(\gamma+\delta)/2) \qquad (3.5.2.8)$$

The overall phase is usually ignored; observe, however, that this phase contains information about the frame orientation with respect to one that is fixed. Thus, $|\psi>$ relates Hilbert space quantum state amplitudes C_α and C_β to the real 3-space unit vector. Note the change from θ to $\theta/2$ implied by the map.

A different situation obtains if the axis **n** stands for an external field of an apparatus (e.g. Stern-Gerlach) that can be changed at will by an experimenter; this is equivalent to a “rotating” frame. But the quantization direction is fixed as we use a canonical base set; but the direction of measurement is different. We want the result expressed in the canonical base so one can compare results with respect to a fixed frame.

Let the direction **n** may signal a rotated 3-axis using an axis perpendicular to the plane made by $\mathbf{e}_3$ and **n**. For $\phi=0$, $\mathbf{e}_1$-axis is the rotation axis.

In this new frame **n** can be taken as spin state quantization direction; note that you will be carrying on the experiments and decide about axes. If we want to measure the spin state with respect to the un-rotated frame the result is embodied in the amplitudes of eq.(3.5.2.5) below. Calculate the spin components after a rotation moving 3-axis to direction **n** with rotation axis perpendicular to the plane ($\mathbf{e}_3$,**n**); the rotation matrix in Hilbert space is given by the matrix elements: $R_{11}=R_{22}= \cos(\theta/2)$, $R_{12} = -\sin(\theta/2)$ and $R_{21}= \sin(\theta/2)$ and the rotated 2-spinor is (fixed frame):

$$[C_\alpha{}^{rot}\ \ C_\beta{}^{rot}] \rightarrow$$
$$[\{C_\alpha\cos(\theta/2)-C_\beta\sin(\theta/2)\}\quad \{C_\alpha\sin(\theta/2) + C_\beta\cos(\theta/2)\}] \qquad (3.5.2.9)$$

Consider the case $C_\alpha = 1$ and $C_\beta = 0$; this spin-polarized system becomes: $[\cos(\theta/2)\ \sin(\theta/2)]$. Now, for $\theta=\pi$ the spinor is [0 1]. Polarization is inverted. Rotating the measuring frame by $\theta=2\pi$ one gets [-1 0], the quantum state is reflected compared to the initial one. And, taking the measuring system frame with $\theta=\pi/2$, a linear superposition with equal amplitudes obtains.

In general, non-zero amplitudes indicate that the canonical quantization direction has been rotated. Moreover, the number of spin states is infinite while the material system is just one "particle" in real space. A particle model is then rather unsuitable in abstract spin space.

3.5.3. Electron-state base functions

An electron base state correspond to angular momentum J=1/2 multiplied by a space base function. The space base function is label with integer Js and a radial function independent from orientation. These are spin ($\hat{S}$) and orbital ($\hat{L}$) angular momenta. The total angular momentum for base states is $\hat{J}= \hat{L} + \hat{S}$.

For a material system with n-electrons, the orbital and spin angular momentum operators are taken as the sum of elementary momentum $\hat{l}_i$ and $\hat{s}_i$:

$$\hat{L} = \Sigma_i\ \hat{l}_i\ ;\ \ \hat{S}.= \Sigma_i\ \ \hat{s}_i\ ; \text{ and}$$
$$\hat{J}= \Sigma_i\ \hat{j}_i = \hat{L} + \hat{S} = \Sigma_i\ (\hat{l}_i + \hat{s}_i) \qquad (3.5.3.1)$$

The eigen value equations are

$$(\hat{l}_i)^2\ |l_i\ m_{li}> = \hbar^2\ l_i(l_i+1)\ |l_i\ m_{li}> \qquad (3.5.3.2)$$

and

$$(\hat{l}_i)_3 |l_i\ m_{li}\rangle = \hbar\ m_{li} |l_i\ m_{li}\rangle \qquad (3.5.3.3)$$

For the spin:

$$(\hat{s}_i)^2 |s_i\ m_{si}\rangle = \hbar^2\ s_i(s_i+1) |s_i\ m_{si}\rangle \qquad (3.5.3.4)$$

and

$$(\hat{s}_i)_3 |s_i\ m_{si}\rangle = \hbar\ m_s |s_i\ m_{si}\rangle \qquad (3.5.3.5)$$

E&E.3.5-1. Calculate atomic states for specific configurations

Consider O^{+3} (OIII) with the configuration $1s^2 2s^2 2p3d$ determine the electronic states $^{2S+1}L_J$. The spectroscopic symbols are: L=1→S; L=2→P; L=3→D; L=4→F.

$L=\Sigma_i\ l_i$ for the present case only open shells contribute. Then L=2+1, and the range for the states is L=3,2,|3-2|. Thus, we have states P,D,F.

$S=\Sigma_i\ s_i = 1/2 + 1/2 = 1$. Possible values S=1,0; multiplicities 3 (triplet) and 1(singlet).

In the Russel-Saunders scheme there are the following states: ^{3}F and ^{1}F; ^{1}D and ^{3}D; ^{1}P and ^{3}P.

Calculate the values of J=L+S.

Take ^{3}F corresponding to 3+1=4=J. Thus J=4,3,|3-1|. We get: $^3F_2$, $^3F_3$, $^3F_4$.

Take ^{1}F corresponds to J=3: $^1F_3$ is the only J-term. Calculate the remaining cases.

3.5.4. Nuclear spin systems

Spin quantum numbers I for nuclei varies from I=0 up in units of spin 1/2: 0,1/2,1,3/2,…. The standard base functions fulfill equations:

$$\hat{I}^2 |I,M_I\rangle = \hbar^2\ I(I+1) |I,M_I\rangle \qquad (3.5.4.1)$$

I=0,1/2,1,3/2,2,5/2,3,…

$$\hat{I}_3 |I,M_I\rangle. = \hbar\ M_S |I,M_I\rangle. \quad -I \le M_I \le I \qquad (3.5.4.2)$$

The commutation relations between the components of $\hat{I}$ and $\hat{I}^2$ are similar to those defined for the generic angular momentum operator, $\hat{J}$.

For a set of m-nuclei relations similar to eqs.(3.3.4.1):

$$\hat{I} = \Sigma_{k=1,m}\ \hat{I}_k \qquad (3.5.4.3)$$

Each individual nuclear angular momentum fulfill the standard equations:

$$(\hat{I}_k)^2 |I_k,M_{Ik}\rangle = \hbar^2\ I_k\ (I_k+1) |I_k,M_{Ik}\rangle \qquad (3.5.4.4)$$

$$(\hat{I}_k)_3 |I_k,M_{Ik}\rangle = \hbar\ M_{Ik} |I_k,M_{Ik}\rangle \qquad (3.5.4.5)$$

Now, the total angular momentum reads, $\hat{J}+\hat{I}=\hat{F}$.

The matrix elements of these operators, including ladder operators are similar to those given in Eqs.(3.3.2-5). We do not need to say anything more in this respect.

So far we have been in the business to calculate base states and quantum numbers helped by invariance properties. Below, we hint at some application of nuclear spins; they are essential in analytical chemistry; the field of nuclear magnetic resonance (NMR) is a chapter important in Physical Chemistry.

E&E.3.5.4-2. Study effects of external magnetic field B on NMR spectra
Full invariance to rotations is lost when the material system is submitted to the field **B**. The NM-spectrum responds by a splitting of the multiplicity covered by $(\hat{I})^2$; for an eigen value I, there are 2I+1 level sharing the same energy; we say that in absence of an external (to the 1-system) magnetic field the energy spectrum is degenerate.

Let E_o be the energy of the 1-system for **B=0**; The interaction Hamiltonian is given by: $\hat{V}$=A $\hat{I}_3$ •**B**. This operator is diagonal. Take first a positive constant A. The energy for a given base state $|I, M_I>|E_o>$ is then given by: $E_{oIMI} = E_o + A\, BM_I$. We take the value of of the field fixed at B, then for the maximum value of M_I=I the energy difference $E_{oIMI=I} - E_o$ is positive for A positive; the lowest value of M_I=-I and the energy level is below E_o and $E_{oIMI=-I} - E_o$ is negative and equal to -A B I. The energy difference between the maximum and minimum is just 2 A B I.

The 1-system in a magnetic field can be put into a linear superposition in the 2I+1 base set for the projections of the angular momentum vector.

3.6. Irreducible tensor operators

So far, the I-frame system has been taken in isolation. The base sets required to represent rotation invariant situations have been worked out. A common situation, however, is to find out an I-frame system interacting with external systems showing lower rotation symmetries. The interaction operators may be scalar (j=0), vector (j=1), quadrupolar (j=2), etc.

In general, generators of the unitary group U(2l+1) are named irreducible tensor operators (ITO) and are defined via commutation relations with the angular momentum operators: $\hat{J}_3$, $\hat{J}_+$ and $\hat{J}_-$. An ITO of rank k is denoted by $\hat{T}^K$ and has (2K+1) components $\hat{T}^K_q$ with the following commutation properties:

$$[\hat{J}_3, \hat{T}^K_q] = q\ \hat{T}^K_q\,;\ [\hat{J}_\pm, \hat{T}^K_q] = ((K\pm q+1)(K\ \mp\ q+1)^{1/2}\ \hat{T}^K_{q\pm1} \qquad (3.6.1)$$

Analogous spin operators, $\hat{T}^K_q$(S), allow for K=0 or 1, only.

In Cartesian frames for a given vector **q** with angular coordinates (θ,ϕ) the irreducible tensor operator is given as: $\hat{T}^K{}_q(\mathbf{q}) = (4\pi/(2K+1))^{1/2}\ Y_K{}^q(\theta,\phi)$.

Tensor operators form two non equivalent classes: angular momentum tensors, e.g. $\hat{T}^K{}_q(J)$ named polar tensor operators and Cartesian tensors, e.g. $\hat{T}^K{}_q(\mathbf{q})$ named axial tensor operators. They fulfill the following commutation properties:

$$[\hat{J}^2, \hat{T}^K{}_q(J)] = 0 \text{ and}$$
$$[\hat{J}^2, \hat{T}^K{}_q(\mathbf{q})] = \hbar^2\,(K(K+1)\ \hat{T}^K{}_q(\mathbf{q})] \qquad (3.6.2)$$

An operator product is defined in analogy to the rules of angular momentum combination:

$$[\hat{T}^{K1}(\alpha) x\, \hat{T}^{K2}(\beta)]^K{}_q =$$
$$\Sigma_{q1\,q2} \langle K_1 q_1 K_2 q_2 | K_1 K_2 K q\rangle\ \hat{T}^{K1}{}_{q1}(\alpha)\ x\ \hat{T}^{K2}{}_{q2}(\beta) \qquad (3.6.3)$$

3.7. Wigner-Eckart theorem

Consider the matrix element of $\langle JM|\hat{T}^K{}_q|J'M'\rangle$. The following equation holds.

$$\langle JM|\hat{T}^K{}_q|J'M'\rangle = (-1)^{J-M} \begin{pmatrix} J & K & J' \\ M & q & M' \end{pmatrix} \langle J||\hat{T}^K||J'\rangle \qquad (3.7.1)$$

Axial tensor operators have only diagonal reduced matrix elements. For polar tensor operators from the properties of spherical harmonics one gets:

$$\langle L|||\hat{T}^K(\mathbf{q})||L'\rangle = (-1)^L\ (2L+1)(2L'+1) \begin{pmatrix} L & K & L' \\ 0 & 0 & 0 \end{pmatrix} \qquad (3.7.2)$$

For $|L-L'| \le K \le L+L'$ and K+L+L' an even integer number, these operators have non-zero reduced matrix elements between states of different angular momenta.

3.8. Discrete Symmetries

So far, continuous transformations have helped finding labels for base states. Translations in space-time and space rotations have been examined. Booster transformation where the angles between time and space axes are changed will be used later on with relativistic equations.

As pointed out in section 3, mapping relating two frames, obtained from one another after translation in time and a general rotation of the space-time frame, defines the set of Lorentz transformations (LTs). Let **a** be a 4-vector representing an origin displacement and $\underline{\underline{\Lambda}}$ a rotation 4x4 matrix. Lorentz transformations $L(\mathbf{a};\underline{\underline{\Lambda}})$ leave invariant ds^2, i.e. the scalar product. The homogeneous LT is defined by: $L(\mathbf{a}=0;\underline{\underline{\Lambda}}) = \Lambda$.

The metric matrix (tensor) in eq.(3.2), named now as G, is invariant to a LT. This translate in the form:

$$\Lambda^T G \Lambda = G \qquad (3.8.1)$$

The matrix elements of G are $G^{oo}= G_{oo} =1$, $G^{11}= G_{11}= G^{22}= G_{22}= G^{33}= G_{33}= -1$; the off-diagonal elements being zero. The matrix Λ^T is the transpose of Λ. The set of matrices satisfying this equation form a group, the homogeneous Lorentz group.

The time component of the LT satisfies the relation:

$$(\Lambda^T G \Lambda)_{oo}= (\Lambda_{oo})^2 - \Sigma_k (\Lambda_{ko})^2 = 1 \qquad (3.8.2)$$

Thus, for real transformations if $\Lambda_{oo} \geq 1$ we have an orthochronous LT transformation; if $\Lambda_{oo} \leq -1$ the LT is non-orthochronous. Together with the condition on the determinant (±1), there are four classes of real transformations. Because the matrix element Λ_{oo} cannot be brought continuously from a value greater than one to a value less than –1 and neither the determinant can be changed continuously from +1 to –1, the four classes are disconnected. These classes can be characterized by one of the four basic transformations: 1, P, T, or TP where P is space inversion (parity) and T is time reversal; 1 is the identity transformation imposed by the group structure of LTs.

Let symbolically characterize the four classes of Lts:

$L^{\uparrow}_{+}$: $\Lambda_{oo} \geq 1$ and det Λ=+1 named as orthochronous proper restricted group, 1;
$L^{\downarrow}_{+}$: $\Lambda_{oo} \leq -1$ and det Λ=+1 named as non-orthochronous proper, TP;
$L^{\uparrow}_{-}$: $\Lambda_{oo} \geq 1$ and det Λ=-1 named as orthochronous, improper, P;
$L^{\downarrow}_{-}$: $\Lambda_{oo} \leq -1$ and det Λ=-1 named as non-orthochronous improper, T.
Note the following mappings:

$$P\,(L^{\uparrow}_{+}) \rightarrow L^{\uparrow}_{-} \qquad (3.8.3)$$
$$T\,(L^{\uparrow}_{+}) \rightarrow L^{\downarrow}_{-} \qquad (3.8.4)$$
$$T\,P\,(L^{\uparrow}_{+}) \rightarrow T(L^{\uparrow}_{-}) \rightarrow L^{\downarrow} \qquad (3.8.5)$$

3.8.1. Parity

Parity transformations $\hat{P}$ belong to the $L^{\uparrow}_{-}$ class. For a base ket $|x^o,x^1,x^2,x^3\rangle = |x^o\rangle\,|x^1,x^2,x^3\rangle$ the operator $\hat{P}$ acts only on the space part:

$$\hat{P}\,|\mathbf{x}\rangle = \hat{P}\,|x^1,x^2,x^3\rangle = |-x^1,-x^2,-x^3\rangle = |-\mathbf{x}\rangle \qquad (3.8.1.1)$$

For the momentum space

$$\hat{P}\,|\mathbf{p}\rangle = \hat{P}\,|p^1,p^2,p^3\rangle = |-p^1,-p^2,-p^3\rangle = |-\mathbf{p}\rangle \qquad (3.8.1.2)$$

With the help of the identity, $(\hat{x}\text{-}\mathbf{x}')|\mathbf{x}'\rangle = (\mathbf{x}'\text{-}\mathbf{x}')\,|\mathbf{x}'\rangle = 0$, we can show that:

$$\hat{P}\;\hat{x}\;(\hat{P})^{-1} = -\;\hat{x} \qquad (3.8.1.3)$$

Analogously,

$$\hat{P}\;\hat{p}\;(\hat{P})^{-1} = -\;\hat{p} \qquad (3.8.1.4)$$

Vector operators changing sign under operation $\hat{P}$ that is equivalent to a full reflection are called polar vector operators.

The operator $\hat{P}$ considered as a reflection operator also is a unitary operator. $\hat{P}^2 = \hat{1}$ and the eigen values are ±1. These eigen values are called parity.

The relationship between parity and reflection operator applies for full reflection. If you take only two axes for reflection, there will be a surprise. The transformations with two axes are related to the unit operator in a continuous manner. These latter do not represent a parity operation. Also, if only one axis is reflected, then you have changed the hand of the I-frame.

Finally, consider an angular momentum base function: |l m>. Projecting in an I-frame with $(\hat{P}\,|\mathbf{x}\rangle)^{\dagger} = \langle\mathbf{x}|\,\hat{P} = \langle-\mathbf{x}|$ we have:

$$\langle\mathbf{x}|\,\hat{P}\,|\,l\;m\rangle = \langle-\mathbf{x}|\,l\;m\rangle = Y_{lm}(-\mathbf{n}_x) \qquad (3.8.1.5)$$

But $Y_{lm}(-\mathbf{n}_x) = Y_{lm}(\pi-\theta,\phi+\pi) = (-1)^l\,Y_{lm}(\theta,\phi)$ and

$$\langle\mathbf{x}|\,\hat{P}\,|l\;m\rangle = \langle-\mathbf{x}|l\;m\rangle = Y_{lm}(-\mathbf{n}_x) = (-1)^l\,Y_{lm}(\theta,\phi) \qquad (3.8.1.6)$$

The parity of the angular momentum base state is $(-1)^l$.

If the Hamiltonian is invariant to reflection, namely, $[\hat{H}\,\hat{P}, \hat{P}\,\hat{H}] = 0$, then the eigen values of $\hat{P}$ can be used to label base quantum states. Base states with different parity are orthogonal.

3.8.2. Time reversal

Unitarity implies introduction of complex numbers. The equation (1.3.1.1), Schrödinger time dependent equation is linear in time axis with imaginary axis: $(i\hbar)\,\partial|\Psi,t\rangle/\partial t$. We know that time inversion is not a simple operation: $T(L^{\uparrow}_{+}) \rightarrow L^{\downarrow}_{-}$. There is a component of time inversion. For the time evolution operator time reversal would imply a reversal of the imaginary axis so that one would expect: $i \rightarrow -i$. But you know that inverting one axis the frame changes hand, or a reflection of space must be expected: $L^{\downarrow}_{-}$.In Hilbert space one takes care of these subtleties with two operations: $\hat{T} = \hat{U}\,\hat{K}$ where $\hat{K}$ complex conjugate everything to its right and $\hat{U}$ is a unitary operator such that $\hat{U}^{-1}\, i\, \hat{U} = i$. This operator just replaces t by –t and it has a phase factor that we choose equals to one. Thus,

$$\hat{T}\exp(i(\mathbf{k}\cdot\mathbf{x}-Et)/\hbar) = \hat{U}\,\hat{K}\exp(i(\mathbf{k}\cdot\mathbf{x}-Et)/\hbar) =$$
$$\hat{U}\exp(-i(\mathbf{k}\cdot\mathbf{x}-Et)/\hbar) = \exp(-i(\mathbf{k}\cdot\mathbf{x}+Et)/\hbar) =$$
$$\exp(i(-\mathbf{k}\cdot\mathbf{x}-Et)/\hbar) \qquad (3.8.2.1)$$

Thus $\psi'(t) \propto \exp(-iEt)$ while $\psi(t) \propto \exp(-iEt)$ has the same behavior. The plane wave is moving opposite to the initial plane wave direction, as it should.

Consider now the non-relativistic spin 1/2 base states (Section 3.5.2):

$$\alpha = \begin{bmatrix}1\\0\end{bmatrix} \text{ and } \beta = \begin{bmatrix}0\\1\end{bmatrix}$$

For time reversal one would expect a spin flip α to β (or vice versa). The operator $\hat{U}$ must be a 2x2 matrix flipping the base functions, namely a Pauli matrix: $\hat{U} = \eta\,\hat{\sigma}_2$. With the matrices defined in (3.5.2.5) we get

$$\hat{T}\begin{bmatrix}1\\0\end{bmatrix} = \hat{U}\,\hat{K}\begin{bmatrix}1\\0\end{bmatrix} = \eta\,\hat{K}\,\hat{\sigma}_2\begin{bmatrix}1\\0\end{bmatrix} =$$
$$\eta\,\hat{K}\,(-i)\begin{bmatrix}0\\1\end{bmatrix} = i\,\eta\begin{bmatrix}0\\1\end{bmatrix} \qquad (3.8.2.2)$$

From this equation we calculate

$$\hat{T}^2 = \hat{U}\,\hat{K}\,\hat{U}\,\hat{K} = = \eta\,\hat{\sigma}_2\hat{K}\,\eta\,\hat{\sigma}_2\hat{K} =$$
$$\eta\,\hat{\sigma}_2\eta^*\,\hat{\sigma}_2^*\,\hat{K}\,\hat{K} = -1 \qquad (3.8.2.3)$$

This is the origin of Kramer's degeneracy for spin 1/2 base states.

Time reversal operation applied to a closed quantum mechanical system lead to a reversible time evolution. In fact, from the structure examined so far, there is no clue as to the way one could distinguish future from past. Special relativity does it. But the theory, so far has not been developed in a fully relativistic framework; see Chapter seven. The point we want to make is the following. A quantum mechanical analysis of a given situation cannot just rest on the special case. From the beginning, all possibilities must be included. Thus, if a measurement is to be done locally, this is all right, but the formalism must contemplate all alternatives that can be measured in the future. By the same token, it must include all possible experimental initial setups. Only the amplitudes will distinguish situations for specific cases. The formalism must necessarily be reversible.

3.8.3. Double groups

For spin 1/2 base functions a rotation by 2π produces the same result as the $\hat{T}^2$-operator, it changes the sign. For molecular systems related to point group symmetries having half-integral angular momentum the group operations must be enlarged so that this $\hat{T}^2$-operator property can be incorporated. In the literature this type of rotation ($\mathfrak{R}$) applied to each group operation double the group dimension. If g is an element of the group, new elements obtain as products $g\mathfrak{R}$; for single-valued representations, characters of elements $g\mathfrak{R}$ are the same as g.

3.8.4. Permutation symmetry

The issue here is the correct definition of base sets for a set of n 1-systems. Material systems that can be decomposed into n-elements each one sharing the same material parameters, mass, charge and spin are of special interest.

The base state |kk'> of each 1-system is used to construct a direct product base set for the n identical 1-systems. This is identified by a set of labels embodied in the symbol $\mathbf{g}_{kk}$:

$$|\mathbf{g}_{kk}> = | k_1k_1', k_2k_2', \ldots, k_hk_h', \ldots, k_nk_n'>$$

characterizing for the k-th member of the set.

Once we have chosen a particular set of 1-system base states and keeping the first label ranged from 1 to n, the assignment of base states chosen from a fixed pool is totally arbitrary. Let us do a permutation 1↔h and get

$$P_{1h} \mid k_1k_1', k_2k_2', \ldots, k_hk_h', \ldots, k_nk_n'> = \\ \mid k_1k_h', k_2k_2', \ldots, k_hk_1', \ldots, k_nk_n'> \qquad (3.8.4.1)$$

Now apply the permutation P_{1h} again:

$$P_{1h}^2 \mid k_1k_1', k_2k_2', \ldots, k_hk_h', \ldots, k_nk_n'> = \\ P_{1h} \mid k_1k_h', k_2k_2', \ldots, k_hk_1', \ldots, k_nk_n'> = \\ \mid k_1k_1', k_2k_2', \ldots, k_hk_h', \ldots, k_nk_n'> \qquad (3.8.4.1)$$

The following identity is fulfilled: $P_{1h}^2 = 1$ and consequently $P_{1h} = \pm 1$. The quantum number of the permutation operator permits identifying symmetric base states ($P_{1h} = +1$) and distinguishing from the anti-symmetric ones $P_{1h} = -1$.

The key to the symmetry property is found in the fact that there are n identical 1-systems. Thus, if you order them in a given manner and then change that order without looking to the internal labels, the new ordering is just the same as the preceding one. The reason is trivial: a particular ordering cannot differentiate identical systems. This is the reason why one chooses the canonical ordering and keeps it as a reference.

Once the canonical order (arbitrary but fixed) is retained, the internal labels may be different. Thus, it makes sense to compare different orderings of the state labels.

We turn now to the projections on to a configuration space with base vectors:

$$|\mathbf{q}> = |\, \mathbf{q}_1, \ldots, \mathbf{q}_h, \ldots, \mathbf{q}_n>.$$

The order used to range the coordinate system is irrelevant, jus as it was above. A base function is given as:

$$<\mathbf{q}|\mathbf{g}_{kk'}> = \\ < \mathbf{q}_1, \ldots, \mathbf{q}_h, \ldots, \mathbf{q}_n| \, k_1k_1', k_2k_2', \ldots, k_hk_h', \ldots, k_nk_n'>.$$

The notation is somewhat redundant and for this reason we simplify it with the replacement $<\mathbf{q}|\mathbf{g}_{kk'}> \rightarrow <\mathbf{q}|\mathbf{g}_{k'}>$:

$$<\mathbf{q}|\mathbf{g}_{k'}> = \\ < \mathbf{q}_1, \ldots, \mathbf{q}_h, \ldots, \mathbf{q}_n| \, k_1', k_2', \ldots, k_h', \ldots, k_n'> \qquad (3.8.4.2)$$

The key lesson is that permutations do not apply to the configuration space but to the base state space. Here, it is understood that it is the set of base state labels that is permuted; the order assigned to the configuration space is kept fixed so that it serves comparison purposes.

One of the most spectacular properties of anti-symmetric base states concerns the individual base functions (labels) that are allowed in. If any two

individual base states are identical, say $k_1'= k_h'= k'$ when applying the P_{1h} operator one gets the result:

$$< \mathbf{q}_1,\ldots, \mathbf{q}_h,\ldots, \mathbf{q}_n| k', k_2',\ldots, k',\ldots, k_n'> =$$
$$-< \mathbf{q}_1,\ldots, \mathbf{q}_h,\ldots, \mathbf{q}_n| k', k_2',\ldots, k',\ldots, k_n'> \qquad (3.8.4.3)$$

There is only one number that is equal to its negative: zero. Thus, all labels used to identify base states must be different from each other.

For spin 1/2 or 3/2 or any odd half integer, an assembly of n-identical 1-systems must show anti-symmetric base states. This is a system of n-fermions.

For fermionic systems, according to eq.(3.8.4.3) base states can only be used once. This is another form of Pauli exclusion principle.

For integer spin, there is no restriction on the number of times a base state can be used. Base states including spin that are symmetric under permutations are known as bosons.

E&E.3.8.4. Show that symmetric and anti-symmetric base states are orthogonal

Let |S> and |A> be two base states whatsoever. A permutation operator $\hat{P}$ acts as follows: $\hat{P}$|S>=+|S> and $\hat{P}$|A>=-|A>. Remember that $\hat{P}^2=\hat{1}= \hat{P}^\dagger \hat{P} = \hat{P}\,\hat{P}^\dagger$. We form now <S|A> and operate as follows:

$$<A|S> = <A|\,\hat{1}\,|S> = <A|\,\hat{P}^\dagger \hat{P}\,|S> = - <A|S>$$

The result is always zero. The base sets belonging to symmetric and anti-symmetric spaces are orthogonal.

3.9. Symmetry principles

Symmetry principles play a fundamental role in the quest for “good” quantum numbers. These are used to label states that in turn are pillars in constructing general quantum states. In previous sections we have tried to differentiate as much as possible the difference between these two elements constituting a Hilbert space. But we have gone along a non-relativistic path; one means with such statement that one treat time and space separately, space-time, while a relativistic approach consider a 4-dimensional spacetime.

The introduction of a 1-system as the set of quantum states sustained by a particular material system permits treating symmetry properties in a general manner. Base states for a 1-system formed by one material object called free particle, are given by unitary irreducible representations of the Poincaré group, namely, the group formed by the translations and Lorentz transformation in the so called Minkowski space. This latter is the rotation group in the space of dimension four.

Thus, if one gets all unitary irreducible representations of the Poincaré group then a complete base set obtains. A little more elaboration can be found in the chapter on relativistic equations.

3.10. Radiation quantum states and interactions

Radiation is a material system showing zero restmass and finite angular momentum.

In this section we take a short cut to present some important aspects of the electromagnetic field as an energy carrier mediating interactions between quantum material systems.

In Special Relativity the finite speed of light relates time to space dimensions. The inertial frame concept has been used to relate quantum states belonging to abstract Hilbert space to projected quantum states associated to a particular I-frame where configuration space comes in. In this chapter, invariance of an arbitrary quantum state to translations and rotations of the I-frame has been used to get explicit forms to the corresponding wave functions (quantum states projected in a configuration space).

Thus, for a material system, a 1-system, supporting quantum states that are able to hold the total mass of its constituents in such a way they can be assigned a location at the origin of the I-frame, or another bound distribution, energy exchange could be described by changing the internal quantum state via interactions. For a radiation field, the problem, if there is one, would be that the material system sustaining the internal quantum states ought to have zero rest mass; the trick used so far does not work in constructing basis states.

Yet, energy exchanges between the EM fielf and a material system elicit a quantization discovered by Planck (1900): the energy exchanges in energy packages dubbed as photons. Thus, energy exchange is quantized.

Experimentally we know that EM radiation is generated by sources located in laboratory (real) space. And detectors located also in real space can sense it.

An I-frame can hence be located at the source and another at the detector; a laboratory distance can naturally be calculated. A direction of emission can be established and designated by $\mathbf{k}$ with origin at the source. From classical electrodynamics we know that to each $\mathbf{k}$ an energy is assigned: $c|\mathbf{k}| = \hbar\omega$. The r.h.s comes from quantum physics. Thus, in the modulus (length) of vector $\mathbf{k}$ one can encode the quantum of energy. Thus, experimentally one determines the origin of emission so that its direction fits the one where a detector is located. Along that direction we know that a quantum of EM energy can be exchanged there; we do not need to put a detector but can make the system interact with another device to change some elements of the system; its quantum state as it were.

We are in front of an interesting situation that is a typical Fence state of affairs. On the one hand there is an energy exchange between a source and a sink that shares clear classical features: systems localized in real space. On the other hand, both the source and sink must have quantum states such that a change affecting them can be described as a quantum process.

A quantum description requires the construction of bases states. In what follows discussion concerning momentum states is presented first to illustrate one way to sense interactions occurred once the system is prepared. Thereafter, we introduce a simple model to construct bases functions that will be used to construct quantum states for the electromagnetic field.

3.10.1 Momentum wave-packets: Uncertainty relationships

Quantum states embody the interactions required to produce them. Let us make clearer this point by examining linear superpositions of planar waves.

Translation symmetry is used to generate base states in position reciprocal space coordinate (Cf.Sect. 3.2.4). The range accorded to configuration space coordinates goes from -∞ to +∞; in reciprocal space k-coordinates have also the range:]-∞,+∞[. The transformation function exp(i**k**.**q**) forms a complete basis set serving to express a given quantum state with amplitudes ϕ(**k**) in k-space to the same quantum state but in **q**-space:

$$\phi(\mathbf{q}) = 1/\sqrt{2\pi} \int_{-\infty}^{+\infty} dk \ \exp(i\mathbf{k}.\mathbf{q})\ \phi(\mathbf{k}) \qquad (3.10.1.1)$$

The eq.(3.10.1.1) reads as a quantum state that is projected onto k-configuration space is determined by the amplitudes ϕ(**k**); this is an input derived from experimental data or representing a particular model situation (see below) and the configuration space representation is then ϕ(**q**). Of course one might have gotten the quantum state projected in configuration space with the set of amplitudes ϕ(**q**) and the relation in **k**-space reads as:

$$\phi(\mathbf{k}) = 1/\sqrt{2\pi} \int_{-\infty}^{+\infty} dq \ \exp(-i\mathbf{k}.\mathbf{q})\ \phi(\mathbf{q}) \qquad (3.10.1.2)$$

Here the wave packet ϕ(**q**) is the input so that in k-space is given by ϕ(**k**). The mathematical forms are different, albeit they represent the same abstract quantum state, different symbols are commonly used to identify them; here, maintain the same symbol (label).

For a time dependent quantum state |ϕ,t> with data obtained from projection in **k**-space one gets the quantum state in configuration space:

$$\phi(\mathbf{q},t) = 1/\sqrt{2\pi} \int_{-\infty}^{+\infty} dk \, \exp(i(\mathbf{k}.\mathbf{q}-\omega t)\, \phi(\mathbf{k}) \qquad (3.10.1.3)$$

In the case that **k** and ω were independent, the separation leading to $\phi(\mathbf{q},t)$ starting from a quantum state prepared in **k**-space would just be an apparent time evolution: the wave packet would come back to $\phi(\mathbf{q},t=0)$ and start up again a new cycle; the amplitudes in absolute value are invariant.

For a Gaussian quantum state, e.g. $\phi_G(\mathbf{q}) = (2/\pi\, \alpha^2)^{3/4} \exp(-|\mathbf{q}|^2/\, \alpha^2)$ as well as $\phi_G(\mathbf{k})$ (Cf. Sect. 3.2.4) the widths at half-maximum, $\Delta\mathbf{q}$ and $\Delta\mathbf{k}$, are controlled by the parameter α, they are roughly inverse to each other so that:

$$\Delta\mathbf{q}\, \Delta\mathbf{k} \approx 1 \qquad (3.10.1.4)$$

The numbers $\Delta\mathbf{q}$ and $\Delta\mathbf{k}$ refer to a property of the quantum state $\phi_G(\mathbf{q})$ or to $\phi_G(\mathbf{k})$ and consequently they embody experimental data. The nature of numbers **q** and **k** differ from $\Delta\mathbf{q}$ and $\Delta\mathbf{k}$; the former belongs to a continuum while the latter correspond to special quantities (i.e. they enter a non-standard analysis where one can find as example the infinitesimals).

This distinction is important to bear in mind. It is at this level that physical situation enters. To talk of particular $\Delta\mathbf{q}$ and $\Delta\mathbf{k}$ one must know that a particular quantum state is involved; in turn, this implies experimental conditions under which the quantum states, not the bases functions, are determined.

It is a common practice to multiply **k** by Planck's constant and using the prescription $\mathbf{p}=\hbar\mathbf{k}$ one get an expression like:

$$\Delta\mathbf{q}\, \Delta\mathbf{p} \approx \hbar \qquad (3.10.1.5)$$

The widths are associated to a preparation of the quantum state and have nothing to do with measurements of any kind. For this reason the name Heisenberg uncertainty relationship is not used here. See Chapter 11 where this and other issues concerning quantum measurement theory are discussed in more detail.

Now the transformation function $\exp(i(\mathbf{k}.\mathbf{q}-\omega t)$ can be used in the frequency-time regime. What is the meaning of $\exp(i\omega t) \rightarrow \langle\omega|t\rangle$? No one, except that we are using frequency and time labels. Assume one can construct a pulse given by the amplitudes $\phi(\omega)$ of a linear superposition the corresponding representation in time-space is:

$$\phi(t) = 1/\sqrt{2\pi} \int_{-\infty}^{+\infty} d\omega \, \exp(-i\omega t)\, \phi(\omega) \qquad (3.10.1.6)$$

Negative and positive frequency labels is one way to signal direction; energy emitted or energy absorbed would be a classical picture but the real numbers used as labels are not relayed to experimental conditions, they provide appropriate mathematical spaces. But the wave packet (quantum state) will show the relationship

$$\Delta\omega\, \Delta t \approx 1 \qquad (3.10.1.7)$$

The width of the pulse is Δt and by multiplying both sides with Planck's constant one obtain

$$\hbar\Delta\omega\, \Delta t \approx \hbar \qquad (3.10.1.8)$$

Taking $\hbar\Delta\omega$ as the amount of energy embodied in the pulse around frequency ω, namely ΔE_ω, we get a form of the energy-time relationships that relate to experimental situations:

$$\Delta E_\omega \Delta t \approx \hbar \qquad (3.10.1.9)$$

Thus, we have a superposition of a bunch of frequencies represented by the function $\phi(\omega)$ in such a way that the pulse width must satisfy eq.(3.10.1.9). This would correspond to a polychromatic EM field. The information is encoded in the amplitudes defining the quantum state. Thus, if you had prepared a "wave packet" $\phi(\omega)=\delta(\omega-\omega')$ the time dependent quantum state would be the fixed amplitude $\exp(-i\omega' t)$, namely a monochromatic state.

3.10.2 Basis sets for EM radiation

What can be a quantum state of the electromagnetic radiation? To this question we dedicate this section. A more detailed presentation is given in Chapter 6.

First, let us evoke some key questions concerning quantum mechanics itself. By now you understand that this is not a scheme designed to describe particles. The quantum states such materials systems may be put in is quite a different story. Thus, the material system over which one is to construct representations of its quantum states are sets of energy quanta an EM field may exchange with massive material systems. You cannot target the photons as particles but you are better off in trying to get the quantum state for such systems.

Let us insist: one should not speak of particles in a radiation field nor for the quantum mechanical description of material systems. Of course, one may use concepts such as particle-state to help the set up of particular algorithms. In the present view of quantum mechanics there would never be a "collapse of the wave function". Material systems do not occupy a given eigenstate when it is being measured.

Experimentally, we know that in real (laboratory) space energy is exchanged between a EM field and a massive material system and that this occurs in energy packets; we call such packets entering the exchange as photons. The question is how to construct a Hilbert-space-like to write down the quantum states.

An answer to the question above is to find out labels for the basis vectors related to photons fields not to particles. A photon filed is a quantum construct; this is all we need to know for the time being.

An energy quantum is characterized by a frequency: ω or ν. The former is a circular frequency (radians per second) the latter has dimension of inverse of time. Select a monochromatic situation. The number of energy quanta it can exchange under determined experimental conditions may characterize the photon field and we use it as a label. One gets:

$$\{|0>, |1>,\ldots, |n-1>, |n>, |n+1>,\ldots\} \qquad (3.10.2.1)$$

This is a complete orthonormal set with $<i|j> = \delta_{ij}$ where the labels may be put in connection with an amount of energy as shown below.

So far we have forgotten to indicate which frequency it is. Let this one be $\mathbf{k}_i$ so that we imply that we may have in real life a photon field whose energy count for $n_{\mathbf{k}i}$ photons, then you relate the labels to the energy with either of the extremes appearing below:

$$n_{\mathbf{k}i} h\nu = n_{\mathbf{k}i} (h/2\pi) (2\pi\nu) = n_{\mathbf{k}i} \hbar\omega \qquad (3.10.2.2)$$

Remember, $\omega \lambda = c$ is a fundamental relationship derived from classical electrodynamics so that the energy can be label with $k_\omega \hbar c = \hbar\omega$. Thus we understand that $|\mathbf{k}|$ labels an energy as well. In what follows the label $n_{\mathbf{k}i}$ is used with the purpose of identifying the frequency implied and to a number of energy quanta (see below). There, we will show that energy-label difference is what matter.

When using label $\mathbf{k}$ one can also refer to as a $\mathbf{k}$-mode. Look now. We have an eigenvector say $|n_{\mathbf{k}}>$ and the energy label $h\nu_{\mathbf{k}}$ and we define the Hamiltonian operator for the $\mathbf{k}$-mode by the following relationship:

$$\hat{H}_{\mathbf{k}} |n_{\mathbf{k}}> = h\nu_{\mathbf{k}} (n_{\mathbf{k}} + 1/2) |n_{\mathbf{k}}> = E_{n\mathbf{k}}|n_{\mathbf{k}}> \qquad (3.10.2.3)$$

The label $n_{\mathbf{k}} = 0$ defines the vacuum, i.e. no energy will be available for exchange. For the $\mathbf{k}$-mode we can construct a quantum state as a linear superposition:

$$|\Psi> = \Sigma_{(n\mathbf{k})} |n_{\mathbf{k}}> <n_{\mathbf{k}}|\Psi> = \Sigma_{(n\mathbf{k})} |n_{\mathbf{k}}> C_{n\mathbf{k}}(\Psi) \qquad (3.10.2.4)$$

The average energy of the EM field if you can prepare in the linear superposition above is given by:

$$<\Psi| \hat{H}_{\mathbf{k}} |\Psi> = \Sigma_{(n\mathbf{k})} C_{n\mathbf{k}}^*(\Psi) C_{n\mathbf{k}}(\Psi) E_{n\mathbf{k}} \qquad (3.10.2.5)$$

The zero-point energy counts by one for normalized quantum states:

$$<\Psi|\ \hat{H}_{\mathbf{k}}\ |\Psi> = \tfrac{1}{2}\, h\nu_{\mathbf{k}} + h\nu_{\mathbf{k}} \Sigma_{(n\mathbf{k})} |C_{n\mathbf{k}}(\Psi)|^2\, n_{\mathbf{k}} \quad (3.10.2.6)$$

This is the average energy associated to the quantum state given by eq. (3.10.2.4). Only amplitudes different from zero contribute to this energy.

It is interesting to see that $|C_{n\mathbf{k}}(\Psi)|^2$ for particular quantum states may be prepared so that a distribution around sets of $n_{\mathbf{k}}$'s covering a finite range; beyond such range the amplitudes are to be taken as zero, this would be a model related to an energy packet. And, as we have emphasized over and over again, the preparation reflects the way real system are manipulated in a laboratory, or simply in the external world.

Now we seek a connection with the energy available in the photon-field (not the photon number!) let us examine the energy ladder. For $n_{\mathbf{k}}=0$ the energy level is just (1/2) $h\nu_{\mathbf{k}}$ which is known as the zero-point energy. Consider the the situation analyzed in **E&E.2.1-1**, namely the commutator: $[\hat{H}_{\mathbf{k}}, |n_{\mathbf{k}}><n_{\mathbf{k}'}|] = (E_{n\mathbf{k}} - E_{n\mathbf{k}'})\, |n_{\mathbf{k}}><n_{\mathbf{k}'}|$. This operator acting on the quantum state eq.(3.10.2.4) from the left yields:

$$\begin{aligned}
&[\hat{H}_{\mathbf{k}}, |n_{\mathbf{k}}><n_{\mathbf{k}}'|]|\Psi> = \\
&(E_{n\mathbf{k}} - E_{n\mathbf{k}'})\, |n_{\mathbf{k}}><n_{\mathbf{k}'}|\ (\Sigma(n_{\mathbf{k}''})\, C_{n\mathbf{k}''}(\Psi)\, |n_{\mathbf{k}''}> = \\
&(E_{n\mathbf{k}} - E_{n\mathbf{k}'})\, C_{n\mathbf{k}'}(\Psi)\, |n_{\mathbf{k}'}> = \\
&(E_{n\mathbf{k}} - E_{n\mathbf{k}'})\, |n_{\mathbf{k}}>\ C_{n\mathbf{k}'}(\Psi) \qquad (3.10.2.7)
\end{aligned}$$

The difference between labels corresponds the excitation operator $|n_{\mathbf{k}}><n_{\mathbf{k}'}|$ that indicates the energy required to shift from one state to another. Let us write $\Delta E_{n,n'}$ to represent an energy that can be directly mapped to energy in the field:

$$\begin{aligned}
\Delta E_{n,n'} &= h\nu_{\mathbf{k}}\, (n_{\mathbf{k}} + 1/2) - h\nu_{\mathbf{k}}\, (n_{\mathbf{k}'} + 1/2) = \\
&h\nu_{\mathbf{k}}\, (n_{\mathbf{k}} - n_{\mathbf{k}'}) \qquad (3.10.2.8)
\end{aligned}$$

If the difference is negative, the field has to give up that energy; if it is positive, the field must accommodate that energy. Thus,

$$[\hat{H}_{\mathbf{k}}, |n_{\mathbf{k}}><n_{\mathbf{k}'}|\ ]|\Psi> = h\nu_{\mathbf{k}}\, (n_{\mathbf{k}} - n_{\mathbf{k}'})\, |n_{\mathbf{k}}>\ C_{n\mathbf{k}'}(\Psi)$$

and the only matrix element different from zero will be $k \neq k'$:

$$\begin{aligned}
&< n_{\mathbf{k}}\ |\ [\hat{H}_{\mathbf{k}}, |n_{\mathbf{k}}><n_{\mathbf{k}'}|\ ]\ |\Psi> = \\
&\qquad h\nu_{\mathbf{k}}\, (n_{\mathbf{k}} - n_{\mathbf{k}'})\, C_{n\mathbf{k}'}(\Psi) \qquad (3.10.2.9)
\end{aligned}$$

In this expression the primed label plays the role of root state. For, if the quantum state had non-zero amplitude there then the transition operator picks up an energy amount $h\nu_{\mathbf{k}}\, (n_{\mathbf{k}} - n_{\mathbf{k}'})$ that can be recovered in laboratory space to the extent that the quantum state of the material system has been constructed this way. All base

state showing zero amplitude do not act as root state, i.e. they would not generate a spectrum.

The energy exchange involving the two base state levels depends on the quantum state. In the present case, if the amplitude for the base state $| n_{k'}>$ is zero, no energy exchange would take place. The energy difference (n_k - $n_{k'}$) may be positive or negative: the field may trap (+) or emit (-) an energy amount: a (bunch of) photon(s).

Therefore, energy available in the field can be extracted if we know the quantum state of the EM field. This state, for the simple 1-mode case is given by eq.(3.10.2.4). "Photons" are not in the base vectors!

Back to the basic operators: $|n_k> <n_{k'}|$. This operator transforms the base state $|n_{k'}>$ into $|n_k>$ multiplied by a constant.

3.10.3 Creation/annihilation operators

The labels of the complete basis set given in eq.(3.10.2.1) corresponds to an ordered integers sequence. The operators $|n_k> <n_{k'}|$ contain too much information if one would like to generate an ordered sequence. Thus, it would be handy to have a set of operators associated to such case.

Consider the case n_k-$n_{k'}$=1, one can relate the base states $|n_k>$ and $|n_{k'}+1>$. By taking $n_{k'}$= 0 the base |0> is associated to a base state for which the EM field at the Fence will have zero energy to be exchanged. The operator onto $|n_k=1> <n_{k'}=0|$ projects the vacuum base state on to |1> that is associated to an EM having one quantum of energy to be exchanged. Observe that the base vectors would be operated in Hilbert (Fock) space where there is no such a thing as exchangeable energy. The mapping between abstract space and real space can be done, for example, with the help of the operator $[\hat{H}_k, |n_k> <n_{k'}|]$ as shown above. However, it is the quantum state |Ψ> that contains the information about the number and types of energy quanta that would be available for a given experiment. Now, given a mode let construct operators that can generate the basis vectors for that mode.

Define an operator to be named as $\hat{a}^\dagger$ such that $\hat{a}^\dagger|0> = cte\ |1>$. We can show that from

$$\hat{a}^\dagger|n_i> = cte\ |\ n_i +1>$$
$$\hat{a}^\dagger|n_i> = \sqrt{(\ n_i +1)}\ |n_i +1> \qquad (3.10.3.1)$$

The operator shifting down one unit $\hat{a}$ annihilates the vacuum and:

$$\hat{a}|0> = 0 \text{ and}$$
$$\hat{a}|n_i> = \sqrt{(n_i)}\ |n_i -1> \text{ for all } n_i > 0 \qquad (3.10.3.2)$$

The operator $\hat{a}$ can be represented as: |0><1|. It is easy to check in this representation that |0><1|0> = $\hat{a}$|0> = 0 due to orthonormality: <1|0> =0.

The base vector |n> can be obtained as follows:

$$(\hat{a}^{\dagger})^n/\sqrt{(n!)}\,|0> = |n> \qquad (3.10.3.3)$$

This is an interesting relationship. It tells us that we can shift the description of the EM field operator space. We have already found this type of situation: Schrödinger and Heisenberg representation in Hilbert space.

This shift is handy. It allows the introduction of electromagnetic quantities via operator forms. In Chapter 6 a detailed description is presented. Here, the operators for the electric field ($\hat{E}(\mathbf{r},t)$), magnetic field ($\hat{H}(\mathbf{r},t)$) and transverse vector ($\hat{A}(\mathbf{r},t)$) are written down:

$$\hat{E}(\mathbf{r},t) = \hat{E}^{+}(\mathbf{r},t) + \hat{E}^{-}(\mathbf{r},t) \qquad (3.10.3.4a)$$

$$\hat{E}^{+}(\mathbf{r},t) = \Sigma_{\mathbf{k},\lambda}\, i\, \mathcal{E}_{\omega k}\, \hat{\varepsilon}_{\mathbf{k}}^{(\lambda)}\, \hat{a}_{\mathbf{k}} \exp(i\, \mathbf{k_k} \cdot \mathbf{r}) \qquad (3.10.3.4b)$$

$$\hat{E}^{-}(\mathbf{r},t) = \Sigma_{\mathbf{k},\lambda}\, -i\, \mathcal{E}_{\omega k}\, \hat{\varepsilon}_{\mathbf{k}}^{(\lambda)}\, \hat{a}_{\mathbf{k}}^{+} \exp(-i\, \mathbf{k_k} \cdot \mathbf{r}) \qquad (3.10.3.4c)$$

λ is a spin polarization label so that the operator $\hat{\varepsilon}_{\mathbf{k}}^{(\lambda)}$ senses spin state; the base vectors becomes a little more complex.

The operators $\hat{E}(\mathbf{r},t)$), $\hat{H}(\mathbf{r},t)$ and $\hat{A}(\mathbf{r},t)$ harbor space-time coordinates and as a consequence they bridge the abstract to the Fence worlds.

3.11. I-frames locations: Sources and sinks

Experiments are performed at particular moments and locations; electromagnetic energy (photons) serves communication purposes; interaction outcomes have character of events.

Events that can be recorded read and/or used to set up further experiments; all these elements use a space-time framework. In the space separating/relating these realms (Fence) the formalism is cast in terms of elements allowing for a bridge linking real to quantum levels. Inertial frames play such a role. For charged matter $\hat{E}(\mathbf{r},t)$), $\hat{H}(\mathbf{r},t)$ and $\hat{A}(\mathbf{r},t)$ are the operators mediating interaction between quantum states found at each side of this Fence. The source is implicitly signaled by the origin of vector **r** the tip of which points to a real space location where a sink might be located,

Two I-frames relate via a communication protocol that corresponds to Lorentz transformations characteristic of special relativity (J.Freund, Special Relativity for Beginners, 2008). The distance between two spacetime events is a fundamental invariant.

In special relativity, the fundamental constant as already noted is the speed of light c. This speed is invariant to the state of uniform motion of the frame where the source is located.

A peculiarity of special relativity resides in the metric. This can be hinted at by comparison of distance measurements. To get a feeling for it, use two tricks:
-i) Measure distance between points 1 and 2 with rods and threads, the squared distance $(\Delta D_{12})^2$ by Pythagoras theorem in 3-space reads: $|\mathbf{x}(1)- \mathbf{x}(2)|^2$; or
-ii) Use light signals so that measuring the space with a clock can be done, i.e. if the signal takes Δt seconds, the square length is $(c\Delta t)^2$.

Let $(\Delta s)^2$ be a proper length square, D_{12}^2 be the distance measured with space tools and $(c\Delta t_{12})^2$ be the same distance measured with the interval $(t(1)- t(2))$ having the precise length so that $D_{12}^2= (c\Delta t_{12})^2$ both must be equal so that the proper length is:

$$(\Delta s)^2 = (c\Delta t_{12})^2 - (x_1(1)- x_1(2))^2 - (x_2(1)- x_2(2))^2 - (x_3(1)- x_3(2))^2 = 0$$

This is a null-vector usually named light vector. The change in sign is characteristic of the metric associated to spacetime.

There are two more cases of interest with $(\Delta s)^2$:
-First, the allocated time interval (lapse) allocated to the measurement is too short with respect to the space interval you want to measure so that the difference between the time and space distance, $(\Delta s)^2$ is now negative:

$$(c\Delta t_{12})^2 - (x_1(1)- x_1(2))^2 - (x_2(1)- x_2(2))^2 - (x_3(1)- x_3(2))^2 = (\Delta s)^2 < 0.$$

The vector with coordinates $(c\Delta t_{12}, x_1(1)- x_1(2), x_2(1)- x_2(2), (x_3(1) - x_3(2))$ fulfilling the inequality above is called *space-like*.
-Second, the time allocated is larger that the one required for a signal to cover the space to be measured, then $\Delta s^2 >0$, thereby defining a time-like vector.

$(\Delta s_{12})^2$ is invariant to a change of origin and rotations in 4-space; the operations are known as Lorentz transformations. Taking point 1 as the origin and an infinitesimal sphere of radius epsilon, the limit is:

$$(ds)^2 = (c\,dt)^2 - d\mathbf{x}^2 = (dx^o\, dx^1\, dx^2\, dx^3)\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix}\begin{bmatrix} dx_0 \\ dx_1 \\ dx_2 \\ dx \end{bmatrix} \quad (3.11.1)$$

The metric matrix is said to have the signature (+ - - -) and $dx^o = dx_o = cdt$. Of course the opposite signature (- + + +) can be chosen, but stick to one all the time. The one chosen here is just conventional.

The equality sign must be understood as mappings of different representations of the same "thing". The speed of light permits time to be incorporated as a fourth space dimension. Column vectors are distinguished from row vectors by the location of labels as shown in eq.(2.4.2). If we want to hide the metric one takes as column vector: $[dx_o\ -dx_1\ -dx_2\ -dx_3]$; this is a four vector. The scalar product between the row and column four vectors for this particular case is: $(dx^o\ dx^1\ dx^2\ dx^3)\ [dx_o\ -dx_1\ -dx_2\ -dx_3] = (ds)^2$.

A subtle shift is accomplished if one takes the spacetime point (x^o, x^1, x^2, x^3) to be the distance between two events, one at the origin the other at (ct, x^1, x^2, x^3) and latter on focus is put on the spacetime point as if it were a massive particle.

Of course one can simply define Minkowski space $\mathbf{M}$ to be a four dimensional vector space over the real number field with a flat Lorentzian metric $\eta_{\mathbf{ab}}$ =diag(1,-1-1,-1) where the bold sub index range over 0,1,2,3. At each point on $\mathbf{R}^4$ there exists a set of basis vectors $\mathbf{e}_o$, $\mathbf{e}_1$, $\mathbf{e}_2$, $\mathbf{e}_3$ belonging to $\mathbf{M}$ (a tetrad) such that any vector $\mathbf{A} \in \mathbf{M}$ by

$$\mathbf{A} = A^o\mathbf{e}_o + A^1\mathbf{e}_1 + A^2\mathbf{e}_2 + A^3\mathbf{e}_3 = A^{\mathbf{a}}\,\mathbf{e}_{\mathbf{a}} \qquad (3.11.2)$$

It follows from eq.(3.2) that the basis vectors fulfill the orthonormalization condition $\mathbf{e}_{\mathbf{a}} \cdot \mathbf{e}_{\mathbf{b}}$ equals to $\eta_{\mathbf{ab}}$.

Reciprocal space and time corresponds to the mappings: length→1/length =(**k**) or wave number; time → 1/time, or frequency ($\omega=\nu/2\pi$). These magnitudes form a 4-vector: $(\omega, \mathbf{k}c) = (\omega, k^1c, k^2c, k^3c)$. The speed of light permits changing wave number dimension into frequency as shown. Thus, the wave number defines spatial intervals while frequency defines time intervals. Observe that these quantities do not define intervals in time and in space because there is nothing like an absolute space and time.

The norm of a four-vector is invariant to the so-called Lorentz transformations (LTs). In fact, a LT is defined as a change of coordinates relating two I-frames that leave the norm of a four-vector invariant. In reciprocal representation the norm of $(\omega, \mathbf{k}c)$ reads:

$$\omega^2 - k^1k_1c^2 - k^2k_2c^2 - k^3k_3c^2 =$$
$$\omega^2 - (k_1c)^2 - (k_2c)^2 - (k_3c)^2 = \text{constant} \qquad (3.11.3)$$

The change is possible because $k^i = k_i$, for i=1,2,3. The speed of light because it is taken to be independent of an I-frame state of (uniform) motion allows dimension change so that **k**c has frequency dimension.

Now let us use Planck's constant $\hbar$ and select momentum by distance dimensions. Thus, $\hbar\mathbf{k}$ is a vector with momentum dimension denoted by **p**. Assign the components of this vector to the space part of a four-vector $(p^0\ p^1\ p^2$

p^3) → **P** and search after the time-like component p^o. To see a connection consider the four-vector (ω, **k**c) $\hbar$ = ($\hbar\omega$,$\hbar k^1 c$, $\hbar k^2 c$, $\hbar k^3 c$) where the time component relates to the energy $\hbar\omega$ = E. Thus, divide this equality by the speed of light to get: (ω, **k**c) $\hbar$ /c = (E/c, $\hbar k^1/c$, $\hbar k^2/c$, $\hbar k^3/c$) = (p^0 p^1/c p^2/c p^3/c) and the covariant column 4-vector: [p_o ($-p_1/c$) ($-p_2/c$) ($-p_3/c$)], the scalar product defines a relativistic invariant (to Lorentz transformations):

$$(\mathbf{P})^2 = (E/c)^2 - (p^1)^2 - (p^2)^2 - (p^3)^2 = \text{constant} \qquad (3.11.4)$$

In the rest frame the linear momentum is the zero vector and (E/c) should correspond to the rest mass momentum $M_o c$. Thus $(E/c)^2 = (M_o c)^2$ and $E = +(M_o c^2)$ so that one can write:

$$(E)^2 - \{(p^1)^2 + (p^2)^2 + (p^3)^2\} c^2 = (M_o c^2)^2 \qquad (3.11.5)$$

These equations relates to the I-frame dynamics considered as a classical system. This part is independent from the internal quantum states sustained by the same material system. This independence is granted for the process of constructing bases sets. In real processes both levels can be made to interact.

At the classical world side it is customary to describe motion in terms of velocity (**v**), or speed (v= |**v**|) of particles (I-frames for us). Here pops up the subtle shift mentioned above leading from event distances to a space I-frames (particles) are located. Thus, at a non-relativistic limit, the mechanical momentum **p** = M**v** and energy E =(1/2)M$\mathbf{v}^2$. Thus, d**p**/d**p** = M**v** = **p**. Take the differential coefficient from eq.(3.11.4) to get:

$$\mathbf{v} = \mathbf{p}c/E \qquad (3.11.6)$$

Using eq.(3.5) one gets:

$$(1-(v/c)^2)\, E^2 = (M_o c^2)^2 \text{ or } \qquad E = \gamma\, M_o c^2 \qquad (3.11.7)$$

The factor gamma is given by:

$$\gamma = (1-(v/c)^2)^{-1/2} = (1-(\beta)^2)^{-1/2} \qquad (3.11.8)$$

The velocity **v** is hence equal to $\boldsymbol{\beta}$c.

Lorentz factor γ is then the ratio between total energy E and rest mass energy $M_o c^2$:

$$\gamma = E/M_o c^2 \qquad (3.11.9)$$

This is a key result from special relativity theory.

E&E.3-1. Find an expression for the momentum vector in terms of the rest mass momentum M_oc.
Consider the relations:1) $dE/d\mathbf{p} = M\mathbf{v} = \mathbf{p}$; 2) $E = \gamma M_oc^2 = Mc^2$. From 2) the total energy M including the kinetic energy of the frame: $M=\gamma M_o$ and from 1) we deduce: $\mathbf{p}= \gamma M_o \mathbf{v}$.

E&E.3.11-2. Use eq.(3.11.9) to discuss a situation where $\beta=1$ and the physical system has a finite energy E.
To make a simple discussion we rewrite the equation as $\gamma M_oc^2 = E$. If the system is going to show a finite energy E in the limit $\beta \rightarrow 1$ the gamma factor goes to infinity according to eq.(3.8). The rest mass of this system in the limit must be zero. Photons are seen this manner, they do not have an inertial frame associated due to their zero rest-mass they transport a finite amount of energy (quantum).

Before dwelling a little more in classical physics aspects observe that we have taken E as a label in the preceding chapters and insist on the claim that it is the difference between two energy levels that import an energy that can be traded between quantum systems and their external energy sources (EM fields for instance). The equation above tells us that mass can also be taken as a label that can be transformed into an energy label. If a quantum process involving two quantum states with mass labels $|M_1>$ and $|M_2>$ in the same I-frame, then if the difference $|M_1-M_2|$ differs from zero we can safely conclude that there is an amount of energy that will be exchanged with an external source (system). A positive value corresponds to an energy release when a process shifting the quantum state $[|M_1> |M_2>](1\ \ 0)$ into a new one $[|M_1> |M_2>](0\ \ 1)$ for $M_1 < M_2$ you will possibly have a blast! By now you can suspect there is need for a lot more before one get this quantum change in action. But the ground idea is there.

A mapping relating two frames, obtained from one another after origin translation and a general rotation of the space-time frame, defines the set of Lorentz equations. Take the 4-vector $\mathbf{a}$ to represent an origin displacement and $\underline{\underline{\Lambda}}$ a 4x4 rotation matrix. The Lorentz transformations $L(\mathbf{a};\underline{\underline{\Lambda}})$ leave invariant $(ds)^2$, i.e. the scalar product $d\mathbf{s}\bullet d\mathbf{s}$ is the same in any rotated frame.

Invariance of the fundamental length to translations and rotations elicits homogeneity and isotropy of (relative) space-time. The location of origin for the laboratory frame is conventional; there is no absolute coordinate representation.

At this stage we do not need more elaborations of kinematics and dynamics. We already used time in a non-relativistic sense (parameter) to explore time displacements invariance when mapped on to Hilbert space. We got the form of a basic law, namely, time-dependent Schrödinger equation. Space-time coordinates serve label purposes in so far defining base vectors in a Hilbert space projected on to an inertial frame. However, because the theory is constructed upon invariableness or symmetries, actual coordinate values are irrelevant, only those

mathematical elements constructed with them that are invariant to Lorentz transformations are relevant.

Quantum states projected onto a multi-dimensional Cartesian coordinate space with origin coinciding with an arbitrary I-frame takes on the form of a wave function. This is a definition. Thus, configuration space is not related to spatiality, there is no location with respect to other elements such as particles or the likes. In clear terms, configuration space is not indicating the positions of a given number of particles. Here, it is an invariant mathematical space supporting any wave functions related to all possible abstract quantum states belonging to Hilbert space that we would like to project out. Furthermore, the time space used so far is a mathematical construct; there is no real space temporality involved, only sequential order.

One objective is to label abstract quantum states with an inertial frame. Therefore, no internal motion is the case and the time axis is never rotated towards the space axis (no boosts). This characterizes a non-relativistic limit case that is used through out in textbooks. The base states are label by space vector **q** with one end at the origin of the I-frame; for a one constituent the coordinate is given by a triad of real numbers (q_1,q_2,q_3), the labels refer to components for three orthogonal unit vectors in column form: $[\mathbf{i}_1, \mathbf{i}_2, \mathbf{i}_3]$. As the complexity of the material systems increases, the dimension of the configuration space also does it. One thing must be clear, once the 1-system is defined, the configuration space is fixed and indexed by the origin of the I-frame; quantum states can change only and projected on the fixed configuration space generates wave functions eliciting changes when the quantum state does it. It is in the nature of the changes that time enters the picture. But changes of detectors set ups are to be monitored at Fences where temporality enforces physical time and spatiality enforces space as locations with respect to a given frame or set of frames.

How is it possible to detect quantum change at any arbitrary reference system? The answer to this question is simple: a quantum state is given by a set of amplitudes affecting the set of base states; they are complex numbers associated to the abstract quantum state. The 1-system base set must be supplemented with the base sets associated to asymptotic states sustained by material systems each one with a respective I-frame so that one always gets the same total number of elements (electrons and nuclei) but new I-frame labels.

The base sets for the multi-I-frame asymptotic systems must be included with the set for the 1-system (supermolecule).

E&E.3.11-1 N-dimensional configuration space

The dimension of a configuration space depends upon the degrees of freedom assigned to a given material system. For the sake of completeness let us give a short presentation of the Euclidean N-dimensional space or Cartesian space.

Definition 1: R^N is a vector space of dimension N where each point x is defined by the N-coordinates $x_1,x_2,\ldots,x_N$;
Def.2: If x and y are two points of R^N their sum x+y is the point $x_1+y_1,x_2+y_2,\ldots,x_N+y_N$;
Def.3:If h is any real number, hx is the point with coordinates $hx_1,hx_2,\ldots,hx_N$;
Def.4: The statement $x\geq 0$ means that $x_1\geq 0,x_2\geq 0,\ldots,x_N\geq 0$;
Def.5: $x\geq y$ means that $x-y\geq 0$;
Def.6: $|x|$ stands for the Euclidean norm: $(x_1^2+x_2^2+\ldots+x_N^2)^{1/2}$; Note that $|x-y|$ is the Euclidean distance between x and y.
Def.7: The hyper volume element $dx_1\ dx_2\ldots dx_N$ is represented by dx in many circumstances; $d^{3N}x$ in others.

Distinguish now between internal quantum states referred to an I-frame from quantum states associated to the I-frame taken as a global physical system. This can be done because a global internal quantum state may be associated to an attractor such that for all practical purposes, the total mass M of the material system can be assigned to the origin of the I-frame. It might as well show mass moments (moments of inertia) in such a way that in real space one can compute classical and/or quantum properties. The coordinates of the laboratory frame are then referred to another frame in real space; configuration base states can hence be introduced with real space locating a composite particle state. At any rate, configuration spaces are supports for quantum states.

Finally, to any configuration space there is a space of reciprocal (wave) vectors related by Fourier transformations.

E&E.3.11-2 Groups

A set of elements g= e, g_1, g_2,… not necessarily countable belong to a group G whenever there is a composition law ($\cdot$) such that
-1. Closure: $g_i\in G$, $g_j\in G \Rightarrow g_i\cdot g_j \in G$
This simply means that taking two elements belonging to the group G when composed with this law there is an element in the set, e.g., $g_i\cdot g_j = g_{ij}$ that is in the definition list; we name this element as g_{ij} just for the sake of notation; for specific cases one has to find out which element in G corresponds to this g_{ij}.

-2. Associativity:	$g_k\cdot (g_i\cdot g_j) = (g_k\cdot g_i)\cdot g_j$
-3. Existence of identity $e\in G$:	$e\cdot g_i = g_i\cdot e$ for all ($\forall$) elements g_i, $e\in G$
-4. Existence of inverse $g_i^{-1}\in G$:	$g_i^{-1}\cdot g_i = g_i\cdot g_i^{-1} = e \ \forall\ g_i\in G$
-5. Commutative (abelian) groups:	$g_i\cdot g_j = g_j\cdot g_i$

If a group consists of a finite number of elements then it is called finite group; G is called infinite otherwise. An example of this latter type is the rotation group $L(\underline{\underline{\Lambda}})$ leaving invariant $(ds)^2$.