4 Symmetries in quantum mechanics

Symmetry transformations - operations that can be done on the system without altering its properties - are important already in classical mechanics and classical field theory as they lead (via the celebrated Noether theorem, to be discussed in Section 11.1) to conservation laws which, in turn, often simplify solving physical problems. They are equally important in quantum mechanics where they allow for example to establish selection rules for quantum transitions (like the ones occurring in atoms interacting with radiation - see Chapter 3), to understand spectra of Hamiltonians and sometimes even to find the exact spectra using group theoretic methods only. Symmetries become even more important in quantum field theories where they usually form the very basis of their formulation by allowing to account for the observed or postulated conservation laws; one also builds quantum field theory models by postulating symmetries (of the action functionals I - see Chapter 11 - defining them) and specifying the number and character of fields (i.e. specifying the field degrees of freedom). Some of the postulated symmetries, whether ordinary or gauge, can be directly read off from the spectrum of the theory Hamiltonan but the consequences of some other may not be directly observable in their spectra due to the phenomenon of spontaneous symmetry breaking.

In this chapter we give a brief introduction to symmetries in quantum theories. Our general considerations will be illustrated here mainly on examples taken from the familiar nonrelativistic quantum mechanics of a single particle, but they apply equally well to nonrelativistic quantum mechanics of systems of many particles developed in Chapter 5 and to quantum field theory. In particular the general results discussed here will be applied to formulate quantum mechanics of interacting relativistic particles, which is one of the possible approaches to the formulation of quantum field theory (presented in Chapters 6 - 9).

4.1 General considerations

In quantum mechanics physical states of a considered system are represented in the Hilbert space appropriate for this system by rays rather than by vectors. Rays are classes of equivalence of vectors which differ one from another by a phase factor:

$$\Psi \sim \Psi' \qquad \text{if} \qquad \Psi = e^{i\delta}\,\Psi',$$

or, in the Dirac notation, $|\Psi\rangle \sim |\Psi'\rangle$ if $|\Psi\rangle = e^{i\delta}\,|\Psi'\rangle$. Observables are represented by linear Hermitian operators O, i.e. operators such that $O = O^\dagger$. The operator $O^\dagger$ conjugate (with respect to the scalar product $(\cdot|\cdot)$ of vectors belonging to the Hilbert space) to a linear operator O is defined by the relation[1]

$$\left(\Phi|O^\dagger\Psi\right) \equiv (O\Phi|\Psi) = (\Psi|O\Phi)^*\,, \tag{4.1}$$

[1]One has to resort here to the mathematical notation Ψ, Φ, etc. instead of $|\Psi\rangle$, $|\Phi\rangle$, etc. for state vectors because the Dirac bra-ket notation is not general enough.

which should hold for all[2] vectors Ψ and Φ. From this definition it follows that eigenvalues of Hermitian operators are real. (To see this, take the scalar product of $O\Psi = \lambda\Psi$ with Ψ, use $O = O^\dagger$ and then apply the definition (4.1) to get $\lambda = \lambda^*$). Another theorem says that different state-vectors, say Ψ_1 and Ψ_2, on which a given Hermitian operator O has different eigenvalues λ_1 and $\lambda_2 \neq \lambda_1$, respectively, are orthogonal to each other. (To show this write: $\lambda_1(\Psi_2|\Psi_1) = (\Psi_2|O\Psi_1) = (O^\dagger\Psi_2|\Psi_1) = (O\Psi_2|\Psi_1) = \lambda_2(\Psi_2|\Psi_1)$; therefore, either $(\Psi_2|\Psi_1) = 0$ or $\lambda_1 = \lambda_2$.)

In classical mechanics one speaks of a symmetry of a given system if, after it is subjected to a transformation S (active view), its transformed counterpart satisfies the same equations of motion as did its original version. For instance, if $\mathbf{r}(t)$ is any trajectory of a pointlike mass m in the gravitational field $-GMm\mathbf{r}/|\mathbf{r}|^3$ of a (pointlike) mass M fixed at the origin of the space, i.e. $m\ddot{\mathbf{r}}(t) = -GMm\mathbf{r}(t)/|\mathbf{r}(t)|^3$, then the trajectory $\mathbf{r}'(t)$ which is obtained by rigidly rotating in space the original trajectory $\mathbf{r}(t)$ by any angle around any axis passing through the origing will also satisfy the same equation: $m\ddot{\mathbf{r}}'(t) = -GMm\mathbf{r}'(t)/|\mathbf{r}'(t)|^3$. Rotations are therefore symmetries of this system.

All transformations S of a system having this property form a group of the system's symmetry transformations: the composition $S_2 \cdot S_1$ of any two such transformations S_1 and S_2 is also a symmetry transformation; each symmetry transformation S has its inverse S^{-1}; there is a trivial transformation - the identity transformation, denoted id, etc. Rotations which are symmetries of the discussed mechanical system form the $SO(3)$ group.

Analogously to the classical case, in Quantum Mechanics, in which the evolution with time of the system's state is represented in the appropriate Hilbert space $\mathcal{H}$ by the changing in time state-vector $\Psi(t)$ or $|\Psi(t)\rangle$, satisfying the Schrödinger equation (1.1), a transformation S of the system is its symmetry, if the state vector $|\Psi'(t)\rangle$ representing the physical state of the transformed system satsfies the same equation (1.1) (with the same Hamiltonian H) as does $\Psi(t)$ ($|\Psi(t)\rangle$) and this should hold for any possible physical state of the system.

A symmetry transformation S which can act on all possible physical states of a given system transforming them into its other possible physical states defines a mapping of the system's Hilbert space $\mathcal{H}$ into itself. Such a mappig must, in addition to being compatible with the time evolution, satisfy also another important requirement. If the physical system is in a state represented by a vector Ψ belonging to the ray R and Φ_n are some vectors belonging to a set of rays R_n, which forms a complete set of orthogonal rays (usually represented by eigenvectors of a Hermitian operator of some particular observable) in the system's Hilbert space, then, according to the rules of Quantum Mechanics, the probability that the system will be found (as a result of a specific measurement) in the state represented by the ray R_n is given by

$$P(R \to R_n) = |(\Phi_n|\Psi)|^2\,, \tag{4.2}$$

[2]We ignore here potential subtleties related to domains on which these operators are defined.

and, due to the completeness of the set of rays R_n,

$$\sum_n P(R \to R_n) = 1\,. \tag{4.3}$$

Symmetry transformations must preserve such probabilities of all possible outcomes of all possible measurements that can be made on the system. Thus, if $R \to R'$ and $R_n \to R'_n$, under the action of a symmetry transformation S, where R, R_n etc. are the rays representing states of the original system and R' and R'_n, etc. are the rays representing states of the transformed system, then the mapping of the Hilbert space generated by S must be such that

$$P(R' \to R'_n) = P(R \to R_n)\,. \tag{4.4}$$

A fundamental theorem by E. Wigner says that mappings of Hilbert spaces satisfying this requirement can only be represented by two types of operators, which obviously act not on ryas but on vectors: either by linear and unitary operators $U(S)$, satisfying the rule

$$U(\alpha\Psi + \beta\Phi) = \alpha\, U\Psi + \beta\, U\Phi\,, \tag{4.5}$$

and such that

$$(U\Phi|U\Psi) = (\Phi|\Psi)\,, \tag{4.6}$$

or by antilinear and antiunitary operators $A(S)$, such that

$$A(\alpha\Psi + \beta\Phi) = \alpha^* A\Psi + \beta^* A\Phi\,, \tag{4.7}$$

and

$$(A\Phi|A\Psi) = (\Psi|\Phi) = (\Phi|\Psi)^*\,. \tag{4.8}$$

If the Hermitian conjugation $A^\dagger$ of an antilinear operator A is defined by (compare with (4.1) - the modification of the definition is necessary to make it compatible with the antilinearity of A)

$$\big(\Phi|A^\dagger\Psi\big) \equiv (A\Phi|\Psi)^* = (\Psi|A\Phi)\,, \tag{4.9}$$

the (anti)unitarity conditions of both types of symmetry operators, linear ones and antilinear ones, read

$$U^\dagger = U^{-1}\,, \qquad\qquad A^\dagger = A^{-1}\,, \tag{4.10}$$

so that

$$\begin{aligned}(U\Phi|U\Psi) &= \big(\Phi|U^\dagger U\,\Psi\big) = \big(\Phi|U^{-1}U\,\Psi\big) = (\Phi|\Psi)\,,\\ (A\Phi|A\Psi) &= \big(\Phi|A^\dagger A\,\Psi\big)^* = \big(\Phi|A^{-1}A\,\Psi\big)^* = (\Phi|\Psi)^*\,.\end{aligned} \tag{4.11}$$

The trivial symmetry transformation - the identity id - is obviously represented by the unit operator $\hat{1}$, which is unitary. It follows, that continuous transformations, which can be continuously deformed to the identity transformation, must also be represented by unitary linear operators. The only known symmetry represented by the antilinear operator is the time reversal transformation (and its composition with other symmetry transformations).

Thus, symmetry operations are represented by unitary (or antiunitary) operators[3] $U(t)$ (even if the operation on the physical system is itself the same at every moment, the Schrödinger picture operator representing it may depend on time - the prominent example being the operators representing boost transformations) such that the equation

$$i\hbar \frac{d}{dt} U(t)|\Psi(t)\rangle = H(t)\, U(t)|\Psi(t)\rangle\,, \tag{4.12}$$

is satisfied if

$$i\hbar \frac{d}{dt} |\Psi(t)\rangle = H(t)\, |\Psi(t)\rangle\,, \tag{4.13}$$

holds. In other words, by unitary (or antiunitary) operators $U(t)$ such that[4]

$$U(t)\, U(t,t_0) = U(t,t_0)\, U(t_0)\,,$$

where $U(t,t_0)$ is the Schrödinger picture evolution operator (defined in Section 1.1) of the system. In most cases when the Hamiltonian of the system does not depend on time this condition is satisfied because $[U(t), H] = 0$ (in which case the symmetry represented by $U(t)$ has direct consequences in the Hamiltonian's spectrum - see Section 4.3), but this need not be always so - again the prominent example are the boost transformations.

We have considered here symmetries which are transformations of the actual physical system. This is the so-called *active view* on symmetry transformations. It is somewhat easier conceptually than the alternative one, called the *passive view*, within which one considers the same system but viewed by another "observer" (who uses another reference frame). In this case the evolution in time of the system's state as seen by the two different "observers" is represented by the respective vectors $|\Psi(t)\rangle$ and $|\Psi'(t)\rangle$ and it is obvious that if $|\Psi(t)\rangle$ satisfies (4.13), $|\Psi'(t)\rangle$ must satisfy a similar equation but with in general a different Hamiltonian H'. It is also clear that probabilities cannot change, that is (4.4), in which R'_n and R' are rays used by the other observer, must hold when the "observer" (the reference frame) changes and therefore such transformations of the states $|\Psi\rangle$ into $|\Psi'\rangle$ must be effected by unitary or antiunitary operators. Operations of changing the "observer" (the reference frame) are symmetry operations if the new Hamiltonian H' is identical with old one H.

4.2 Continuous symmetry transformations

Suppose a (more or less) abstract group of continuous transformations of a given physical system has been identified and we try to realize it on vectors belonging to the system's

[3]Do not confuse symmetry operators with the evolution operator $U(t_2,t_1)$ which has, however, two time arguments.

[4]This readily follows from the general solution (see Section 1) $U(t)|\Psi(t)\rangle = U(t,t_0)U(t_0)|\Psi(t_0)\rangle$ of the equation (4.12) after substituting $|\Psi(t)\rangle = U(t,t_0)|\Psi(t_0)\rangle$ into the left hand side.

Hilbert space. The group structure of the symmetry transformations must be reflected in the properties of the operators representing them: if

$$S_1 : \;\; R_n \to R'_n \,, \qquad \text{and} \qquad S_2 : \;\; R'_n \to R''_n \,,$$

so that

$$S_2 \cdot S_1 : \;\; R_n \to R''_n \,,$$

then the operator $U(S_1)$ should transform vectors forming R_n into vectors forming R'_n and $U(S_2)$ vectors from R'_n into vectors from R''_n. Correspondingly, the operator $U(S_2 \cdot S_1)$ should transform vectors of the ray R_n directly into vectors of R''_n. However, since operators act on vectors rather than on rays, one cannot exclude that

$$U(S_2)\, U(S_1)\, \Psi_n = e^{-i\phi_n(S_2,S_1)}\, U(S_2 \cdot S_1)\, \Psi_n \,, \tag{4.14}$$

that is, there can be a phase factor in the composition law of the operators representing the symmetry transformations. It is easy to see that the phase factor $\phi_n(S_2, S_1)$ must be the same for all Hilbert space vectors that can be superposed:

$$\begin{aligned} e^{-i\phi_{nm}(S_2,S_1)}\, U(S_2 \cdot S_1)\, (\Psi_n + \Psi_m) &= U(S_2)\, U(S_1)\, (\Psi_n + \Psi_m) \\ &= U(S_2)\, U(S_1)\, \Psi_n + U(S_2)\, U(S_1)\, \Psi_m \\ &= e^{-i\phi_n(S_2,S_1)}\, U(S_2 \cdot S_1)\, \Psi_n + e^{-i\phi_m(S_2,S_1)}\, U(S_2 \cdot S_1)\, \Psi_m \,. \end{aligned} \tag{4.15}$$

Acting on both sides of this equality with $U^{-1}(S_2 \cdot S_1)$ and rearranging the terms, we get

$$\left(e^{-i\phi_{nm}(S_2,S_1)} - e^{-i\phi_n(S_2,S_1)}\right) \Psi_n + \left(e^{-i\phi_{nm}(S_2,S_1)} - e^{-i\phi_m(S_2,S_1)}\right) \Psi_m = 0 \,.$$

If the vectors Ψ_n and Ψ_m are linearly independent, this can hold only if the coefficients of Ψ_n and Ψ_m vanish, that is, if the three phase factors are equal. Therefore, in general, the composition law of symmetry operators takes the form

$$U(S_2)\, U(S_1) = e^{-i\phi(S_2,S_1)}\, U(S_2 \cdot S_1) \,, \tag{4.16}$$

with the phase depending only on the transformations being composed and their concrete representation by operators in the subspace spanned by all vectors of the Hilbert space that can be superposed (i.e. the superposition of which can represent physically realizable states of the quantum system - see the discussion following the formulae (4.32) and (4.33)).

Associativity of the symmetry transformations reflected in the corresponding property $U(S_3)[U(S_2)U(S_1)] = [U(S_3)U(S_2)]U(S_1)$ of the symmetry operators $U(S)$, implies that the phase factors $\phi(S_2, S_1)$ satisfy the relation

$$\phi(S_3,\, S_2 \cdot S_1) + \phi(S_2,\, S_1) = \phi(S_3,\, S_2) + \phi(S_3 \cdot S_2,\, S_1) \,. \tag{4.17}$$

If the phases $\phi(S_2, S_1)$ cannot be absorbed by a redefinition of the operators $U(S)$ - this would be possible if they could be represented in the form

$$\phi(S_2, S_1) = \varphi(S_2 \cdot S_1) - \varphi(S_2) - \varphi(S_1) \,,$$

- that is when they form a nontrivial *two-cocycle*, one has to do with a *projective* representation of the symmetry group by operators acting in the system's Hilbert space.

Projective representations can always be avoided by appropriately enlarging the symmetry group (i.e. by replacing the original symmetry group by its - usually more abstract - universal covering group) without changing physical implications of the symmetries as such. (This will be demonstrated below on the important example of the Gaileo group and its rotation subgroup.) At this point we assume that the symmetry group we are discussing is just the enlarged one.

Continuous symmetry transformations form Lie groups that can be identified with differentiable manifolds. The real parameters θ_a, $a = 1, \ldots, n$ varying continuously in some domain - for notational convenience they can be viewed as forming together a vector $\boldsymbol{\theta}$ - and parametrizing symmetry transformations $S(\boldsymbol{\theta})$ provide then the coordinate system on the group manifold. As it is customary, we assume they are such that $\boldsymbol{\theta} = \mathbf{0}$ corresponds to the identity transformation (id). In a given parametrization (a map on the group manifold) the composition rule $S_2 \cdot S_1 = S$, when written as $S(\boldsymbol{\theta}_2) \cdot S(\boldsymbol{\theta}_1) = S(\boldsymbol{\theta}) = S(h(\boldsymbol{\theta}_2, \boldsymbol{\theta}_1))$ defines the composition function $h_a(\boldsymbol{\theta}_2, \boldsymbol{\theta}_1) = \theta_a$, which must have the following obvious property:

$$h_a(\mathbf{0}, \boldsymbol{\theta}) = h_a(\boldsymbol{\theta}, \mathbf{0}) = \theta_a \,. \tag{4.18}$$

Operators[5] $U(\boldsymbol{\theta})$ representing in the Hilbert space infinitesimal (close to the identity) continuous symmetry transformations $S(\boldsymbol{\theta})$ with $|\theta_a| \ll 1$, can always be written as

$$U(S(\boldsymbol{\theta})) = \hat{1} - i\,\theta_a Q^a - \frac{1}{2}\theta_a\theta_b Q^{ab} + \mathcal{O}(\theta^3) \,. \tag{4.19}$$

The operators Q^a are called *symmetry generators*. As follows from the symmetry $\theta_a\theta_b = \theta_b\theta_a$, the operators Q^{ab} must be symmetric in their indices, $Q^{ab} = Q^{ba}$. Unitarity of $U(S)$ (up to $\mathcal{O}(\theta^2)$ terms) requires the generators Q^a to be Hermitian operators. For this reason, symmetry generators are always candidates for quantum mechanical observables. (One can even risk the statement that the only legitimate observables of a given quantum theory are indicated in this way by its symmetries.)

Applying the expansion (4.19) to the compositions rule (recall, we have assumed for the moment the absence of possible phase factors)

$$U(S(\boldsymbol{\theta}'))\, U(S(\boldsymbol{\theta})) = U(S(h(\boldsymbol{\theta}', \boldsymbol{\theta}))) \,, \tag{4.20}$$

and using the property (4.18) of the composition function $h_a(\boldsymbol{\theta}', \boldsymbol{\theta})$, which implies that its Taylor expansion has the form

$$h_a(\boldsymbol{\theta}', \boldsymbol{\theta}) = \theta'_a + \theta_a + C_a{}^{bc}\,\theta'_b\theta_c + \ldots \,, \tag{4.21}$$

[5]We omit in the notation their possible dependence on time.

we find

$$\left(1 - i\,\theta'_a Q^a - \frac{1}{2}\theta'_a\theta'_b Q^{ab} + \ldots\right)\left(1 - i\,\theta_a Q^a - \frac{1}{2}\theta_a\theta_b Q^{ab} + \ldots\right)$$
$$= 1 - i\,(\theta'_a + \theta_a + C_a{}^{bc}\theta'_b\theta_c)Q^a - \frac{1}{2}(\theta'_a + \theta_a)(\theta'_b + \theta_b)Q^{ab} + \ldots \tag{4.22}$$

Comparison of the coefficients of the same combinations of the θ's on both sides determines the operators Q^{ab}

$$Q^{bc} = Q^b Q^c - iC_a{}^{bc}Q^a = Q^c Q^b - iC_a{}^{cb}Q^a\,, \tag{4.23}$$

where the second equality follows from the requirement of the symmetry of Q^{ab} in its indices. Thus, the law of the composition of symmetry operations determines (but not completely, as will be seen shortly) the algebraic properties of the Hilbert space operators Q^a (generating transformations of state-vectors corresponding to infinitesimal symmetry transformations) of these symmetries:

$$\left[Q^a,\ Q^b\right] = i\left(C_c{}^{ab} - C_c{}^{ba}\right)Q^c \equiv if_c{}^{ab}Q^c\,. \tag{4.24}$$

The factors $f_a{}^{ab} = -f_a{}^{ba}$ are called the *structure constants* of the symmetry group *Lie algebra*.[6] The *Jacobi identity*

$$\left[Q^a,\ \left[Q^b,\ Q^c\right]\right] + \left[Q^c,\ \left[Q^a,\ Q^b\right]\right] + \left[Q^b,\ \left[Q^c,\ Q^a\right]\right] = 0\,, \tag{4.25}$$

(satisfied identically by any three operators Q^a, Q^b and Q^c) imposes then the following relation on the structure constants

$$\sum_{d=1}^{r}\left(f_e{}^{ad}f_d{}^{bc} + f_e{}^{cd}f_d{}^{ab} + f_e{}^{bd}f_d{}^{ca}\right) = 0\,. \tag{4.26}$$

The generators Q^a form the representation (by the operators acting in the Hilbert space) of the Lie algebra of the group of symmetry transformations which geometrically is identified with the vector space tangent to the Lie group manifold at its point representing the identity transformaion.

Finally, we note that if the group structure is such that the composition function $h_a(\boldsymbol{\theta}', \boldsymbol{\theta})$ is additive: $h_a(\boldsymbol{\theta}', \boldsymbol{\theta}) = \theta'_a + \theta_a$ (i.e. $f_a{}^{bc} \equiv 0$) - the whole symmetry group is Abelian, or we consider only an Abelian subgroup of it - one can write

$$U(S(\boldsymbol{\theta}_2))\,U(S(\boldsymbol{\theta}_1)) = U(S(h(\boldsymbol{\theta}_2, \boldsymbol{\theta}_1))) = U(S(\boldsymbol{\theta}_2 + \boldsymbol{\theta}_1))\,.$$

This allows to immediately find the explicit form of the operator $U(S(\boldsymbol{\theta}))$ representing finite transformations:

$$U(S(\boldsymbol{\theta})) = \lim_{N\to\infty}\left[U(S(\boldsymbol{\theta}/N))\right]^N = \lim_{N\to\infty}\left(1 - i\,\frac{\theta_a Q^a}{N}\right)^N = e^{-i\theta_a Q^a}. \tag{4.27}$$

[6] If the symmetry group is compact, like the rotation groups $SO(N)$ or special unitary groups $SU(N)$, the generators Q^a can be chosen in such a way that the structure constants are totally antisymmetric in all three indices. In these cases they can simply be written as f^{abc}.

We now return to the problem of projective representations. They can appear for two different reasons: the algebraic one and the topological one. The logic is as follows. We take from "the reality" a group of symmetry transformations which we think should be the symmetry group also in the quantum version of the problem (e.g. when considering the motion of a particle in a rotationally symmetric potential we take for it the $SO(3)$ group because this is the symmetry group considered in this context in classical mechanics). To find algebraic properties, in their possibly most general form, of the operators Q^a generating the unitary operators U, which should represent the symmetry transformations in the quantum theory, we expand both sides of the equality

$$U(S(\boldsymbol{\theta}'))\,U(S(\boldsymbol{\theta})) = e^{-i\phi(S',S)}\,U(S(h(\boldsymbol{\theta}',\boldsymbol{\theta})))\,, \tag{4.28}$$

similarly as in (4.21) and (4.22) but this time allowing for a possible phase factor, because its presence cannot *a priori* be excluded by physical requirements. Taking into account that the expansion of the phase factors must take the form

$$\phi(S(\boldsymbol{\theta}'),\, S(\boldsymbol{\theta})) = h^{ab}\theta'_a\theta_b + \ldots \tag{4.29}$$

(because if any of the two operators on the left-hand side of the formula (4.28) is the unit operator, the phase ϕ should be zero) and repeating the steps used in (4.22) which led to (4.24) we now find

$$\left[Q^a,\ Q^b\right] = i\left(C_c{}^{ab} - C_c{}^{ba}\right)Q^c + i\,(h^{ab} - h^{ba})\hat{1} \equiv i\,f_c{}^{ab}Q^c + i\,f^{ab}\hat{1}\,, \tag{4.30}$$

with $f^{ab} = h^{ab} - h^{ba}$. The terms proportional to the unit operator $\hat{1}$ are called the *central charges* (of the algebra of generators).

The Jacobi identity (4.25) imposes on central charges certain constraints which usually eliminate a number of them. Furthermore, some central charges not excluded by the Jacobi identity can be removed from the commutation relations by redefining the generators Q^a (without changing the $if_c{}^{ab}$ parts of their commutation rules which is uniquely determined by the composition law of the symmetry transformations). For example, they can all be removed in the case of the $SO(3)$ and the Poincaré groups, but not in the case of the Galileo group (as we will show shortly). If they cannot be removed, one has to do with the projective representation and the group is represented projectively already in the neighbourhood of the identity transformation.

Even if all central charges are ecluded or can be removed, the symmetry group representation can still be projective for topological reasons. This can happen if the group manifold is not simply connected, that is, when its *first homotopy group* (called also the *path group*) $\pi_1(G)$ is nontrivial. To ascribe a Hilbert space operator $U(S)$ to a point S (to a symmetry transformation) on the group manifold in a given coordinate system $\boldsymbol{\theta}$, in which S is characterized by $\boldsymbol{\theta}^S$, one chooses some standard path $\boldsymbol{\theta} = \boldsymbol{\theta}(\xi)$ with $\boldsymbol{\theta}(0) = \mathbf{0}$ and $\boldsymbol{\theta}(1) = \boldsymbol{\theta}^S$ connecting S with the identity transformation and solves along it the differential equation

$$\frac{d}{d\xi}\,U(\boldsymbol{\theta}(\xi)) = -iQ^a\,U(\boldsymbol{\theta}(\xi))\,f_a{}^b(\boldsymbol{\theta}(\xi))\,\frac{d\theta_b(\xi)}{d\xi}\,, \tag{4.31}$$

defining U for every point on the path (the input for ξ close to zero being the formula (4.19)). The equation (4.31) arises as follows. The operator $U(\boldsymbol{\theta}(\xi + d\xi)) \approx U(\boldsymbol{\theta}(\xi)) + (dU/d\xi)d\xi$ should be obtained as the composition

$$U(\delta\boldsymbol{\theta})\, U(\boldsymbol{\theta}(\xi)) \approx (1 - i\delta\theta_a Q^a)\, U(\boldsymbol{\theta}(\xi))\,,$$

with $\delta\theta_a$ determined by the condition

$$\begin{aligned}\theta_a(\xi + d\xi) \approx \theta_a(\xi) + \frac{d\theta_a(\xi)}{d\xi}\, d\xi = h_a(\delta\boldsymbol{\theta}, \boldsymbol{\theta}(\xi)) \\ \approx h_a(\mathbf{0}, \boldsymbol{\theta}(\xi)) + \left.\frac{\partial h_a(\tilde{\boldsymbol{\theta}}, \boldsymbol{\theta}(\xi))}{\partial \tilde{\theta}_b}\right|_{\tilde{\theta}_b=0} \delta\theta_b\,,\end{aligned}$$

where $h_a(\boldsymbol{\theta}_1, \boldsymbol{\theta}_2)$ is the group composition function. Due to its property (4.18) one gets

$$\delta\theta_a = f_a{}^b(\boldsymbol{\theta}(\xi))\, \frac{d\theta_b(\xi)}{d\xi}\, d\xi\,,$$

where $f_a{}^b(\boldsymbol{\theta}(\xi))$ is the matrix inverse to $\left.(\partial h_a(\tilde{\boldsymbol{\theta}}, \boldsymbol{\theta}(\xi))/\partial\tilde{\theta}_b)\right|_{\tilde{\theta}_b=0}$. This leads to (4.31). It can be shown, that if another path going from the identity to S is chosen and used to define $U(S)$, the same operator is obtained provided this new path and the standard one can be continuously deformed to each other.

To a composition $S_2 \cdot S_1$ of two transformations S_1 and S_2 there correspond, therefore, in principle two different operators: $U(S_2 \cdot S_1)$ obtained by integrating the defining differential equation along the standard path going from the identity directly to $S = S_2 \cdot S_1$ and the operator $U(S_2)\, U(S_1)$, which can be thought of as being obtained by integrating the defining differential equation along the path[7] $\mathrm{id} \to S_1 \to S_2 \cdot S_1$. If the group manifold is not simply connected, the latter path may not be continuously deformable to the standard one. If this is the case, the operator $U(S(\theta_2))\, U(S(\theta_1))$ obtained along the non-standard path $\mathrm{id} \to S_1 \to S_2 \cdot S_1$ may differ by a phase factor $\phi(S(\theta_2), S(\theta_1))$ from the operator $U(S_2 \cdot S_1)$ obtained using the standard path. Furthermore, if a path $\mathrm{id} \to S_1 \to S_2 \cdot S_1 = S$ is continuously deformable to another path $\mathrm{id} \to S_1' \to S_2' \cdot S_1' = S$, then, on the basis of what has already been said, they give rise to the same operator $U(S_2)\, U(S_1) = U(S_2')\, U(S_1')$, that is their relative phase factors with respect to $U(S_2 \cdot S_1)$

[7] This path can be realized as follows. Let the path $\theta_a^{\mathrm{stand}(S_1)}(\xi)$, such that $\theta_a^{\mathrm{stand}(S_1)}(0) = 0$ and $\theta_a^{\mathrm{stand}(S_1)}(1) = \theta_a^{S_1}$, be the standard path from id to S_1, and analogously, let $\theta_a^{\mathrm{stand}(S_2)}(\xi)$, such that $\theta_a^{\mathrm{stand}(S_2)}(0) = 0$ and $\theta_a^{\mathrm{stand}(S_2)}(1) = \theta_a^{S_2}$, be the standard path from id to S_2. Then the path $\theta_a(\xi)$ corresponding to $\mathrm{id} \to S_1 \to S_2 \cdot S_1$ is

$$\theta_a(\xi) = \begin{cases} \theta_a^{\mathrm{stand}(S_1)}(2\xi)\,, & \xi \in [0, \frac{1}{2}] \\ h_a(\boldsymbol{\theta}^{\mathrm{stand}(S_2)}(2\xi - 1),\, \boldsymbol{\theta}^{S_1})\,, & \xi \in [\frac{1}{2}, 1] \end{cases},$$

where $h_a(\boldsymbol{\theta}', \boldsymbol{\theta})$ is the group composion function.

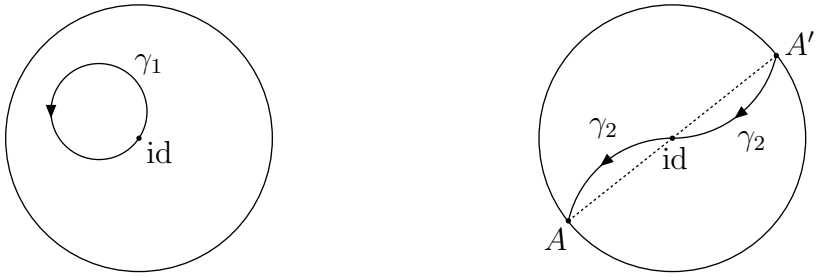

Figure 4.1: Two closed paths in the $SO(3)$ group manifold starting from the point $P \equiv$ identity (id). The path γ_1 is contractible to the trivial path. The path γ_2 is noncontractible due to the jump it makes from A to A'; the points A and A' in the figure represent the same point (transformation) in the group manifold.

(obtained using the standard path from the identity to S) must be equal. Thus, the phase factors that may appear in the formula (4.28) share the properties of the homotopy group of the group manifold of the considered symmetry transformations. It is therefore easy to understand that the phase factors form a one dimensional representation of the first homotopy group $\pi_1(G)$ of the manifold of the symmetry transformations (that is, of G).

For example, the group manifold of the three-dimensional rotations is doubly connected: $\pi_1(SO(3)) = \mathbb{Z}_2$, where $\mathbb{Z}_2$ is the group consisting of two elements: the identity id and another element, call it a, and the group composition law reads: $\mathrm{id}\cdot a = a\cdot\mathrm{id}$, $\mathrm{id}\cdot\mathrm{id} = \mathrm{id}$, $a \cdot a = \mathrm{id}$. This group has two one-dimensional representations: the faithful one in which id is represented by 1 and a by -1 and another one which is trivial because both elements, id and a, are represented by 1. That $\pi_1(SO(3)) = \mathbb{Z}_2$ can be seen by representing each rotation by the vector the length of which is equal to the rotation angle α and pointing in the direction of the rotation axis $\mathbf{n}$. All such vectors fill a ball of radius $R = \pi$. The topology of this manifold is however complicated by the fact that a rotation by $\alpha = \pi$ around $\mathbf{n}$ is equivalent to the rotation by $\alpha = \pi$ around the direction $-\mathbf{n}$. Therefore, the antipodal points of the surface of the ball have to be identified. This leads to its double connectedness: imagine a path starting from a point P somewhere inside the ball and returning to P which reaches somewhere the surface of the ball. Because the point on the surface is equivalent to its antipodal point, the path can make a "jump" from one side of the surface to the other side where it can again reimmerse into the ball to reach P. Such a path cannot be continuously deformed to another path going also from P back to P, but which remains entirely inside the ball (cf. Figure 4.1). However, a path which makes two "jumps" can be continuously deformed to it (see Figure 4.2). Thus, $\pi_1(SO(3)) = \mathbb{Z}_2$ and the phase factors $e^{-i\phi}$ in the composition law (4.16) of the operators representing rotations in the Hilbert space can only form one of the two possible one-dimensional representations of the $\mathbb{Z}_2$ group, that is, either be simply unity or take the values 1 and -1.

This is indeed confirmed when the commutation relations (4.24) of the rotation group

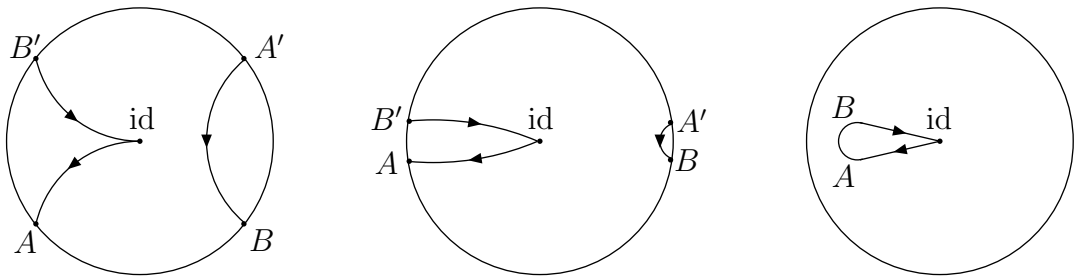

Figure 4.2: Consecutive stages of contracting to the point a path in the $SO(3)$ group manifold which makes two jumps.

- cf. also Section 4.4 and the formulae (4.81) - are explicitly solved:[8] one finds that the representations labeled by half-integer j ($j = \frac{1}{2}, \frac{3}{2}, \ldots$) are projective. Take e.g. as S_1 and S_2 the rotations around the z axis by the angles α_1 and α_2, respectively. From (4.27) it then follows that

$$U(S(\alpha)) = \exp\left(-\frac{i}{\hbar}\alpha J^z\right).$$

Denoting $|j, j_z\rangle$ the common eigenvectors (for simplicity we assume they are normalizable and suppress other labels needed to fully specify them) of the $\mathbf{J}^2$ and J^z operators, one gets that if $j = \frac{1}{2}$, $\langle \frac{1}{2}, j_z|J^z|\frac{1}{2}, j'_z\rangle = \frac{\hbar}{2}(\sigma^3)_{j_z j'_z}$. If the angles α_1 and α_2 are such that $\alpha_1 + \alpha_2 = 2\pi$, one obtains that

$$\langle \tfrac{1}{2}, j_z|U(S(\alpha_2))U(S(\alpha_1))|\tfrac{1}{2}, j'_z\rangle = \left(\exp -2\pi\frac{i}{2}\sigma^3\right)_{j_z j'_z} = -\left(I_{2\times 2}\right)_{j_z j'_z}, \qquad (4.32)$$

whereas $S(\alpha_2) \cdot S(\alpha_1) =$ id and therefore the operator ascribed to $S(\alpha_2) \cdot S(\alpha_1)$ along the standard path is simply the unit operator the matrix elements of which between the $\mathbf{J}^2$ and J^z eigenvectors with $j = \frac{1}{2}$ form simply the 2×2 unit matrix $I_{2\times 2}$. The same is also true for all half integer values of j. Thus, in the case of half-integer j representations (realized in a Hilbert space on state-vectors representing states of an odd number of fermions, which have half-integer spins) of the rotation group $SO(3)$ the phase factor $e^{-i\phi}$ is indeed equal $+1$ or -1.

If one considers instead representations characterized by $j = 0, 1, \ldots$ composing two rotations by α_1 and by α_2 around the z-axis with $\alpha_1 + \alpha_2 = 2\pi$ one gets

$$\langle j, j_z|U(S(\alpha_2))U(S(\alpha_1))|j, j'_z\rangle = \left(I_{(2j+1)\times(2j+1)}\right)_{j_z, j'_z}, \qquad (4.33)$$

[8] Solving the commutation relations of a symmetry group means (in the context of quantum mechanics) finding the explicit form of elements of the symmetry group generators Q^a in the basis (formed by normalizable or nonnormalizable vectors) of a subspace of the Hilbert space in which basis the group generators belonging to the Cartan subalgebra are diagonal - see the discussion following the formula (4.58).

so in this case the phase factors $e^{-i\phi}$ are always equal $+1$. The proof (4.15) that the phase factors cannot depend on the vector in the Hilbert space on which operators are acting (but are only intrinsic properties of the operators and the transformations) relied on the possibility of forming a superposition of the two vectors. Because in composing the same two operators $U(S_2)$ and $U(S_1)$ representing the rotations S_2 and S_1 one can apparently meet with two different representations of $\pi_1(SO(3))$ by the phase factors - the trivial one, in which $e^{-i\phi} = +1$ and the faithful one in which $e^{-i\phi} = \pm 1$, (depending on whether the operators act on vectors corresponding to integer or half integer j), one is tempted to think that it is the structure of the rotation group that imposes a *superselection rule* which forbids forming superpositions of state-vectors corresponding to integer and half integer values of j.[9] However, as a matter of facts, the impossibility of forming superpositions of state vectors corresponding to integer and half integer spins does not follow from the topological properties of the rotation group. The point is (as already said) that the symmetry group $SO(3)$ can be replaced by its universal covering group, the $spin(3)$ group isomorphic withe the $SU(2)$ group, which has the same physical implications, but is simply-connected (i.e. its first homotopy group is trivial) and, for this reason, has only non-projective representations. We have the full right to *declare* that the group of symmetry transformations of the quantum system is not $SO(3) = SU(2)/\mathbb{Z}_2$, but $SU(2)$ and the $spin(3) \simeq SU(2)$ group would not impose any selection rule. Nevertheless, we still do believe that preparing physical systems in states which are superpositions of states corresponding to integer and half-integer spin values is physically impossible although it would now not cause any contradiction[10] (*transitions* between such states and other "normal" states are then, obviously, forbidden by the rotational invariance which ensures conservation the total angular momentum).

It is easy to demonstrate that the $SU(2)$ group is indeed simply-connected and constitutes the twofold covering of the rotation group $SO(3)$. By definition the $SU(2)$ group is the group formed by all unitary 2×2 matrices with unit determinant (unimodular). Any such matrix M can be represented in the form

$$M = \exp(-iH)\,, \qquad \text{where} \qquad H = H^\dagger \qquad \text{and} \qquad \mathrm{tr}(H) = 0\,. \tag{4.34}$$

[9]This problem does not arise, of course, in ordinary quantum mechanics of a single particle in which all vectors of the Hilbert space are superpositions of $\hat{\mathbf{J}}^2$ eigenvectors characterized all by integer or all by half-integer j. It appears however already in nonrelativistic quantum mechanics of many-particle systems within which one can consider interactions of bosons and fermions (e.g. electrons and phonons) which have integer and half-integer spins, respectively. In this case the superselection rule says that a superposition of the state of, say, two bosons and one fermion with the state of one bosons and two fermions is not allowed (it cannot be realized experimentally).

[10]If $SU(2)$ is taken for the system's symmetry group nontrivial transformation properties of states formed as superpositions of interger and half-integer spin states under rotations by 2π: e.g. (schematically)

$$|j = 1\rangle + |j = \frac{1}{2}\rangle \longrightarrow |j = 1\rangle - |j = \frac{1}{2}\rangle\,,$$

which would be strange if such rotations were identity transformations, would be acceptable because the rotations by 2π are then not the identity symmetry transformation.

Matrices H satisfying these requirements can in turn always be written linear combinations with real coefficients of the three Pauli matrices σ^i. Hence, the $SU(2)$ group has 3 generators and its Lie algebra is isomorphic with the one of $SO(3)$ (determined by the composition law of three-dimensional rotations of a macroscopic body). However, $SU(2)$ has "twice as many" elements as does $SO(3)$: given a three-dimensional vector $\mathbf{r}$ we can form a 2×2 matrix[11] $V = -\mathbf{r} \cdot \boldsymbol{\sigma} = \sigma_i \, r^i$, where $\boldsymbol{\sigma}$ is the vector formed by three Pauli matrices. Of course, V is Hermitian, $\mathrm{tr}(V) = 0$ and $\det(V) = -\mathbf{r}^2$. Take now a 2×2 matrix M belonging to $SU(2)$. The matrix V'

$$V' = M \cdot V \cdot M^\dagger \,, \tag{4.35}$$

is also Hermitian and traceless, so it defines a new vector $\mathbf{r}'$ through the formula $V' = -\mathbf{r}' \cdot \boldsymbol{\sigma}$. Since $\det(V') = \det(V)$, it follows that $\mathbf{r}^2 = \mathbf{r}'^2$. Hence, M defines a rotation $R(M)$ such that $R(M) \cdot \mathbf{r} = \mathbf{r}'$. In fact every rotation can be represented by a matrix M belonging to $SU(2)$. From (4.35) it is clear, however, that the $SU(2)$ matrices M and $-M$ (both belonging to the $SU(2)$ matrix group) define the same rotation: $R(M) = R(-M)$. Therefore, one says that the $SU(2)$ group is the (universal) twofold covering of the rotation group $SO(3)$.

The group $SU(2)$ is simply-connected, its topology being that of a three-dimensional sphere[12] ($\pi_1(S_n)$ for $n > 2$ is trivial, i.e. consists of a single element only), so it has only non-projective representations. The elements of $SU(2)$ corresponding to the rotation R around the z axis by an angle α are the matrices $\exp(-\frac{i}{2}\sigma^3\alpha)$ and $\exp(-\frac{i}{2}\sigma^3(\alpha + 2\pi)) = -\exp(-\frac{i}{2}\sigma^3\alpha)$. The ranges of the parameters θ_a, $a = 1, 2, 3$ parametrizing elements of the $SU(2)$ group are $[0, 4\pi)$ because all θ_a in this range give different unitary, unimodular matrices. The $SO(3)$ group is obtained from $SU(2)$ as $SU(2)/\mathbb{Z}_2$ where $\mathbb{Z}_2$ is the (trivially) invariant subgroup[13] of $SU(2)$ consisting of the matrices I and $-I$. Thus, if we declare that the true symmetry of the quantum system is $SU(2)$ instead of $SO(3)$, there are only non-projective representations but the superselection rule still remains (as we believe) valid.

[11] In view of the $SL(2, C)$ construction of spinor representations of the Lorentz group - see Section 8.6 - it is convenient to introduce already here the matrices $\sigma_i = -\sigma^i$ and also the matrices $\bar{\sigma}^i = -\sigma^i$ so that $\delta^i{}_j = \frac{1}{2}\mathrm{tr}(\bar{\sigma}^i \sigma_j)$.

[12] The most general form of a unitary unimodular 2×2 matrix $M^\dagger = M^{-1}$ is

$$M = \begin{pmatrix} d + ie & f + ig \\ -f + ig & d - ie \end{pmatrix},$$

with the parameters d, e, f and g satisfying the constraint $d^2 + e^2 + f^2 + g^2 = 1$ (ensuring that $\det(M) = 1$), which is just the definition of the three-dimensional sphere S_3 (immersed in the four-dimensional Euclidean space).

[13] A group $H \subset G$ is an invariant subgroup of the group G if $ghg^{-1} \in H$ for every $h \in H$ and every $g \in G$. The quotient group G/H consists of the equivalence classes of elements of G defined by the equivalence relation $g \sim g'$ if $g' = gh$ for some $h \in H$.

4.3 The Galileo group

In this Section we apply the general formalism outlined above to a nonrelativistic quantum theory. As the examples we will consider mainly one-particle systems, but the general considerations will apply to many-particle systems as well.

We consider first the transformations which form the Galileo group and which are assumed to be the symmetry transformations of some physical system. These transformations are rotations of the system in the three-dimensional space, translations in three space directions, translations in time and transformations corresponding to boosting the considered physical system to an arbitrary velocity. The elements composing a transformation S belonging to the Galileo group can be, therefore, represented as

$$S = (O,\, \mathbf{V},\, \mathbf{a},\, \tau)\,, \tag{4.36}$$

where[14] O is an orthogonal rotation preserving the Euclidean scalar product of three-dimensional vectors and $\mathbf{V}$ and $\mathbf{a}$ are two three-vectors with the components V^i and a^i, $i = 1, 2, 3$, in a fixed base $\mathbf{e}_1$, $\mathbf{e}_2$, $\mathbf{e}_3$ of the three-dimensional space. On the space and time coordinates x^i, $i = 1, 2, 3$, and the time t of an event occuring in the considered physical system the element S of the Galileo group (a transformation) acts in the following way

$$\begin{cases} x'^i = O^i{}_j\, x^j + V^i\, t + a^i \\ t' \;\; = t + \tau \end{cases}. \tag{4.37}$$

The 3×3 matrix O satisfies the relation $O^T \cdot O = O \cdot O^T = I$. We take here the *active view* on the transformations. x'^i, t' are thus the space-time coordinates of the same event occuring in the system translated forward in time by τ (i.e. the event occurs in it later than the one in the original system) and first rotated by O, then boosted to acquire a (additional) velocity $\mathbf{V}$ and then shifted in space by a vector $\mathbf{a}$. In the *passive view* on transformations x'^i and t' are the space-time coordinates of the event occuring in the system as seen by another observer which in the reference frame, the axes $\mathbf{e}'_i$ of which are given by $O^{-1} \cdot \mathbf{e}_i$, moves with respect to the original frame with the velocity $-\mathbf{e}'_i V^i$, uses the coordinate system shifted by $-\mathbf{e}'_i a^i$ and whose clock is late by τ (i.e. according to this clock the event occurs earlier) with respect to the clock of the original observer.

The composition law of the group elements S_2 and S_1 can be easily deduced by considering the action of two successive transformations $S_1 = (O_1,\, \mathbf{V}_1,\, \mathbf{a}_1,\, \tau_1)$ and $S_2 = (O_2,\, \mathbf{V}_2,\, \mathbf{a}_2,\, \tau_2)$ on the space-time coordinates: the transformations

$$\begin{cases} x'^i = (O_1)^i{}_j\, x^i + V_1^i\, t + a_1^i \\ t' \;\; = t + \tau_1 \end{cases}, \qquad \begin{cases} x''^k = (O_2)^k_{\;i}\, x'^i + V_2^i\, t' + a_2^i \\ t'' \;\; = t' + \tau_2 \end{cases} \tag{4.38}$$

[14] We will denote O (from polish "obrót") active rotations which are linear mappings O of vector spaces into themselves. (A rotation O of a "live" vector $\mathbf{V}$ is written as $O \cdot \mathbf{V}$.) Matrices $O^i{}_j$ of such rotations, also denoted O, are then to be understood (using the notation of my "iconic" algebra notes) as matrices $[O_{(\mathbf{e})(\mathbf{e})}]^i{}_j$ given (on "both sides") in the same basis $\mathbf{e}_i$ of the vector space in which O acts.

when combined give

$$\begin{cases} x''^k = (O_2{\cdot}O_1)^k_{\ j}\, x^j + (O_2)^k_{\ j} V_1^j\, t + (O_2)^k_{\ j} a_1^j + V_2^k\, t + V_2^k\, \tau_1 + a_2^k \\ t'' = t + \tau_2 + \tau_1 \end{cases} .$$

Hence,

$$S_2 \cdot S_1 = (O_2{\cdot}O_1,\, \mathbf{V}_2 + O_2{\cdot}\mathbf{V}_1,\, \mathbf{a}_2 + O_2{\cdot}\mathbf{a}_1 + \mathbf{V}_2\, \tau_1,\, \tau_2 + \tau_1)\,, \tag{4.39}$$

and the transformation inverse to $S = (O, \mathbf{V}, \mathbf{a}, \tau)$ is (check that $S^{-1}{\cdot}S = \mathrm{id} \equiv (I, \mathbf{0}, \mathbf{0}, 0)$ as well as $S \cdot S^{-1} = \mathrm{id}$)

$$S^{-1} = (O^{-1},\ -O^{-1}{\cdot}\mathbf{V},\ -O^{-1}{\cdot}\mathbf{a} + O^{-1}{\cdot}\mathbf{V}\,\tau,\ -\tau)\,. \tag{4.40}$$

We now parametrize the infinitesimal transformation S, or in other words, introduce a local coordinate system on the Galileo group manifold in the vicinity of the identity transformation. An infinitesimal rotation can be most conveniently parametrized by the three components (angles) θ^1, θ^2 and θ^3 given in the (orthonormal) basis $\mathbf{e}_1$, $\mathbf{e}_2$ and $\mathbf{e}_3$ of the vector $\boldsymbol{\theta}$ specifying it (recall that a vector $\mathbf{u}$ rotated by an infinitesimal angle θ around the axis $\boldsymbol{\theta}/\theta$ is given by $\mathbf{u}' \approx \mathbf{u} + \boldsymbol{\theta} \times \mathbf{u}$):

$$\begin{pmatrix} x'^1 \\ x'^2 \\ x'^3 \end{pmatrix} \approx \begin{pmatrix} 1 & -\theta^3 & \theta^2 \\ \theta^3 & 1 & -\theta^1 \\ -\theta^2 & \theta^1 & 1 \end{pmatrix} \begin{pmatrix} x^1 \\ x^2 \\ x^3 \end{pmatrix}, \tag{4.41}$$

so that the matrix o of an infinitesimal rotation in (4.37) takes the form[15]

$$o^i_{\ j} = \delta^i_{\ j} - \delta^{il}\epsilon_{lkj}\,\theta^k \equiv \delta^i_{\ j} - \delta^{il}\omega_{lj} \equiv \delta^i_{\ j} + \omega^i_{\ j}\,, \tag{4.42}$$

(antisymmetry of ω_{lj} in the l and j indices ensures orthogonality of $o^i_{\ j}$ up to the terms of second order in ω_{lj}). The remaining elements of the infinitesimal symmetry transformation can be most naturally parametrized by the three components of the boost velocity v^i, the three components ε^i of the space translation and the infinitesimal time shift δ. In the quantum theory there should exist such Hermitian operators J^l (or $J^{ki} \equiv \epsilon^{kil}J^l$), K^l, P^l and H playing the same role as do the generators Q^a in (4.19) and allowing to write the operator $U(S(o, \mathbf{v}, \boldsymbol{\varepsilon}, \delta))$ of the infinitesimal transformation (in the chosen parametrization), in which the matrix $o = I + \omega$ of the infinitesimal rotation is parametrized by $\boldsymbol{\theta}$ as indicated in (4.42), in the form

$$U(o, \mathbf{v}, \boldsymbol{\varepsilon}, \delta) = \hat{1} - \frac{i}{\hbar}\,\theta^l J^l - \frac{i}{\hbar}\,v^l K^l - \frac{i}{\hbar}\,\varepsilon^l P^l + \frac{i}{\hbar}\,\delta\, H\,. \tag{4.43}$$

Compared to our general notation introduced in (4.19) we have factorized here $1/\hbar$ and chosen the signs in front of the generators so that J^l, P^l, and H will coincide with

[15] In view of its Minkowskian four-dimensional generalization it is convenient to define the Levi-Civita tensors with upper and lower indices as $\epsilon^{123} = +1 = -\epsilon_{123}$, so that $\epsilon^{kij}\epsilon_{mij} = -2\delta^k_{\ m}$.

the operators of the total angular momentum, the momentum and the Hamiltonian, respectively (the true symmetry generators are $J^l/\hbar$, $P^l/\hbar$ and $H/\hbar$).

Deriving the explicit form of the composition function h_a (defined above the formula (4.18)) from the Galileo group composition rule (4.39) we could now find the commutation relations between the generators J^i, K^i, P^i, and H. There is however a simpler method of finding them. Since we know how the phase factors can affect the commutation rules (by giving rise to the appearance of central charges) we will temporarily ignore them and consider the following product of operators

$$U(S)\,U(o,\mathbf{v},\boldsymbol{\varepsilon},\delta)\,U^{-1}(S)\,,$$

in which $S=(O,\mathbf{V},\mathbf{a},\tau)$. This can be represented in two different ways. Firstly, one can use (4.43) to write the above composition in the form

$$\begin{aligned}&\hat{1}-\frac{i}{\hbar}\,\theta^l\,U(S)J^lU^{-1}(S)-\frac{i}{\hbar}\,v^l\,U(S)K^lU^{-1}(S)\\&\quad-\frac{i}{\hbar}\,\varepsilon^l\,U(S)P^lU^{-1}(S)+\frac{i}{\hbar}\,\delta\,U(S)HU^{-1}(S)\,.\end{aligned}\tag{4.44}$$

Secondly, one can apply the composition rule (4.39) and (4.40) to write

$$U(S)\,U(o,\,\mathbf{v},\,\boldsymbol{\varepsilon},\,\delta)\,U^{-1}(S)=U(\tilde{O},\,\tilde{\mathbf{V}},\,\tilde{\mathbf{a}},\,\tilde{\tau})\,,\tag{4.45}$$

where

$$\begin{aligned}\tilde{O}^i{}_j&\equiv\delta^i{}_j+(O\cdot\omega\cdot O^{-1})^i{}_j\equiv\delta^i{}_j+\tilde{\omega}^i{}_j\,,\\\tilde{V}^i&\equiv O^i{}_jv^j-(O\cdot\omega\cdot O^{-1})^i{}_jV^j\,,\\\tilde{a}^i&\equiv O^i{}_j(\varepsilon+v\tau)^j+V^i\delta-(O\cdot\omega\cdot O^{-1})^i{}_j(a-V\tau)^j\,,\\\tilde{\tau}&\equiv\delta\,.\end{aligned}$$

As the parameters of this new transformation all vanish for vanishing $\omega^i{}_j$, v^i, ε^i and δ, they are all infinitesimal. Owing to this one can write

$$U(\tilde{O},\,\tilde{\mathbf{V}},\,\tilde{\mathbf{a}},\,\tilde{\tau})=\hat{1}-\frac{i}{\hbar}\,\tilde{\theta}^kJ^k-\frac{i}{\hbar}\,\tilde{V}^kK^k-\frac{i}{\hbar}\,\tilde{a}^kP^k+\frac{i}{\hbar}\,\tilde{\tau}H\,.\tag{4.46}$$

Comparing the coefficients of θ^l, v^l, ε^l and δ in (4.44) and in (4.46) one finds

$$\begin{aligned}U(S)\,J^{ij}\,U^{-1}(S)&=\big(J^{kl}-V^kK^l+V^lK^k\\&\qquad-(a+V\tau)^kP^l+(a+V\tau)^lP^k\big)\,R^{ki}R^{lj}\,,\\U(S)\,K^i\,U^{-1}(S)&=\big(K^j+\tau P^j\big)\,R^{ji}\,,\\U(S)\,P^i\,U^{-1}(S)&=P^jR^{ji}\,,\\U(S)\,H\,U^{-1}(S)&=H+V^iP^i\,.\end{aligned}\tag{4.47}$$

Taking now the parameters of S itself to be infinitesimal, that is, writing: $R^{ij} = \delta^{ij} - \omega^{ij}$, $V^i = v^i$, $a^i = \varepsilon^i$ and $\tau = \tau$, expanding both sides of the equalities (4.47) to the first order in these small parameters and comparing the corresponding coefficients on both sides, we arrive at the following commutation relations

$$\begin{aligned}
&\big[J^i,\ J^j\big] = i\hbar\,\epsilon^{ijk} J^k\,, && \big[P^i,\ P^j\big] = 0\,,\\
&\big[J^i,\ P^j\big] = i\hbar\,\epsilon^{ijk} P^k\,, && \big[K^i,\ K^j\big] = 0\,,\\
&\big[J^i,\ K^j\big] = i\hbar\,\epsilon^{ijk} K^k\,, && \big[K^i,\ P^j\big] = 0\,,\\
&\big[J^i,\ H\big] = 0\,, && \big[P^i,\ H\big] = 0\,,\\
& && \big[K^i,\ H\big] = -i\hbar P^i\,.
\end{aligned} \tag{4.48}$$

To account for possible phases in the formula (4.16) we have to supplement the right hand side of each of the above commutation relations with a c-number term times the unit operator $\hat{1}$ - a possible central charge. We have, however, to check whether such central charges are allowed by the Jacobi identity (4.25). Let us consider the first commutator of (4.48) in the modified form

$$\big[J^i,\ J^j\big] = i\hbar\,\epsilon^{ijk} J^k + i\hbar\, f^{ij}_{JJ}\,\hat{1}\,, \tag{4.49}$$

where $f^{im}_{JJ} = -f^{mi}_{JJ}$. Inserting this form of the commutators into the Jacobi identity (4.25) with three generators J we find that the combination

$$\epsilon^{ijm} f^{km}_{JJ} + \epsilon^{kim} f^{jm}_{JJ} + \epsilon^{jkm} f^{im}_{JJ}\,, \tag{4.50}$$

should vanish. Contracting it with δ^{ki} gives

$$\epsilon^{ijm} f^{im}_{JJ} + \epsilon^{jim} f^{im}_{JJ}\,.$$

Because this is automatically zero (owing to the antisymmetry of ϵ^{ijm}), we conclude[16] that the Jacobi identity does allow for a nonzero f^{im}_{JJ}. In contrast, the Jacobi identity with J, P and H shows that $f^{i}_{PH} = 0$ and the one with two J's and H eliminates f^{i}_{JH}. We consider next the modified commutation relation

$$\big[P^i,\ P^j\big] = i\hbar\, f^{ij}_{PP}\,\hat{1}\,. \tag{4.51}$$

The Jacobi identity with P^i, K^j and H shows then that $f^{ij}_{PP} = 0$ - the central charge in the commutation rule of two P operators is forbidden by the Jacobi identity. The same follows by taking the Jacobi identity with J^x, P^x and P^y which implies that that $f^{xz}_{PP} = 0$, etc. Similar argument eliminates also f^{ij}_{KK}. However the equality $\epsilon^{kij} f^{ij}_{KP} = 0$ (which can be obtained in the same way) does not imply vanishing of the central charge f^{ij}_{KP}, because $f^{ij}_{KP} \neq -f^{ji}_{KP}$; the central charge f^{ij}_{KP} can have a nonzero symmetric part, which, taking the physical dimensions of the operators into account can be written as

$$\big[K^i,\ P^j\big] = -i\hbar M\,\delta^{ij}\,\hat{1}\,, \tag{4.52}$$

[16] One can check that the combination (4.50) does indeed vanish in all possible cases.

with M being some real mass parameter (the sign is chosen for the latter convenience). Similarly, the Jacobi identities do not exclude the central charges f^{ij}_{JP}, f^{ij}_{JK} nor f^{i}_{KH}.

In the next step we try to redefine the generators to eliminate central charges. It is easy to see that defining

$$\tilde{J}^i = J^i + \frac{1}{2}\epsilon^{ijk} f^{jk}_{JJ}\,\hat{1}\,, \qquad \tilde{P}^i = P^i + \frac{1}{2}\epsilon^{ijk} f^{jk}_{JP}\,\hat{1}\,, \qquad \tilde{K}^i = K^i + \frac{1}{2}\epsilon^{ijk} f^{jk}_{JK}\,\hat{1}\,,$$

we obtain the commutation rules $[\tilde{J}^i,\ \tilde{J}^j] = i\hbar\epsilon^{ijk}\tilde{J}^k$, $[\tilde{J}^i,\ \tilde{P}^j] = i\hbar\epsilon^{ijk}\tilde{P}^k$, $[\tilde{J}^i,\ \tilde{K}^j] = i\hbar\epsilon^{ijk}\tilde{K}^k$, and also $[\tilde{K}^i,\ H] = -i\hbar\tilde{P}^k$, since the Jacobi identity with J, K and H relates appropriately f^{ij}_{JP} with f^{i}_{KH} (check it!). Thus, the only commutation rule from which the central charge cannot be eliminated is (4.52), because there is no operator on its right hand side that could be redefined. From now on, we will assume that the generators have been redefined and will omit the tildas.[17]

The consequence of the modified commutation rule (4.52) is the following. Take $S_2 = (I,\ \mathbf{V},\ \mathbf{0},\ 0)$ and $S_1 = (I,\ \mathbf{0},\ \mathbf{a},\ 0)$. Geometrically, that is according to the rule (4.39), $S_2 \cdot S_1 = (I,\ \mathbf{V},\ \mathbf{a},\ 0)$. Since K^i commute with K^j and P^i commute with P^j, (4.27) can be used to write $U(S_2)$ and $U(S_1)$ separately in the exponentiated forms. (4.52) then implies that[18]

$$U(S_2)\,U(S_1) = e^{-\frac{i}{\hbar}\mathbf{V}\cdot\mathbf{K}}\,e^{-\frac{i}{\hbar}\mathbf{a}\cdot\mathbf{P}} = e^{-\frac{i}{2\hbar}\mathbf{a}\cdot\mathbf{V}M}\,e^{-\frac{i}{\hbar}(\mathbf{V}\cdot\mathbf{K}+\mathbf{a}\cdot\mathbf{P})}\,. \tag{4.53}$$

The right hand side differs by the phase factor from the operator ascribed to $S_2 \cdot S_1$ with the help of (4.27) parametrizing the standard path from id to the transformation $S_2 \cdot S_1$ as $(R(\xi), \mathbf{V}(\xi), \mathbf{a}(\xi), \tau(\xi)) = (I, \xi\mathbf{V}, \xi\mathbf{a}, 0)$, with $0 \le \xi \le 1$. This shows that because of the presence of the central charge f^{ij}_{KP} we have to do with a projective representation.

The extension of the Galileo group which allows to avoid projective representations is obtained by, besides the replacement of the $SO(3)$ group factor by the $SU(2)$ one, as discussed at the end of Section 4.2, the formal inclusion into the algebra of generators of the mass operator $M\hat{1}$, which commutes with all other generators of the Galileo group and which acting on a state of a particle (of many particles - in the case of quantum mechanics of a many-particle system) gives its mass (the sum of masses of particles represented by this state). This extends the Galileo group by an additional $U(1)$ factor. In a quantum theory of a many-particle system such a mass operator which commutes with H forbids

[17]The above analysis was completely general, not relaying on any concrete realization of the Galileo group by operators in a particular Hilbert space. When a quantum theory of a system is constructed by quantizing its given classical theory, the symmetries of which are known (or postulated), the Noether theorem combined with the canonical quantization rules gives a concrete prescription for constructing the system's symmetry group generators and obtaining their algebra i.e. their commutation relations; the form of the central charges follows then automatically from the construction. This will be illustrated in Chapter 11 in the case of fields quantization.

[18]In the second step we have used the standard formula $e^{A+B} = e^{-\frac{1}{2}[A,\,B]}e^A e^B$ valid provided the operator $C = [A,\ B]$ commutes with A and B.

transitions between states of different masses implying the mass conservation law (and, therefore, the conservation of the numbers of particles of each kind separately). In addition, one imposes the superselection rule (which does not follow from the symmetry group itself but rather reflects the experimental reality) which forbids forming superpositions of states corresponding to different masses.

If the Galileo group is indeed the symmetry group of a concrete physical system (which may also posses other symmetries, called *internal symmetries* to distinguish them from the ones related to the space-time transformatios forming the Galileo group or, in the relativistic case, the Poincaré group) it should be possible to construct (usually by appealing to the Noether theorem and the procedure of the canonical quantization) Hermitian symmetry generators H, J^i, P^i, K^i acting in the system's Hilbert space and satisfying, up to the allowed central charges, the commutation rules (4.48) which have been determined on the basis of the "geometric" properties of these symmetry transformations. Whether this is indeed possible and what is the interpretation of these generators, depends, of course, on the physical situation specified primarily by the Hamiltonian H of the considered system. Some Hamiltonians (e.g. singling out a point or a direction in the space) can make it impossible to find operators satisfying all the requirements simultaneously. Usually it is then possible to satisfy the requirements for a subgroup (consisting e.g. of rotations and time translations only) of the full Galileo group.[19]

We now illustrate these general considerations on examples. Instead of appealing to the Noether theorem, to find how the operators realizing in the Hilbert space assumed symmetry transformations should act on states of the system we shall simply require that matrix elements of operators (corresponding to measurable quantities) between states of the transformed system agree in the expected way with the corresponding matrix elements of these operators between states of the original system. We will continue to employ the *active* point of view on symmetry transformations, as conceptually it is somewhat easier: to check whether the action on states of the found putative symmetry operators satisfying these requirements is compatible, as discussed in Section 4.1, with the dynamics we will simply ask whether the transformed system is also physically realizable and whether the time evolution of its states is a solution of the original Schrödinger equation.

We begin with time translations. Physically the state vector $|\Psi'\rangle$ of the system translated in time by τ and the state vector $|\Psi\rangle$ of the original system should be related in such a way that for $t' = t + \tau$ the matrix elements of (time independent) operators O

[19] Because there are then less symmetry generators, and therefore less commutators determined by the symmetry group properties (composition rule), some restrictions imposed by the Jacobi identity may be absent (the operators like e.g. the momentum operator or the total angular momentum operator which still can be constructed, but do not generate symmetries may have commutators with the symetry generators which have different form they would have to have, if they too were symmetry generators) and additional central charges may become allowed.

corresponding to observables satisfy[20]

$$O_{\psi'}(t') \equiv \langle \Psi'(t')|O|\Psi'(t')\rangle = \langle \Psi(t)|O|\Psi(t)\rangle \equiv O_{\psi}(t)\,, \tag{4.54}$$

i.e. the result of a measurement made on the time-translated system at time t' should coincide with the result of the same measurement made on the original system at t. Validity of (4.54) for all superpositions of states is ensured by the relation $|\Psi'(t')\rangle = |\Psi(t)\rangle$, where $t' = t + \tau$. In agreement with our general discussion, if time translations are symmetries of the physical system, there should exists a unitary operator $U(\tau)$, such that

$$|\Psi'(t)\rangle = |\Psi(t-\tau)\rangle = U(\tau)|\Psi(t)\rangle\,. \tag{4.55}$$

Writing the Taylor expansion of $|\Psi(t-\tau)\rangle$ we find

$$\begin{aligned} |\Psi'(t)\rangle &= |\Psi(t)\rangle + \frac{i}{\hbar}\,\tau\left(i\hbar\frac{d}{dt}\right)|\Psi(t)\rangle + \frac{1}{2}\left(\frac{i}{\hbar}\,\tau\right)^2\left(i\hbar\frac{d}{dt}\right)^2|\Psi(t)\rangle + \ldots \\ &= |\Psi(t)\rangle + \frac{i}{\hbar}\,\tau H|\Psi(t)\rangle + \frac{1}{2}\left(\frac{i}{\hbar}\,\tau\right)^2\left(i\hbar\frac{d}{dt}\right)H|\Psi(t)\rangle + \ldots\,, \end{aligned} \tag{4.56}$$

where H is the Hamiltonian. Comparing with the infinitesimal form of $U(\tau)$ we see that it is the Hamiltonian that is the candidate for the generator of time translations. However, H is the time translation generator only if it is time independent: the composition law (4.39) tells us that time translations form an Abelian subgroup of the Galileo group. Therefore, as follows from the formula (4.27), we should have $U(\tau) = \exp((i/\hbar)\tau H)$. From the last term in (4.56) it is however clear that this is possible only if $dH/dt = 0$. It is also obvious that in such a case if $|\Psi(t)\rangle$ satisfies the Schrödinger equation, so will do also $|\Psi'(t)\rangle = U(\tau)|\Psi(t)\rangle$. Thus, if the Hamiltonian is time independent translations in time are symmetries of the quantum theory and are obviously generated by the Hamiltonian itself. This result is completely general and applies to any quantum theory.

In principle one can envisage situations in which H does depend on time (time translation symmetry is explicitly broken), whereas the other operations (e.g. rotations and/or space translations) remain good symmetries (that is, the operators having the properties required for the generators of these symmetries can be constructed). However, in such a case instantaneous energy eigenstates are not of direct physical interest and, therefore, consequences of the remaining symmetries are not immediately clear.[21] In the following we will assume that time translations are good symmetries of the considered physical system. As required by the commutation rules (4.48), the generators of space translations and/or rotations (if these operations are good symmetries) as well as other generators Q^a of possible internal symmetries (see the examples of the harmonic oscillators and the nonrelativistic Hydrogen atom) should then commute with the Hamiltonian.

[20] If the (Schrödinger picture) operator O depends on time, one should equate matrix elements of $O(t')$ and $O(t)$, respectively.

[21] But symmetries the generators Q^a of which commute with $H(t)$ at a particular instant t have, of course, standard implications for the spectrum of the instantaneous eigenvalues of $H(t)$ at that instant.

This is a good place to discuss the implications for the spectrum of the Hamiltonian H of a set of generators Q^a, $a = 1, \ldots, o$ which all commute with it and form by themselves a closed algebra in the sense of satisfying the commutation relations (4.24):

$$\left[Q^a,\ Q^b\right] = i f_c{}^{ab} Q^c\,, \tag{4.57}$$

with some structure constants $f_c{}^{ab}$. The considerations presented below are again fairly general and will apply also to the relativistic quantum field theory of interactions of elementary particles. The role of the generators Q^a can be played by the rotation group generators J^i of the Galileo group (or of the Poincaré group in the relativistic case), or by generators of some additional internal symmetries, like e.g. the isospin symmetry or the "Eightfold-Way" symmetries of strong interactions, the physical system uder considerations may possess.[22]

Suppose a set of such generators Q^a acting in the Hilbert space and commuting with the system's Hamiltonian is given. Of course, if $H|n\rangle = E_n|n\rangle$ (n labeling the energy levels can also be a multi-index), then also $HU(\boldsymbol{\theta})|n\rangle = E_n U(\boldsymbol{\theta})|n\rangle$, where $U(\boldsymbol{\theta})$ is the unitary operator built out of the generators Q^a and the continuous parameters $\boldsymbol{\theta} = (\theta_1, \ldots, \theta_o)$ realizing a symmetry transformation. This does not mean that the degeneracy of the energy levels of the system is infinite (parametrized by the continuous parameters $\boldsymbol{\theta}$) but only that each energy level (treated as a subspace of the Hilbert space) is spanned by state-vectors (forming its basis) $|n, i\rangle$ (all satisfying $H|n, i\rangle = E_n|n, i\rangle$) labeled by a discrete index i (which in general is a multi-index $i = (i_1, \ldots, i_r)$, see below), such that for any $\boldsymbol{\theta}$ the state $U(\boldsymbol{\theta})|n, i\rangle$ is a linear combination of the vectors $|n, j\rangle$. In fact, all basis vectors $|n, j\rangle$ can be obtained from a given one by successively acting on it with the generators Q^a.

Consider now matrices formed out of the matrix elements of the generators Q^a between the basis vectors $|n, i\rangle$ of an energy level E_n:

$$T^a_{ij} \equiv \langle n, i|Q^a|n, j\rangle\,. \tag{4.58}$$

The matrices T^a_{ij} obviously share the algebraic properties of the generators Q^a. In partic-

[22]The question whether internal symmetries can combine with the space-time ones to form a larger group of symmetries (with nonzero commutators of the space-time symmetry generators with the internal symmetry generators) finds in the relativistic case the answer in the negative in the important Coleman - Mandula "no-go" theorem which says that any algebra of generators of internal and Poincaré space-time symmetries can only have the form of a direct sum of the separate algebras (that is, generators of these two kinds of symmetries must necessarily commute); correspondingly, the full symmetry group must have the form of the direct product of the groups formed by space-time and internal symmetries. In the nonrelativistic case, when space-time symmetries form the Galileo group the Coleman - Mandula is not valid and in the past there were attempts (not especially successful) within the nonrelativistic quark model to combine the Gell-Mann $SU(3)$ internal symmetry with the space-time ones. In the relativistic case the only possibility to circumvent the Coleman - Mandula "no-go" theorem is to allow for graded symmetry Lie algebras which consist of generators of bosonic and fermionic types (fermionic generators satisfy then the anticommutation relations). This is the basis of supersymmetric theories.

ular, they satisfy the commutation relations[23]

$$T^a_{ik}T^b_{kj} - T^b_{ik}T^a_{kj} = if_c{}^{ab}T^c_{ij}\,, \tag{4.59}$$

with the same structure constants $f_c{}^{ab}$ as in (4.57). Hence, they form a *matrix representation* of the Lie algebra of the symmetry group generated by Q^a's. Mathematically speaking, at each energy level E_n of the system the state-vectors $|n,i\rangle$ span the space (i.e. form its basis) of a matrix representation of the Lie algebra of the symmetry group (physicists say: they span a representation or, shortly, they form a representation). Possible matrix (i.e. finite-dimensional) representations of various Lie algebras are well known from group theory. For example, if $[H,\,\mathbf{J}] = 0$, rotations are good symmetry transformations and the matrix representations of the Lie algebra of the rotation group we are familiar with are $2j+1$ dimensional with $j = 0, \frac{1}{2}, 1, \ldots$, and the state-vectors $|n,i\rangle \equiv |j,j_z\rangle$ are labeled by the eigenvalues of the operator J^z.

In more complicated cases one defines the *rank* r of the Lie algebra (assigned also to the group generated by this algebra) as the maximal number of its generators (or of their linear combinations) which commute with one another. The maximal set of mutually commuting generators form what in group theory is called the *Cartan subalgebra*; the rank r of the group is simply the dimension of its Cartan subalgebra. It follows from the general rules of quantum mechanics that the state-vectors $|n,i\rangle$ can be chosen in such a way that all generators belonging the the Cartan subalgebra have only diagonal elements between these vectors. Therefore, the eigenvalues of these generators are used to label the state-vectors $|n,i\rangle$ (i.e. define the index i) within a given representation of the Lie algebra. In other words, i is in fact a multi-index $i = (i_1, \ldots, i_r)$ specifying the eigenvalues on the state $|n, i_1, \ldots, i_r\rangle$ of each of these r Cartan subalgebra generators. In the case of the rotation group any two generators do not commute and the group rank equals 1. J^z is then chosen as the single generator of the Cartan subalgebra. In the $SU(3)$ group, the rank of which is 2, there are two commuting generators and the states within a given representation are labeled by two indices - the eigenvalues of the two Cartan subalgebra generators.

Finally, the fundamental theorem of Racah states that for every simple group of rank r exactly r independent operators[24] can be built out of its generators Q^a (not necessarily as their linear or bilinear combinations), which commute with all the generators Q^a and, because they are built out of Q^a's (assumed to commute with H), also with the Hamiltonian H. These operators called the *Racah operators*, being constructed from Q^a's, cannot map vectors belonging to a given representation into vectors belonging to another representation. Moreover, since they commute with all Q^a's, they cannot map a vector from a given representation into another vector of the same representation either (commuting in particular with all Cartan subalgebra generators, they cannot change their eigenvalues

[23]Recall, that we have assumed that the symmetry group is already the enlarged one, so that the central charges are absent (i.e. they are included into the set of generators Q^a).

[24]Independent means that they are not powers of each other nor products of (powers) of others.

and, therefore, cannot map one basis vectors of a given representation into another one because these are distinguished by the eigenvalues of the Cartan subalgebra generators and all vectors can be written as superpositions of these basis vectors); the same follows also from the mentioned fact that all basis vectors of a given representation can be obtained by successively acting with all Q^a's on one vector of this representation). Hence, all the vectors of a given representation must be eigenvectors with the same eigenvalues of the Racah operators. For this reason the eigenvalues of the Racah operators are used to distinguish different representations (their eigenvalues are different on vectors belonging to different representations) of the Lie algebra of the symmetry group that are realized on various energy levels of the system. A simplifying circumstance is the fact that, as found by Casimir, one of the Racah operators is always given in the form of a biliner combination of the generators Q^a. It is called the *Casimir operator*. In the case of the rotation group generated by $\mathbf{J}$ this Casimir operator is just $\mathbf{J}^2 = (J^x)^2 + (J^y)^2 + (J^z)^2$. Since the $SU(2)$ group is of rank $r = 1$, this is the only Racah operator and representations of $SU(2)$ are completely specified by the $\mathbf{J}^2$ eigenvalues.

After these general remarks we return to our considerations of the Galileo group transformations, using now as nonrelativistic quantum mechanics of a single particle as an example.

The first one is the symmetry with respect to space translations in quantum mechanics of a single particle. Physically the wave function ψ' (the state vector $|\psi'\rangle$) of the translated system and the wave function ψ ($|\psi\rangle$) of the original system should be related by $|\psi'(\mathbf{r}')| \equiv |\langle\mathbf{r}'|\psi'\rangle| = |\langle\mathbf{r}|\psi\rangle| \equiv |\psi(\mathbf{r})|$, where $\mathbf{r}' = \mathbf{r}+\mathbf{a}$. If translation are to be symmetry operations, this must hold for all possible superpositions of states. This implies that $\psi'(\mathbf{r}') = \psi(\mathbf{r})$. Therefore, the unitary operator $U(\mathbf{a})$ realizing translations in the Hilbert space: $|\psi'\rangle = U(\mathbf{a})|\psi\rangle$, must be such that

$$\psi'(\mathbf{r}) = \langle\mathbf{r}|\psi'\rangle = \langle\mathbf{r}|U(\mathbf{a})|\psi\rangle = U(\mathbf{a})\,\psi(\mathbf{r}) = \psi(\mathbf{r}-\mathbf{a})\,, \tag{4.60}$$

where the last $U(\mathbf{a})$ here is understood to be the operator in the position representation. Proceeding as in the case of time translations we find

$$U(\mathbf{a}) \approx 1 - \frac{i}{\hbar}\,\mathbf{a}\cdot(-i\hbar\boldsymbol{\nabla}) = \hat{1} - \frac{i}{\hbar}\,\mathbf{a}\cdot\hat{\mathbf{p}} \approx \exp\left(-\frac{i}{\hbar}\,\mathbf{a}\cdot\hat{\mathbf{p}}\right), \tag{4.61}$$

where the fact that $[\hat{p}^i,\ \hat{p}^j] = 0$ enabled us to use (4.27) to get $U(\mathbf{a})$ for finite transformations. This shows that it is the ordinary momentum operator which plays the role of space translations generator. However, if time translations are also symmetries of the system then, as we have found, the structure of the Galileo group requires that H and $\mathbf{P}$ commute, which can be the case only if H is the Hamiltonian of a free particle.[25] (This needs not be the case for systems of many particles interacting one with another by forces

[25] In the case of quantum mechanics of a single neutral particle with spin and a nonzero magnetic moment $\boldsymbol{\mu}$ (as e.g. neutron), $\mathbf{P}$ commutes with H also if the particle interacts with a uniform, constant external magnetic field through the interaction $V_{\rm int} = -\boldsymbol{\mu}\cdot\mathbf{B}$.

depending only on $\mathbf{r}_i - \mathbf{r}_j$.) Generalizing to arbitrary systems, we conclude that for time-independent Hamiltonians, space translations are symmetries of the quantum theory only if the momentum operator $\mathbf{P}$ commutes with the Hamiltonian. If it does, then the state vector of the transformed system is

$$|\Psi'(t)\rangle = U(\mathbf{a})|\Psi(t)\rangle\,, \tag{4.62}$$

with the translation operator given (in the general case) by

$$U(\mathbf{a}) = \exp\left(-\frac{i}{\hbar}\,\mathbf{a}\cdot\hat{\mathbf{P}}\right), \tag{4.63}$$

with $\hat{\mathbf{P}}$ the operator of the total momentum of the system.

One can next try to represent boosts. Physically (cf.4.37) the wave functions of the boosted system and of the original one should be related by $|\langle\mathbf{r}+\mathbf{V}t|\psi'(t)\rangle| = |\langle\mathbf{r}|\psi(t)\rangle|$ that is, by

$$|\langle\mathbf{r}|\psi'(t)\rangle| \equiv |\psi'(t,\mathbf{r})| = |\psi(t,\mathbf{r}-\mathbf{V}t)| = |\langle\mathbf{r}-\mathbf{V}t|\psi(t)\rangle|\,, \tag{4.64}$$

so that if the boost are symmetries of the system a unitary operator $U(\mathbf{V})$ should exist, such that $|\psi'\rangle = U(\mathbf{V})|\psi\rangle$ with the property (in the position representation)

$$U(\mathbf{V})\,\psi(t,\mathbf{r}) = \psi(t,\mathbf{r}-\mathbf{V}t)\,. \tag{4.65}$$

For infinitesimal transformations one should be able to write $U(\mathbf{V}) \approx \hat{1} - (i/\hbar)V^i\hat{K}^i$. By analogy with (4.60) it is clear that the generators $\hat{K}^i$ acting in the Hilbert space of a single particle should have a part of the form $\hat{K}^i \sim t\,\hat{p}^i$, which will ensure the proper shift of the space argument of ψ. However, this is not enough, as one has to satisfy also the commutation relations of K^i with H and P^i given in (4.48) and (4.52). It turns out that in the case of quantum mechanics of a single spinless particle (but not in general, of course!) this is possible only if H is the Hamiltonian of a free particle, in which case

$$\hat{K}^i = -M\hat{x}^i + t\hat{p}^i\,, \tag{4.66}$$

and its commutation rule with $H = \hat{\mathbf{P}}^2/2M$ requires that the mass parameter in (4.52) coincides with the mass of the particle. It is then easy to check that

$$\begin{aligned}\psi'(t,\mathbf{r}) &= \exp\left(-\frac{i}{\hbar}V^i(-M\hat{x}^i + t\,\hat{p}^i)\right)\psi(t,\mathbf{r}) \\ &= \exp\left(-i\frac{M\mathbf{V}^2}{2\hbar}\,t\right)\exp\left(\frac{i}{\hbar}MV^ix^i\right)\psi(t,\mathbf{r}-\mathbf{V}t)\,,\end{aligned} \tag{4.67}$$

satisfies the free Schrödinger equation if $\psi(t,\mathbf{r})$ does (check it!).

Finally we consider rotations which most frequently are symmetry transformations of the system (in particular if it is a single particle moving in an external spherically

symmetric potential), even if translations and boosts are not. Consider first a spinless nonrelativistic particle. Its wave functions has only one component (with the usual probabilistic interpretation). The wave function of the original and rotated systems should, on physical grounds, be related by $|\psi'(\mathbf{r}')| \equiv |\langle \mathbf{r}'|\psi'\rangle| = |\langle R\cdot\mathbf{r}|\psi'\rangle| = |\langle \mathbf{r}|\psi\rangle| \equiv |\psi(\mathbf{r})|$. This equality holds for arbitrary superpositions of the state vectors provided

$$\psi'(\mathbf{r}) \equiv \langle \mathbf{r}|\psi'\rangle = \langle R^{-1}\cdot\mathbf{r}|\psi\rangle \equiv \psi(R^{-1}\cdot\mathbf{r})\,, \tag{4.68}$$

which in turn must be ensured by the the rotation operator $U(R)$ such that $|\psi'\rangle = U(R)|\psi\rangle$ or, in the position representation, that $\psi'(\mathbf{r}) = U(R)\psi(\mathbf{r})$. The matrix R of an infinitesimal rotation is of the form (4.41). Defining the vector $\boldsymbol{\theta} \equiv (\theta^x, \theta^y, \theta^z)$ we can write

$$R^{-1}\cdot\mathbf{r} \approx \mathbf{r} - \boldsymbol{\theta}\times\mathbf{r}\,, \tag{4.69}$$

and the right hand side of (4.68) becomes

$$\psi(\mathbf{r}) - (\boldsymbol{\theta}\times\mathbf{r})\cdot\boldsymbol{\nabla}\psi(\mathbf{r}) + \ldots = \psi(\mathbf{r}) - \frac{i}{\hbar}(\boldsymbol{\theta}\times\mathbf{r})\cdot\hat{\mathbf{P}}\,\psi(\mathbf{r}) + \ldots \tag{4.70}$$

or, in the Dirac notation, $\langle\mathbf{r}|\left(\hat{1} - (i/\hbar)(\boldsymbol{\theta}\times\hat{\mathbf{r}})\cdot\hat{\mathbf{P}}\right)|\psi\rangle$. With a straightforward vector algebra we get therefore

$$\psi'(\mathbf{r}) \approx \left(\hat{1} - \frac{i}{\hbar}\,\boldsymbol{\theta}\cdot\hat{\mathbf{L}}\right)\psi(\mathbf{r})\,, \tag{4.71}$$

(where $\mathbf{L} = \mathbf{r}\times\mathbf{P}$ is the familiar orbital angular momentum operator), that is,

$$|\psi'\rangle = U(R)|\psi\rangle \approx \left(\hat{1} - \frac{i}{\hbar}\,\boldsymbol{\theta}\cdot\hat{\mathbf{L}}\right)|\psi\rangle\,. \tag{4.72}$$

Obviously, if rotations are symmetries of the physical system the operators $\mathbf{L}$ and, hence, also $U(R)$, commute with the system's Hamiltonian H. The proper form of the commutators of the operators L^i, which play in this case the roles of J^i, with the operators P^i and K^i (which must take the form specified in (4.48), if translations and boosts are also symmetries) are ensured by the vector character of these operators (see Section 4.6).

If the particle has a nonzero spin, its wave function has more components labeled by an index σ. In the appropriate basis in the internal space $|\psi_\sigma(\mathbf{r})|^2 \equiv |\langle\mathbf{r},\sigma|\psi\rangle|^2$ is the probability density of finding the particle at $\mathbf{r}$ with spin projection in the z-direction equal $\sigma\hbar$, i.e. of finding it in the state $|\mathbf{r},\sigma\rangle$ (strictly speaking this interpretation is valid only in nonrelativistic quantum mechanics). On physical grounds, and generalizing (4.68), if rotations are symmetries of the system, the wave function components ψ_σ transform under rotations one into another forming a linear, finite-dimensional (and unitary - because the

rotation group is compact) matrix representation of the rotation group. In other words, one must then have

$$\langle \mathbf{r}, \sigma | \psi' \rangle = \sum_{\sigma'=-j}^{j} D_{\sigma\sigma'}(R) \, \langle R^{-1}\cdot\mathbf{r}, \sigma' | \psi \rangle \qquad \text{or}$$

$$\psi'_\sigma(\mathbf{r}) = \sum_{\sigma'=-j}^{j} D_{\sigma\sigma'}(R) \, \psi_{\sigma'}(R^{-1}\cdot\mathbf{r}) \, . \tag{4.73}$$

Expanding (4.73) to the first order in θ^i and using the formula (4.69) together with the form

$$D^{(s)}_{\sigma\sigma'}(\boldsymbol{\theta}) \approx \delta_{\sigma\sigma'} - \frac{i}{\hbar}\,\theta^i S^{(s)i}_{\sigma\sigma'} + \dots \tag{4.74}$$

of the $D^{(s)}_{\sigma\sigma}$ matrices (for spin s) valid for infinitesimal rotations R parametrized by three angles θ^i, one finds in this case that the Hilbert space generators $\mathbf{J}$ of the rotation (sub)group

$$U(\boldsymbol{\theta}) \approx \hat{1} - \frac{i}{\hbar}\,\theta^i J^i \, , \tag{4.75}$$

such that $U(\boldsymbol{\theta})|\psi\rangle = |\psi'\rangle$ must have the form

$$J^i = L^i + S^{(s)i} \, , \tag{4.76}$$

with L^i acting on the space variable $\mathbf{r}$ and $S^{(s)i}$ acting on the discrete variables σ. Thus, $[L^i,\ S^{(s)j}] = 0$ and in order to satisfy the commutation relation $[J^i,\ J^j] = i\hbar\,\epsilon^{ijk}J^k$ the operators S^i must, because the operators L^i satisfy such relations separately, satisfy the rules

$$[S^{(s)i},\ S^{(s)j}] = i\hbar\,\epsilon^{ijk}S^{(s)k} \, . \tag{4.77}$$

J^i's are simply the operators of the total angular momentum split (in nonrelativistic quantum mechanics) into the orbital angular momentum operators L^i and the spin operators $S^{(s)i}$. The latter, being matrices in the spin indices σ must form a finite dimensional, unitary representation of the commutation relations (4.77) which are the commutation relations of the $SU(2)$ group. All such representations are well known. They are labeled by $s = 0, \frac{1}{2}, 1, \frac{3}{2}, 2 \dots$ and have dimension $2s+1$. In standard textbooks one finds the matrices $S^i_{\sigma\sigma'}$ of the group generators in these representations by solving explicitly the commutation relations (4.77). One then finds that the matrices S^i corresponding to $s = \frac{1}{2}$ are the familiar Pauli matrices $S^i_{\sigma\sigma'} = \frac{1}{2}\sigma^i_{\sigma\sigma'}$; if $s = 1$, the S^i matrices read

$$S^x = \frac{\hbar}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \quad S^y = \frac{\hbar}{\sqrt{2}}\begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}, \quad S^z = \hbar\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix},$$

and so on.

In the next section we will discuss the realization of the rotation group in Hilbert spaces in more details.

4.4 The rotation group

In many applications it is the rotation group which is a good symmetry of the nonrelativistic systems. Moreover, rotations form also an important subgroup of the Lorentz group relevant for relativistic systems. It is therefore worthwhile to complete with some details its discussion begun in Section 4.2 and to derive some useful formulae.

We first chose the parametrization of the rotation group proposed in connection with the discussion of its double-connectedness in Section 4.2. In this parametrization the rotation is specified by giving the direction $\mathbf{n}$ of the rotation axis and the rotation angle $0 \leq \psi \leq \pi$. In turn, the direction $\mathbf{n}$ is specified by giving two polar angles $0 \leq \vartheta \leq \pi$ and $0 \leq \varphi \leq 2\pi$. This parametrization (the map on the group manifold) is not globally defined: at $\psi = 0$ the angles ϑ and φ are ill defined. Alternatively, one can specify the three Cartesian coordinates (ψ^x, ψ^y, ψ^z) of the rotation vector $\boldsymbol{\psi} \equiv \psi \mathbf{n}$. These coordinates are restricted to the domain $|\boldsymbol{\psi}| \leq \pi$. This map is well defined everywhere, except for the points such that $|\boldsymbol{\psi}| = \pi$ because, as already explained, $\boldsymbol{\psi}$ and $-\boldsymbol{\psi}$ define then the same rotation.

In this parametrization the most natural "standard" path along which one defines the Hilbert space operator $U(\boldsymbol{\psi})$ corresponding to a given rotation $R(\boldsymbol{\psi})$ is the path $\boldsymbol{\psi}(\xi) = \xi\, \boldsymbol{\psi}$ with $0 \leq \xi \leq 1$. It defines a one-parameter Abelian subgroup of rotations, so that integration of the differential equation (4.31) reduces to the formula (4.27) and one gets

$$U(\boldsymbol{\psi}) = \exp\left(-\frac{i}{\hbar}\, \boldsymbol{\psi}\cdot\mathbf{J}\right), \tag{4.78}$$

where J^i are the Hilbert space rotation group generators. In agreement with our discussion (around eq. (4.57)), if rotations are symmetries of the considered quantum system, one can find in the Hilbert space the state-vectors $|n, j, m\rangle$ (the label n distinguishes e.g. different Hamiltonian eigenvalues; it will be omitted in the following), which under (active) rotations transform into one another

$$U(\boldsymbol{\psi})|j, m\rangle \equiv e^{-\frac{i}{\hbar}\psi^i J^i}|j, m\rangle = \sum_{m'=-j}^{+j} |j, m'\rangle\, D^{(j)}_{m'm}(\boldsymbol{\psi})\,. \tag{4.79}$$

Closing this relation from the left with $\langle j, m'|$ (assuming that these states are normalized to unity) we get the rotation matrices[26]

$$D^{(j)}_{m'm}(\boldsymbol{\psi}) = \langle j, m'|e^{-\frac{i}{\hbar}\psi^i J^i}|j, m\rangle\,, \tag{4.80}$$

[26]Of course, the matrices $D^{(j)}_{m'm}(\boldsymbol{\psi})$ do not depend on the (hidden) label n. Once they are found using one set of vectors $|(n), j, m\rangle$, e.g. ones corresponding to a discrete energy level of the Hamiltonian, they can be used in the relations (4.79) in which the vectors $|(\tilde{n}), j, m\rangle$ may e.g. be nonnormalizable belonging to the continuous part of the Hamiltonian spectrum.

in the $\boldsymbol{\psi}$-parametrization. Using matrix elements of the generators J^i (they are obtained in standard textbook by solving the algebra of J^i's in the basis in which J^z is diagonal) given by

$$\begin{aligned}
\left(J^z_{(j)}\right)_{m'm} &\equiv \langle j,m'|J^z|j,m\rangle = m\hbar\,\delta_{m',m}\,,\\
\left(J^x_{(j)} \pm iJ^y_{(j)}\right)_{m'm} &\equiv \langle j,m'|J^x \pm iJ^y|j,m\rangle \\
&= \hbar\sqrt{(j\mp m)(j\pm m+1)}\;\delta_{m'm\pm1}\\
&= \hbar\sqrt{j(j+1)-m(m\pm1)}\,\delta_{m'm\pm1}\,,
\end{aligned} \tag{4.81}$$

the matrices $D^{(j)}_{m'm}(\boldsymbol{\psi})$ can be obtained by exponentiating (with the help of the standard methods) the matrices $\left(\psi^i J^i_{(j)}\right)_{m'm}$ (built out of matrix elements of the generators J^i) contracted with the components of the rotation vector $\boldsymbol{\psi}$. In the $j=\frac{1}{2}$ case one finds in this way ($\psi\equiv|\boldsymbol{\psi}|$, $\mathbf{n}\equiv\boldsymbol{\psi}/|\boldsymbol{\psi}|$)

$$D^{(1/2)}(\boldsymbol{\psi}) = \cos\frac{\psi}{2} - i\,\mathbf{n}\cdot\boldsymbol{\sigma}\sin\frac{\psi}{2}\,. \tag{4.82}$$

Another parametrization of the rotation group is provided by the Euler angles α, β and γ. In this parametrization a given *active* rotation $R(\alpha,\beta,\gamma)$ is composed of three successive rotations: first by the angle α around the axis $\mathbf{n}_1\equiv\mathbf{e}_z$, then by the angle β around the axis $\mathbf{n}_2\equiv-\mathbf{e}_x\sin\alpha+\mathbf{e}_y\cos\alpha$ and finally by γ around the axis $\mathbf{n}_3\equiv\mathbf{e}_x\cos\alpha\sin\beta+\mathbf{e}_y\sin\alpha\sin\beta+\mathbf{e}_z\cos\beta$:

$$R(\alpha,\beta,\gamma) = R(\gamma,\mathbf{n}_3)\cdot R(\beta,\mathbf{n}_2)\cdot R(\alpha,\mathbf{n}_1)\,. \tag{4.83}$$

Using the general property of rotations

$$R(\theta,\mathbf{n})\cdot R(\psi,\mathbf{k})\cdot R^{-1}(\theta,\mathbf{n}) = R(\psi,R_{\rm vec}(\theta,\mathbf{n})\cdot\mathbf{k})\,, \tag{4.84}$$

where $R_{\rm vec}(\theta,\mathbf{n})$ is the active rotation realized on three-vectors, it can be shown that[27]

$$R(\alpha,\beta,\gamma) = R(\alpha,\mathbf{e}_z)\cdot R(\beta,\mathbf{e}_y)\cdot R(\gamma,\mathbf{e}_z)\,. \tag{4.85}$$

By convention the ranges of the angles in the Euler parametrization are: $0\le\gamma,\alpha<2\pi$ and $0\le\beta\le\pi$. Also this parametrization is not globally defined: as is clear from (4.85), if $\beta=0$, the rotation depends only on $\alpha+\gamma$ (modulo 2π), while if $\beta=\pi$, it depends only on $\alpha-\gamma$. The rotation inverse to $R(\alpha,\beta,\gamma)$ is given by[28]

$$[R(\alpha,\beta,\gamma)]^{-1} = R(\varepsilon(\gamma)-\gamma,\,\beta,\,\varepsilon(\alpha)-\alpha)\,, \tag{4.86}$$

[27] Evidently the order of angles in notation $R(\alpha,\beta,\gamma)$ stems from this way of realizing the rotation (4.83).

[28] As usually with rotations there are different "schools"; we stick here to the one represented by a booklet of K. Zalewski.

with $\varepsilon(\theta) = \pi$ if $0 \leq \theta < \pi$ and $\varepsilon(\theta) = 3\pi$ if $\pi \leq \theta < 2\pi$ (to keep the angles in the prescibed ranges).

In this parametrization, as the "standard path", along which one ascribes to a given rotation $R(\alpha, \beta, \gamma)$ the corresponding Hilbert space operator $U(\alpha, \beta, \gamma)$, it is natural to chose the path id $\to R(\gamma, \mathbf{e}_z) \to R(\beta, \mathbf{e}_y) \cdot R(\gamma, \mathbf{e}_z) \to R(\alpha, \mathbf{e}_z) \cdot R(\beta, \mathbf{e}_y) \cdot R(\gamma, \mathbf{e}_z)$. The operator $U(\alpha, \beta, \gamma)$ is then the product

$$U(\alpha, \beta, \gamma) = \exp\left(-\frac{i}{\hbar}\,\alpha J^z\right) \exp\left(-\frac{i}{\hbar}\,\beta J^y\right) \exp\left(-\frac{i}{\hbar}\,\gamma J^z\right). \tag{4.87}$$

It then follows, that (as can be easily verified)

$$U(\varepsilon(\gamma) - \gamma,\, \beta,\, \varepsilon(\alpha) - \alpha)\, U(\alpha,\, \beta,\, \gamma) = e^{-i(\varepsilon(\gamma)+\varepsilon(\alpha))J^z}. \tag{4.88}$$

This is the unit operator only when acting on the states with integer j; in action on the half-integer j states it is the unit operator only if $\varepsilon(\gamma) + \varepsilon(\alpha) = 4\pi$; if $\varepsilon(\gamma) + \varepsilon(\alpha) = 2\pi$ or 6π it is the minus unit operator.

The rotation matrices $D^{(j)}_{m'm}(\alpha, \beta, \gamma)$ take in this parametrization the form

$$\begin{aligned} D^{(j)}_{m'm}(\alpha, \beta, \gamma) &\equiv \langle j, m'| e^{-\frac{i}{\hbar}\alpha J^z} e^{-\frac{i}{\hbar}\beta J^y} e^{-\frac{i}{\hbar}\gamma J^z} |j, m\rangle \\ &= e^{-im'\alpha}\, d^{(j)}_{m'm}(\beta)\, e^{-im\gamma}\,, \end{aligned} \tag{4.89}$$

where the matrices $d^{(j)}_{m'm}(\beta)$ are defined by the formula

$$d^{(j)}_{m'm}(\beta) \equiv \langle j, m'| e^{-\frac{i}{\hbar}\beta J^y} |j, m\rangle\,. \tag{4.90}$$

As in the $\boldsymbol{\psi}$-parametrization, since the matrix elements of J^y between the $|j, m\rangle$ states are known, the matrices $d^{(j)}_{m'm}(\beta)$ can be obtained just by exponentiating the matrices $\left(\beta J^y_{(j)}\right)_{m'm}$. In the $j = \frac{1}{2}$ case with $J^y_{(\frac{1}{2})} = (\hbar/2)\sigma^y$ the matrix $d^{(1/2)}_{m'm}(\beta)$ is easy to find and reads

$$d^{(1/2)}(\beta) = \begin{pmatrix} \cos\frac{\beta}{2} & \sin\frac{\beta}{2} \\ -\sin\frac{\beta}{2} & \cos\frac{\beta}{2} \end{pmatrix}. \tag{4.91}$$

The matrices $d^{(j)}_{m'm}(\beta)$ corresponding to higher values of j can be found straightforwardly using the trick presented in Appendix B, where the properties of the $d^{(j)}_{m'm}(\beta)$ and $D^{(j)}_{m'm}(\alpha, \beta, \gamma)$ matrices are also collected.

An important concept (allowing to formulate e.g. the orthogonality relations satisfied by the $D^{(j)}_{m'm}(\alpha, \beta, \gamma)$ matrices) is the integration over the group of a function $f(g)$ of the group element g. This requires defining on the group manifold a measure which is compatible with the group composition rules. If the group G is compact, like the rotation

group, the integral which is both left- and right- invariant can be defined on it (on every group left- and right- invariant measured can be defined but are in the general case they are different). This means the following property

$$\int d\mu(g)\, f(g) = \int d\mu(g)\, f(g'g) = \int d\mu(g)\, f(gg')\,, \tag{4.92}$$

where $d\mu(g)$ is the appropriate measure and g' is an arbitrary element of G. In a given parametrization of the group elements by continuous parameters θ^a, $a = 1, \ldots, o$, the integral is given by

$$\int d\mu(g)\, f(g) = \int d^o\boldsymbol{\theta}\, \rho(\boldsymbol{\theta})\, f(\boldsymbol{\theta})\,, \tag{4.93}$$

where $\rho(\boldsymbol{\theta})$ is some density determined by the requirement that the integral is left- and right- invariant. For example, left-invariance means that the following equality must hold

$$\int d^o\boldsymbol{\theta}\, \rho(\boldsymbol{\theta})\, f(\tilde{\boldsymbol{\theta}}(\boldsymbol{\theta}', \boldsymbol{\theta})) = \int d^o\tilde{\boldsymbol{\theta}}\, \rho(\tilde{\boldsymbol{\theta}})\, f(\tilde{\boldsymbol{\theta}})\,, \tag{4.94}$$

with $\tilde{\theta}_a = h_a(\boldsymbol{\theta}', \boldsymbol{\theta})$, where h_a is the composition function introduced in Section 4.2. After changing in the right integral the integration variables to $\boldsymbol{\theta}$, (4.94) is equivalent to

$$\rho(\boldsymbol{\theta}) = \rho(h(\boldsymbol{\theta}', \boldsymbol{\theta}))\left|\frac{\partial h_a(\boldsymbol{\theta}', \boldsymbol{\theta})}{\partial \theta_b}\right|. \tag{4.95}$$

The right-hand side must be of course independent of $\boldsymbol{\theta}'$. Assuming that a density ρ fulfilling this condition exists, one can determine it by considering only infinitesimal values of the parameters $\boldsymbol{\theta}$ (i.e. $\boldsymbol{\theta} \to \mathbf{0}$). Evaluating both sides of (4.95) at $\boldsymbol{\theta} = \mathbf{0}$ gives then

$$\rho(\boldsymbol{\theta}') = \rho(\mathbf{0})\left|\frac{\partial h^a(\boldsymbol{\theta}', \boldsymbol{\theta})}{\partial \theta^b}\right|^{-1}_{\boldsymbol{\theta}=\mathbf{0}}. \tag{4.96}$$

This fixes ρ up to an arbitrary (inessential) multiplicative constant $\rho(\mathbf{0})$.

In the parametrization of the rotations by the vector $\boldsymbol{\psi} = (\psi^x, \psi^y, \psi^z)$ one finds in this way (normalizing the measure so that in this particular parametrization $\rho(\mathbf{0}) = 1$)

$$\begin{aligned} d\psi^x d\psi^y d\psi^z\, \rho(\boldsymbol{\psi}) &= d\psi^x d\psi^y d\psi^z\, \frac{2(1-\cos|\boldsymbol{\psi}|)}{|\boldsymbol{\psi}|^2} \\ &\equiv d|\boldsymbol{\psi}|\, d\Omega_{\boldsymbol{\psi}}\, 2(1-\cos|\boldsymbol{\psi}|)\,. \end{aligned} \tag{4.97}$$

The volume of the rotation group $SO(3)$ is then

$$\mathrm{Vol}(SO(3)) = \int_0^{2\pi} d\varphi \int_0^{\pi} d\vartheta \sin\vartheta \int_0^{\pi} d|\boldsymbol{\psi}|\, 2(1-\cos|\boldsymbol{\psi}|) = 8\pi^2\,. \tag{4.98}$$

In the parametrization by the Euler angles one finds

$$d\alpha\, d\beta\, d\gamma\, \rho(\alpha,\beta,\gamma) = d\alpha\, d\beta\, d\gamma\, \sin\beta\,, \tag{4.99}$$

and the rotation group volume is given by

$$\int_0^{2\pi} d\alpha \int_0^{\pi} d\beta \int_0^{2\pi} d\gamma\, \sin\beta = 8\pi^2\,. \tag{4.100}$$

If a function is defined on the $SU(2)$ group instead of $SO(3)$, which means that it takes different values on those $SU(2)$ elements which correspond to the same element of $SO(3)$,[29] the range of integration over ψ in the first parametrization[30] is $(0, 2\pi)$; the $SU(2)$ group volume is $16\pi^2$.

The matrices $D^{(j)}_{m'm}(\alpha,\beta,\gamma)$ can be viewed as a collection of $(2j+1)^2$ functions defined on the group and can therefore be integrated over it. Moreover, the product of two such matrices $D^{(j_1)}_{m'_1 m_1}$ and $D^{(j_2)}_{m'_2 m_2}$ with j_1 and j_2 both integer or both half integer (in view of the superselection rule the only cases of interest) is a single-valued function and can be, therefore, integrated over $SO(3)$. Their product satisfies then the following orthogonality relation

$$\int_0^{2\pi} d\alpha \int_0^{\pi} d\beta \int_0^{2\pi} d\gamma \sin\beta\, D^{(j_2)*}_{m'_2 m_2}(\alpha,\beta,\gamma) D^{(j_1)}_{m'_1 m_1}(\alpha,\beta,\gamma) = \frac{8\pi^2}{2j_1+1}\,\delta^{j_1 j_2}\delta_{m_1 m_2}\delta_{m'_1 m'_2}, \tag{4.101}$$

which exemplifies the general orthogonality relation satisfied by matrices of finite dimensional unitary representations of a compact group: the coefficient of the delta functions is always given by the volume of the group divided by the dimension of the representation. The completeness relation reads

$$\frac{1}{8\pi^2}\sum_j \sum_{m=-j}^{+j}\sum_{m'=-j}^{+j} (2j+1) D^{(j)*}_{m'm}(\bar\alpha,\bar\beta,\bar\gamma) D^{(j)}_{m'm}(\alpha,\beta,\gamma) = \delta(\bar\alpha-\alpha)\delta(\cos\bar\beta-\cos\beta)\delta(\bar\gamma-\gamma)\,. \tag{4.102}$$

Since the dependence of the $D^{(j)}$ functions on the angles α and γ is trivial, the integrals over these angles can be taken explicitly giving the relation

$$\int_0^{\pi} d\beta \sin\beta\, d^{(j')*}_{m'm}(\beta)\, d^{(j)}_{m'm}(\beta) = \frac{2}{2j+1}\,\delta^{j'j}\,. \tag{4.103}$$

[29] In some textbooks such functions are termed double-valued because from the point of view of $SO(3)$ they assume two different values on every its element.

[30] In the parametrization by the Euler angles the extension to $SU(2)$ is realized depending on the "school" either by extending the range on the angle α to 4π or by letting β to cover two ranges: $[0,\pi]$ and $[2\pi, 3\pi]$.

The appropriate inverse relation is

$$\sum_j (j+\frac{1}{2})\, d^{(j)*}_{m'm}(\beta)\, d^{(j)}_{m'm}(\bar\beta) = \delta(\cos\bar\beta - \cos\beta)\,. \tag{4.104}$$

4.5 Composing angular momenta

We recall first some general features of group representations. Consider two three-dimensional vectors $\mathbf{V} = \mathbf{e}_i V^i$ and $\mathbf{W} = \mathbf{e}_i W^i$. Under an arbitrary (active) rotation $O \in SO(3)$ the vectors are transformed into $\mathbf{V}' = \mathbf{e}_i V'^i$ and $\mathbf{W}' = \mathbf{e}_i W'^i$ whose components are given by by $V'^i = \sum_j O^{ij}_{\rm vec} V^j$ and $W'^i = \sum_j O^{ij}_{\rm vec} W^j$ with $O^{ij}_{\rm vec}$ the orthogonal 3×3 matrix representing rotations on three-vectors (in the chosen orthonormal basis $\mathbf{e}_i$). This obviously determines also the transformation law of the nine components $T^{ij} = V^i W^j$ in the basis $\mathbf{t}_{ij} \equiv \mathbf{e}_i \otimes \mathbf{e}_j$ of the tensor $\mathbf{T} = \mathbf{V} \otimes \mathbf{W}$ formed out of these two vectors:

$$T'^{ij} = \sum_{(kl)} O^{(ij),(kl)}_{\rm tens} T^{kl}\,.$$

Indeed, the elements of the 9×9 matrix $O^{(ij),(kl)}_{\rm tens}$ are given by $O^{(ij),(kl)}_{\rm tens} = O^{ik}_{\rm vec}\, O^{jl}_{\rm vec}$. It is however possible to change the basis $\mathbf{t}_{ij}$ of the 9 dimensional tensor product of the vector spaces to $\tilde{\mathbf{t}}_{ij} = \mathbf{t}_{kl}[R^{-1}]^{(kl)(ij)}$ which induces the corresponding changes of the components of tensors:

$$T^{kl} = \sum_{(mn)} R^{(kl),(mn)}\, \tilde T^{mn}\ , \qquad T'^{ij} = \sum_{(mn)} R^{(ij),(mn)}\, \tilde T'^{mn}\,,$$

so that

$$\tilde T'^{ij} = \sum_{(kl)} [\tilde O_{\rm tens}]^{(ij),(kl)} \tilde T^{kl}\,,$$

with

$$\tilde O^{(ij),(kl)}_{\rm tens} = \sum_{(mn)} \sum_{(rs)} R^{(ij),(mn)}\, O^{(mn),(rs)}_{\rm tens}\, [R^{-1}]^{(rs),(kl)}\,. \tag{4.105}$$

This change of the basis can be chosen in such a way that all 9×9 matrices $\tilde O_{\rm tens}$ corresponding to all rotations (which have all the properties necessary for a representation of the rotation group) assume the block-diagonal structure with one 1×1 block, one 3×3 block and one 5×5 block. Therefore the 9-dimensional representation of the rotation group spanned by the 9 components $V^i W^j$ is reducible and decomposes into three irreducible representations: one 1-dimensional, one 3-dimensional and one 5-dimensional. The elements of the orthogonal matrix R of the change of basis are what in the context of the $SU(2)$ group covering the rotation group is called the Clebsch-Gordan coefficients.

The block-diagonal structure of the matrices $\tilde{O}_{\rm tens}$ means that after the linear change of the basis the nine components of the tensor are grouped into a one component which does not change under rotations, 3 components which transform among themselves and 5 other components which also transform among themselves. (In the case of the tensor V^iW^j these 1, 3 and 5 component objects correspond, of course, to the scalar $\mathbf{V}\cdot\mathbf{W}$, the antisymmetric tensor $A^{ij} = V^iW^j - V^jW^i$ which has 3 independent components and the symmetric traceless tensor $S^{ij} = V^iW^j + V^jW^i - \frac{2}{3}(\mathbf{V}\cdot\mathbf{W})\delta^{ij}$ which has 5 independent components). This illustrates a general rule: a representation (of any group) formed by taking the tensor product of two (irreducible) representations is in general reducible and can be decomposed into irreducible ones by an appropriate change of the basis.

Basically the same can be repeated in the Dirac notation for the eigenstates of the angular momentum operators. In this case we have state vectors of the general form $|n, j_1, m_1, j_2, m_2\rangle$ depending on two[31] different sets of labels, j_1, m_1 and j_2, m_2, of which the first set forms a complete representation of the $su(2)$ Lie algebra generated by the operators $\mathbf{J}_1$ and the second set has the same property with respect to the algebra generated by $\mathbf{J}_2$. An example is provided by quantum mechanics of a particle with a nonzero spin (see the formulae (4.73)) whose state can be written as a superposition

$$|\psi\rangle = \sum_n \sum_{l=0} \sum_{m_l=-l}^{+l} \sum_{\sigma=-s}^{+s} c_{nlm_l\sigma} |n, l, m_l, s, \sigma\rangle \,, \tag{4.106}$$

of the states $|n, l, m_l, s, \sigma\rangle$ (with fixed s corresponding to the particle's spin) such that

$$\begin{aligned} e^{\frac{i}{\hbar}\psi^i L^i} |n, l, m_l, s, \sigma\rangle &= \sum_{m_l'=-l}^{+l} |n, l, m_l', s, \sigma\rangle D^{(l)}_{m_l' m_l}(\boldsymbol{\psi}) \,, \\ e^{\frac{i}{\hbar}\psi^i S^i} |n, l, m_l, s, \sigma\rangle &= \sum_{\sigma'=-s}^{+s} |n, l, m_l, s, \sigma'\rangle D^{(s)}_{\sigma'\sigma}(\boldsymbol{\psi}) \,, \end{aligned} \tag{4.107}$$

with the matrices $D^{(j)}_{m_l' m_l}$ introduced in subsection 4.4. In quantum mechanics of many particles, nonrelativistic (see section 5) or relativistic, the two sets of states may represent e.g. angular momentum states of two different spinless particles. More complicated cases of angular momenta of more then two particles and/or of two or more particles with nonzero spins can be treated by applying successively the rules formulated in this subsection for two sets of states.

Obviously, in the example of a single particle with spin $\mathbf{J}_1 = \mathbf{L}$ and $\mathbf{J}_2 = \mathbf{S}$ act on different sets of labels. Mathematically the states $|j_1, m_1; j_2, m_2\rangle$ have the structure of the tensor product

$$|j_1, m_1; j_2, m_2\rangle \equiv |j_1, m_1\rangle \otimes |j_2, m_2\rangle \,, \tag{4.108}$$

[31] n labels the state vectors with respect e.g. to their Hamiltonian eigenvalues; as we will be now considering state vectors with the same value of n this label will be not explicitly indicated.

and the operators $\mathbf{J}_1$ act on $|j_1, m_1\rangle$ while $\mathbf{J}_2$ act on $|j_2, m_2\rangle$. The basis of states (4.108) called the product basis (of the subspace of the Hilbert space corresponding to fixed label n) is formed by the states which under the $SU(2)$ transformations behave as an $SU(2)$ representations constructed as the tensor product of two irreducible $SU(2)$ representations: one characterized by j_1 and the second one characterized by j_2. As in the example with two vectors, it is possible to change the basis in the (sub)space spanned by the vectors (4.108), so that this representation of $SU(2)$ explicitly decomposes into a direct sum of irreducible representations, which (as all irreducible $SU(2)$ representations) are characterized by integers j. This change of basis is written (in the Dirac notation) as

$$|j_1, m_1; j_2, m_2\rangle = \sum_j \sum_{m=-j}^{j} |j, m\rangle\langle j, m|j_1, m_1; j_2, m_2\rangle \,, \tag{4.109}$$

where $|j, m\rangle$ are the eigenstates of $\mathbf{J}^2 = (\mathbf{J}_1 + \mathbf{J}_2)^2$ with the eigenvalues $j(j+1)\hbar^2$ and of $J^z = J_2^z + J_1^z$ with the eigenvalues $m\hbar$.

The scalar products on the right hand side are just the (complex conjugate of the) Clebsch-Gordan coefficients:

$$C_{j_2 j_1}(m_2, m_1|j, m) \equiv \langle j_1, m_1; j_2, m_2|j, m\rangle \,. \tag{4.110}$$

The following reasoning tells us which representations j appear in the sum (4.109) for a given pair j_2 and j_1, i.e. determines for which j the Clebsch-Gordan coefficients are nonzero. As will become clear, in the decomposition of into irreducible representations of a tensor product of any two $SU(2)$ representations each representation with a given j can appear at most once. Acting with the operator $J^z = J_2^z + J_1^z$ on both sides of (4.109) we get

$$(J_2^z + J_1^z)|j_2, m_2; j_1, m_1\rangle = \sum_j \sum_{m=-j}^{+j} J^z |j, m\rangle\langle j, m|j_2, m_2; j_1, m_1\rangle \,.$$

Action of $J_z^z + J_2^z$ (of J^z) on the left (right) hand side reduces to multiplication by $m_2 + m_1$ (m) and expressing next the state $|j_2, m_2; j_1, m_1\rangle$ on the left hand side using (4.109) we arrive at the relation

$$\sum_j \sum_{m=-j}^{+j} (m - m_2 - m_1)|j, m\rangle\langle j, m|j_2, m_2; j_1, m_1\rangle = 0 \,, \tag{4.111}$$

which, in view of the completeness of the $|j, m\rangle$ states, means that in (4.109) only the terms with $m = m_2 + m_1$ can appear. In other words, the Clebsch-Gordan coefficients (4.110) vanish for $m \neq m_2 + m_1$. This expresses the obvious fact that the z-axis projection of the total angular momentum of the system is the sum of the z-axis projections of the angular momenta of its components. This enables us to find the representations $|j, m\rangle$ by comparing the numbers of states with the same value of $m = m_2 + m_1$ in the two bases.

As the maximal values of m_1 and m_2 on the left hand side of (4.109) equal j_1 and j_2, respectively, it follows that the maximal value of m on the right hand side of (4.109) is $j_2 + j_1$. Hence, the maximal j in the sum must also be equal $j_2 + j_1$. Consider now $m = j_2 + j_1 - 1$. In the original product basis (4.108) there are two states corresponding to this value of the z-axis projection of the total angular momentum: $|j_2, j_2 - 1; j_1, j_1\rangle$ and $|j_2, j_2; j_1, j_1 - 1\rangle$. After changing the basis one their linear combination becomes the state $|j = j_2 + j_1, m = j_2 + j_1 - 1\rangle$ and combines with the state $|j = j_2 + j_1, m = j_2 + j_1\rangle$ to form the $j = j_2 + j_1$ representation. The other linear combination must be the state $|j = j_2 + j_1 - 1, m = j_2 + j_1 - 1\rangle$ and it is the state of maximal z-axis spin projection of the representation with $j = j_2 + j_1 - 1$. It is easy to see, that this process continues so long as lowering m by one unit increases the number of states with the new value of m: at each step a new representation with j lower by one unit appears. In order to see when this process stops, or, in other words, what is the minimal value of j, we can simply compare the total number of states. In the original product basis (4.108) there are $(2j_2+1)(2j_1+1)$ states. This number must equal the total number of the $|j, m\rangle$ states in the irreducible representations found in the decomposition of the direct product. Thus

$$(2j_2 + 1)(2j_1 + 1) = \sum_{j=?}^{j=j_2+j_1} (2j + 1)\,, \tag{4.112}$$

(we already know the maximal value of j). Since on the right hand side $j = j_2 + j_1$, $j_2 + j_1 - 1$, ..., it is easy to find that the lowest possible $j = |j_2 - j_1|$. Hence, when two angular momenta j_2 and j_1 are composed, one gets all irreducible representations $|j, m\rangle$ with

$$|j_2 - j_1| \le j \le j_2 + j_1\,, \tag{4.113}$$

and j changing in unit steps. It follows, that the sum over j in (4.109) extends to such values of j only, or, equivalently, that

$$C_{j_2 j_1}(m_2, m_1|j, m) \neq 0 \quad \text{ only for } \quad \begin{cases} m = m_1 + m_2 \\ |j_1 - j_2| \le j \le j_1 + j_2 \end{cases}. \tag{4.114}$$

Using the unitarity of the Clebsch-Gordan coefficients (being the matrix of the change of basis, they must be unitary)

$$\begin{aligned} \sum_{j=|j_1-j_2|}^{j_1+j_2} \sum_{m=-j}^{+j} C_{j_2 j_1}(m_2, m_1|j, m)\, C^*_{j_2 j_1}(m_2', m_1'|j, m) &= \delta_{m_1 m_1'} \delta_{m_2 m_2'}\,, \\ \sum_{m_2=-j_2}^{+j_2} \sum_{m_1=-j_1}^{+j_1} C_{j_2 j_1}(m_2, m_1|j, m)\, C^*_{j_2 j_1}(m_2, m_1|j', m') &= \delta_{jj'} \delta_{mm'}\,, \end{aligned} \tag{4.115}$$

the relation (4.109) can be inverted to give

$$|j, m\rangle = \sum_{m_1=-j_1}^{+j_1} \sum_{m_2=-j_2}^{+j_2} |j_2, m_2; j_1, m_1\rangle\, C_{j_2 j_1}(m_2, m_1|j, m)\,. \tag{4.116}$$

Acting on both sides of (4.116) with $J_\pm = (J_2^x + J_1^x) \pm i(J_2^y + J_1^y)$ and using again the completeness of the states $|j_1, m_1; j_2, m_2\rangle$ we can obtain useful relations between the Clebsch-Gordan coefficients:

$$\begin{aligned}\sqrt{j(j+1) - m(m\pm 1)}\, C_{j_2 j_1}(m_2, m_1|j, m\pm 1) \\ = \sqrt{j_2(j_2+1) - m_2(m_2\mp 1)}\, C_{j_2 j_1}(m_2\mp 1, m_1|j, m) \\ + \sqrt{j_1(j_1+1) - m_1(m_1\mp 1)}\, C_{j_2 j_1}(m_2, m_1\mp 1|j, m)\,.\end{aligned} \tag{4.117}$$

From the construction it is also obvious that the Clebsch-Gordan coefficients can be chosen so that

$$C_{j_2 j_1}(j_2, j_1|j = j_1 + j_2, m = j_1 + j_2) = 1\,. \tag{4.118}$$

This condition plus the recurrence relations (4.117) allow to determine completely (up to some arbitrary phase factors) the factors $C_{j_2 j_1}(m_2, m_1|j, m)$. By convention arbitrary phase factors are chosen so that all the Clebsch-Gordan coefficients are real.

Clebsch-Gordan coefficients allow also to write down a decomposition of a product of two D-functions defined in (4.89) (see also (4.79) and (4.80)). Acting on both sides of the relation

$$|j_1, m_1\rangle \otimes |j_2, m_2\rangle = \sum_{j=|j_1-j_2|}^{j_1+j_2} |j, m_1 + m_2\rangle\, C^*_{j_1 j_2}(m_1, m_2|j, m_1 + m_2)\,, \tag{4.119}$$

with a rotation operator $U(R)$ and expanding both sides one gets the relation

$$\begin{aligned}\sum_{m_1'}\sum_{m_2'} |j_1, m_1'\rangle \otimes |j_2, m_2'\rangle\, D^{(j_1)}_{m_1', m_1} D^{(j_2)}_{m_2', m_2} \\ = \sum_{j=|j_1-j_2|}^{j_1+j_2} \sum_{m'} |j, m'\rangle\, D^{(j)}_{m', m_1+m_2}\, C^*_{j_1 j_2}(m_1, m_2|j, m_1 + m_2)\,.\end{aligned}$$

Closing now this relation from the left with the conjugation of the relation (4.119) one obtains the equality

$$\begin{aligned}D^{(j_1)}_{m_1', m_1} D^{(j_2)}_{m_2', m_2} = \sum_{j=|j_1-j_2|}^{j_1+j_2} C_{j_1 j_2}(m_1, m_2|j, m_1 + m_2) \\ C_{j_1 j_2}(m_1', m_2'|j, m_1' + m_2') D^{(j)}_{m_1'+m_2', m_1+m_2}\,.\end{aligned} \tag{4.120}$$

Using the relation $D^{(j)}_{m'm} = (-1)^{m-m'} D^{(j)*}_{-m', -m}$ this can be rewritten also in the alternative form

$$\begin{aligned}D^{(j_1)}_{m_1', m_1} D^{(j_2)*}_{m_2', m_2} = (-1)^{m_2 - m_2'} \sum_{j=|j_1-j_2|}^{j_1+j_2} C_{j_1 j_2}(m_1, -m_2|j, m_1 - m_2) \\ C_{j_1 j_2}(m_1', -m_2'|j, m_1' - m_2') D^{(j)}_{m_1'-m_2', m_1-m_2}\,.\end{aligned} \tag{4.121}$$

As an illustrative example of the use of the Clebsch-Gordan coefficients let us consider the Hydrogen atom taking into account the electron spin. We first treat the problem in nonrelativistic quantum mechanics. Since both, $\mathbf{L}$ and $\mathbf{S}$ (where the spin operators $S^i = (\hbar/2)\sigma^i$) commute with the Hamiltonian $H = \mathbf{P}^2/2M - e^2/r$, the basis of states at a given energy level n is formed by the states

$$|n, l, m\rangle \otimes |s, \sigma\rangle\,, \quad -l \leq m \leq l\,, \quad s = \frac{1}{2}\,, \quad \sigma = \pm\frac{1}{2}\,. \tag{4.122}$$

They are eigenstates of $\mathbf{L}^2$, L^z, $\mathbf{S}^2$ and S^z with the eigenvalues $l\,(l+1)\hbar^2$, $m\hbar$, $\frac{3}{4}\hbar^2$ and $\sigma\hbar$, respectively. In contrast to H, the Dirac Hamiltonian H_D, which describes the Hydrogen atom in relativistic quantum mechanics commutes only with the total angular momentum operators $\mathbf{J} = \mathbf{L} + \mathbf{S}$ but not with $\mathbf{L}$ and $\mathbf{S}$ separately. Hence, in the nonrelativistic limit the eigenfunctions of H_D do not reduce to the states (4.122), but rather to their linear combinations which are eigenfunctions of H, J^z and $\mathbf{J}^2$: rotational invariance requires exact degeneracy of groups of states with the same $\mathbf{J}^2$ only and one should expect that the first order relativistic corrections will split energies of those groups of eigenstates of the nonrelativistic Hamiltonian H which correspond to different values of the $\mathbf{J}^2$ operator.[32] The wave functions of these states could be, of course, constructed just by taking the Clebsch-Gordan coefficients from tables. Instead, we will find them here by solving directly the appropriate equations. In so doing we will also obtain explictly some of the Clebsch-Gordan coefficients.

We begin by noticing that since $J^z = L^z + S^z$, its eigenstates corresponding to the eigenvalue $j_z\hbar$ must necessarily have the form

$$|n, l, s, j, j_z\rangle = A|n, l, j_z - \tfrac{1}{2}\,\rangle \otimes |s,\, \tfrac{1}{2}\,\rangle + B|n, l, j_z + \tfrac{1}{2}\,\rangle \otimes |s,\, -\tfrac{1}{2}\,\rangle\,,$$

with some constants A and B. In position representation $\psi_\sigma(\mathbf{r})$ with the upper ($\sigma = +\frac{1}{2}$) component representing the projection onto the $|s, \frac{1}{2}\rangle$ spin state, the wave function takes the form

$$\psi_\sigma^{(jj_z)}(\mathbf{r}) = \begin{pmatrix} A\,R_{nl}(r)\,Y_{lj_z-\frac{1}{2}}(\theta,\phi) \\ B\,R_{nl}(r)\,Y_{lj_z+\frac{1}{2}}(\theta,\phi) \end{pmatrix},$$

where R_{nl} are the nonrelativistic radial wave functions and Y_{lm} are the spherical harmonics. The coefficients A and B should be such that $\psi_\sigma^{(jj_z)}(\mathbf{r})$ is the eigenfunction of $\mathbf{J}^2$ with the eigenvalue $j(j+1)\hbar^2$. Using the decomposition

$$\mathbf{J}^2 = (\mathbf{L} + \mathbf{S})^2 = \mathbf{L}^2 + \mathbf{S}^2 + 2L^zS^z + L_+S_- + L_-S_+\,,$$

[32] The fact that the spectrum of the nonrelativistic Hydrogen atom exhibits large degeneracy, not required by the rotational invariance generated by the $\mathbf{L}$ operator (extra degeneracy of states with different values of the orbital angular momentum l) is due to an extra dynamical symmetry discussed in subsection 4.7. Moreover, even the spectrum of the full Dirac Hamiltonian H_D exhibits some extra degeneracy not required by the rotational invariance. Consequently, this degeneracy is preserved also by the lowest order relativistic corrections to the energy levels. This extra degeneracy is removed only by corrections to the energy levels predicted by the full Quantum Electrodynamics.

where

$$S^z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad S_+ = \hbar\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \quad S_- = \hbar\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix},$$

we get

$$\mathbf{J}^2 = \begin{pmatrix} \mathbf{L}^2 + \mathbf{S}^2 + \hbar L^z & \hbar L_- \\ \hbar L_+ & \mathbf{L}^2 + \mathbf{S}^2 - \hbar L^z \end{pmatrix}.$$

In action on $\psi_\sigma^{(jj_z)}$ one can replace $\mathbf{S}^2$ by $\frac{3}{4}\hbar^2$. Moreover, the action of $\mathbf{L}^2$, $L_\pm$ and L^z on the spherical harmonics Y_{lm} is also known. The eigenequation $\mathbf{J}^2\psi_\sigma^{(jj_z)} = j(j+1)\psi_\sigma^{(jj_z)}$ therefore reduces to

$$\hbar^2\begin{pmatrix} [l(l+1) + \frac{3}{4} + j_z - \frac{1}{2} - j(j+1)]A\, Y_{lj_z-\frac{1}{2}} + p\, B\, Y_{lj_z-\frac{1}{2}} \\ p\, A\, Y_{lj_z+\frac{1}{2}} + [l(l+1) + \frac{3}{4} - j_z - \frac{1}{2} - j(j+1)]B\, Y_{lj_z+\frac{1}{2}} \end{pmatrix} = 0\,,$$

where $p \equiv \sqrt{l(l+1) - (j_z + \frac{1}{2})(j_z - \frac{1}{2})} = \sqrt{(l+\frac{1}{2})^2 - j_z^2}$. Dividing the upper (lower) equation by $Y_{lj_z-\frac{1}{2}}$ ($Y_{lj_z+\frac{1}{2}}$) we obtain

$$\begin{pmatrix} [l(l+1) + \frac{1}{4} + j_z - j(j+1)] & p \\ p & [l(l+1) + \frac{1}{4} - j_z - j(j+1)] \end{pmatrix}\begin{pmatrix} A \\ B \end{pmatrix} = 0\,,$$

For a nontrivial solution to exist, the determinant of the matrix on the left hand side should vanish:

$$\left[l(l+1) + \frac{1}{4} - j(j+1)\right]^2 - \left(l + \frac{1}{2}\right)^2 = 0\,,$$

(notice that the determinant does not depend on j_z!). Thus, either $j = l - \frac{1}{2}$ or $j = l + \frac{1}{2}$. For example, for $j = l - \frac{1}{2}$ the coefficients A and B are related by

$$A\left(l + \frac{1}{2} + j_z\right) + B\sqrt{\left(l + \frac{1}{2}\right)^2 - j_z^2} = 0\,.$$

Hence, for $j = l - \frac{1}{2}$ one can take

$$A = N\sqrt{l + \frac{1}{2} - j_z}\,, \qquad B = -N\sqrt{l + \frac{1}{2} + j_z}\,,$$

with N fixed by the normalization of the wave function

$$1 = \int d^3\mathbf{r}\,\left(\left|\psi_{\frac{1}{2}}^{(jj_z)}\right|^2 + \left|\psi_{-\frac{1}{2}}^{(jj_z)}\right|^2\right) = |A|^2 + |B|^2 = |N|^2(2l+1)\,,$$

where we have assumed that the wave functions $R_{nl}(r)\,Y_{lj_z\pm\frac{1}{2}}$ are properly normalized. Thus, we finally find

$$\psi_\sigma^{(j=l-\frac{1}{2},\,j_z)} = \begin{pmatrix} \sqrt{\frac{l+\frac{1}{2}-j_z}{2l+1}}\,R_{nl}(r)\,Y_{lj_z-\frac{1}{2}}(\theta,\phi) \\ -\sqrt{\frac{l+\frac{1}{2}+j_z}{2l+1}}\,R_{nl}(r)\,Y_{lj_z+\frac{1}{2}}(\theta,\phi) \end{pmatrix},$$

and, similarly, or just by noticing that the two functions $\psi_\sigma^{(j=l-\frac{1}{2},\,j_z)}$ and $\psi_\sigma^{(j=l+\frac{1}{2},\,j_z)}$ must be orthogonal to each other,

$$\psi_\sigma^{(j=l+\frac{1}{2},\,j_z)} = \begin{pmatrix} \sqrt{\frac{l+\frac{1}{2}+j_z}{2l+1}}\,R_{nl}(r)\,Y_{lj_z-\frac{1}{2}}(\theta,\phi) \\ \sqrt{\frac{l+\frac{1}{2}-j_z}{2l+1}}\,R_{nl}(r)\,Y_{lj_z+\frac{1}{2}}(\theta,\phi) \end{pmatrix}.$$

Comparing these explicit solutions with the general formula

$$|n,l,s,j,j_z\rangle = \sum_{m=-l}^{+l}\sum_{\sigma=\pm\frac{1}{2}} |n,l,m\rangle\otimes|s,\sigma\rangle\,C_{l\frac{1}{2}}(m,\sigma|j,j_z)\,,$$

we can read off the explicit expressions of nonzero Clebsch-Gordan coefficients coupling the angular momenta l and $s=\frac{1}{2}$:

$$\begin{aligned} C_{l\frac{1}{2}}(j_z-\tfrac{1}{2}\,,\,+\tfrac{1}{2}\,|l\mp\tfrac{1}{2}\,,\,j_z) &= \sqrt{\frac{l+\frac{1}{2}\mp j_z}{2l+1}}\,, \\ C_{l\frac{1}{2}}(j_z+\tfrac{1}{2}\,,\,-\tfrac{1}{2}\,|l\mp\tfrac{1}{2}\,,\,j_z) &= \mp\sqrt{\frac{l+\frac{1}{2}\pm j_z}{2l+1}}\,. \end{aligned}$$

The C-G coefficients obtained in this way could, of course, differ by a phase factor as compared to those listed in standard tables. It is however easy to check that for $j_z = l+\frac{1}{2}$ we have obtained $C_{l\frac{1}{2}}(j_z-\frac{1}{2},\frac{1}{2}|l+\frac{1}{2},j_z)=1$, as in the the standard convention.

4.6 Tensor operators and the Wigner-Eckart theorem

The physical information in quantum mechanics is contained in matrix elements of various operators and not in state vectors and operators separately. It is therefore possible to introduce a sort of the "Heisenberg" picture for symmetry transformations by defining the transformed operators O' by the equality

$$\langle\chi|O'|\psi\rangle = \langle\chi'|O|\psi'\rangle\,, \tag{4.123}$$

that is, so that the matrix elements of the transformed operators O' between the original states are the same as the matrix elements of the original operators between the

transformed states. Since $|\psi'\rangle = U|\psi\rangle$ with the appropriate symmetry operator U, one gets

$$O' = U^\dagger O\, U \approx O + i\theta^a \left[Q^a,\ O\right], \tag{4.124}$$

where in the last step we have assumed that the transformation is infinitesimal. In agreement with the intuition, in quantum mechanics of a single nonrelativistic particle, in the case of translations the formula (4.124) gives

$$\hat{\mathbf{r}}' = U^\dagger(\mathbf{a})\, \hat{\mathbf{r}}\, U(\mathbf{a}) = \hat{\mathbf{r}} - \mathbf{a}\,, \tag{4.125}$$

whereas for rotations one finds

$$\hat{\mathbf{r}}' = U^\dagger(R)\, \hat{\mathbf{r}}\, U(R) = R{\cdot}\hat{\mathbf{r}}\,. \tag{4.126}$$

Classification of operators with respect to their behaviour under rotations proves very useful. It is precisely this property property that determines the selection rules for their various matrix elements. This leads us naturally to consider the so-called tensor operators, i.e. sets of operators which under rotations transform one into another, and the Wigner-Eckart theorem.

From the formulae (4.124) and (4.75) it follows that under infinitesimal rotations

$$O' = O - \frac{i}{\hbar}\theta^i \left[J^i,\ O\right], \tag{4.127}$$

that is, the behaviour under rotations of the operator O is determined by its commutator with the rotation generators J^i, i.e. the operators of the total angular momentum. One defines therefore the tensor operator $T(j,m)$ or $T^{(j)}_m$ of the type j as the set of $2j+1$ operators having the following commutation rules with $\mathbf{J}$:

$$\begin{aligned}
\left[J^z,\ T^{(j)}_m\right] &= m\hbar\, T^{(j)}_m\ , \\
\left[J_+,\ T^{(j)}_m\right] &= \hbar\sqrt{j(j+1) - m(m+1)}\ T^{(j)}_{m+1}\,, \\
\left[J_-,\ T^{(j)}_m\right] &= \hbar\sqrt{j(j+1) - m(m-1)}\ T^{(j)}_{m-1}\,.
\end{aligned} \tag{4.128}$$

The above formulae can succinctly be rewritten in the form

$$\left[J^i,\ T^{(j)}_m\right] = \sum_{m'=-j}^{+j} T^{(j)}_{m'}\, \langle j, m'|J^i|j, m\rangle\,, \tag{4.129}$$

Using this form and the formula (4.78) the rule (4.124) of the transformation of the tensor operator under a rotation can be cast in the form

$$e^{-\frac{i}{\hbar}\psi^i J^i}\, T^{(j)}_m\, e^{\frac{i}{\hbar}\psi^i J^i} = T^{(j)}_m - \frac{i}{\hbar}\left[\boldsymbol{\psi}{\cdot}\mathbf{J},\ T^{(j)}_m\right]$$

$$+\frac{1}{2}\left(-\frac{i}{\hbar}\right)^2\left[\boldsymbol{\psi}\cdot\mathbf{J},\ \left[\boldsymbol{\psi}\cdot\mathbf{J},\ T^{(j)}_m\right]\right]+\dots$$
$$=T^{(j)}_m-\frac{i}{\hbar}\sum_{m'}T^{(j)}_{m'}\left(\psi^i J^i_{(j)}\right)_{m'm}$$
$$+\frac{1}{2}\left(-\frac{i}{\hbar}\right)^2\sum_{m''}\sum_{m'}T^{(j)}_{m''}\left(\psi^i J^i_{(j)}\right)_{m''m'}\left(\psi^i J^i_{(j)}\right)_{m'm}+\dots$$

In this way we get the transformation rule

$$U^\dagger(R)\,T^{(j)}_m\,U(R)=\sum_{m'=-j}^{+j}T^{(j)}_{m'}\,\langle j,m'|U^\dagger(R)|j,m\rangle$$
$$=\sum_{m'=-j}^{+j}T^{(j)}_{m'}D^{(j)}_{m'm}(R^{-1})\,. \tag{4.130}$$

valid for all parametrizations of the rotation R.

The operators $T^{(j)}_m$ are the analogs of the irreducible representations of the $SU(2)$ rotation group on state vectors; operators of the type $T^{(j)}_m$ behave as if they had the angular momentum j. Indeed, it follows from the definition (4.128) that[33]

$$\sum_{i=x,y,z}\left[J^i,\ \left[J^i,\ T^{(j)}_m\right]\right]=j(j+1)\hbar^2\,T^{(j)}_m\,. \tag{4.131}$$

The simplest example are, of course, scalar operators which commute with $\mathbf{J}$: they are the $T^{(0)}_0$ tensor operators. Another example are vector operators V^i which, similarly as the momentum operator P^i or the boost operator K^i in (4.48), satisfy

$$\left[J^i,\ V^j\right]=i\hbar\epsilon^{ijk}V^k\,. \tag{4.132}$$

Vector operators V^i are the tensor operators of the type $T^{(1)}_m$:

$$T^{(1)}_1=-\frac{1}{\sqrt{2}}(V^x+iV^y)\,,$$
$$T^{(1)}_0=V^z\,, \tag{4.133}$$
$$T^{(1)}_{-1}=\frac{1}{\sqrt{2}}(V^x-iV^y)\,.$$

Let us consider now the following combination of two different tensor operators of the type $T^{(j_1)}_{m_1}$ and $T^{(j_2)}_{m_2}$:

$$T^{(j)}_m\equiv\sum_{m_2=-j_2}^{+j_2}\sum_{m_1=-j_1}^{+j_1}T^{(j_2)}_{m_2}\,T^{(j_1)}_{m_1}\,C_{j_2j_1}(m_2,m_1|j,m)\,. \tag{4.134}$$

[33]The formula (4.131) is the direct analog of the formula $\mathbf{J}^2|j,m\rangle=j(j+1)\hbar^2|j,m\rangle$ if one takes into account that the action of the generators J^i on tensor operators is through the commutator.

Using the standard identity

$$[\mathbf{J},\ O_2O_1] = O_2\,[\mathbf{J},\ O_1] + [\mathbf{J},\ O_2]\,O_1\,, \tag{4.135}$$

and the relations (4.117) it is possible to show that $T^{(j)}_m$ defined by (4.134) is indeed a tensor operator of the type $T^{(j)}_m$. Similarly, using the unitarity relation (4.115) one can write

$$T^{(j_2)}_{m_2}\,T^{(j_1)}_{m_1} = \sum_{j=|j_1-j_2|}^{j_1+j_2}\ \sum_{m=-j}^{+j} C_{j_2j_1}(m_2,m_1|j,m)\,T^{(j)}_m\,, \tag{4.136}$$

which shows that the product of two tensor operators can be decomposed into the sum of irreducible tensor operators.

The formula most important in applications is

$$|j_2,m_2\rangle^b \equiv \sum_{m=-j}^{+j}\ \sum_{m_1=-j_1}^{+j_1} T^{(j)}_m\,|j_1,m_1\rangle\,C_{jj_1}(m,m_1|j_2,m_2)\,. \tag{4.137}$$

In the manner similar as (4.134), but by using instead of (4.135) the relation

$$\mathbf{J}\,O|\psi\rangle = [\mathbf{J},\ O]\ |\psi\rangle + O\,\mathbf{J}|\psi\rangle\,,$$

the states $|j_2,m_2\rangle^b$ can be shown to be eigenstates of $\mathbf{J}^2$ and J^z with the eigenvalues $j_2(j_2+1)\hbar^2$ and $m_2\hbar$, respectively. It is important, however, that in general the states $|j_2,m_2\rangle^b$ are *not* properly normalized (by definition the states $|j_2,m_2\rangle$ are normalized states):

$$\langle j_2,m_2|j_2,m_2\rangle^b = \mathcal{N}(j_2,j,j_1,T) \neq 1\,. \tag{4.138}$$

On the other hand, because the states $|j_2,m_2\rangle^b$ with higher m_2 can be obtained from the ones with lower m_2 by acting on them successively with J_+, their normalization does not depend on m_2. Therefore, as indicated in (4.138) the normalization factor $\mathcal{N}(j_2,j,j_1,T)$ depends only on j_2, j_1 and on the operator T and its type j (but not on the operator component labeled by m).[34]

Inverting the relation (4.137) using the unitarity relations (4.115) of the Clebsch-Gordan coefficient we get

$$T^{(j)}_m\,|j_1,m_1\rangle = \sum_{j_2=|j-j_1|}^{j+j_1}\ \sum_{m_2=-j_2}^{+j_2} |j_2,m_2\rangle^b\ C_{jj_1}(m,m_1|j_2,m_2)\,. \tag{4.139}$$

[34]The factor $\mathcal{N}(j_2,j,j_1,T)$ does depend also on quantum numbers other than those directly related to the angular momentum; this additional dependence is the same for all kets with the same j (i.e. it is independent of m_1).

Closing this relation from the left with a properly normalized state $\langle j_2, m_2|$ we finally obtain

$$\langle j_2, m_2|T^{(j)}_m\,|j_1, m_1\rangle = C_{jj_1}(m, m_1|j_2, m_2)\,\mathcal{N}(j_2, j, j_1, T)\,. \tag{4.140}$$

This is the content of the Wigner-Eckart theorem which says that the matrix elements of a tensor operator $T^{(j)}_m$ between properly normalized eigenstates of the total angular momentum operators $\mathbf{J}^2$ and J^z are determined, up to a single number $\mathcal{N}(j_2, j, j_1, T)$, by the Clebsch-Gordan coefficients. Since there are in principle $(2j_2 + 1)(2j + 1)(2j_1 + 1)$ matrix elements this is an enormous simplification.

The number $\mathcal{N}(j_2, j, j_1, T)$ which is sometimes written as

$$\mathcal{N}(j_2, j, j_1, T) \equiv (-1)^{j+j_2-j_1}\,\frac{1}{\sqrt{2j_2+1}}\,\langle j_2||T||j_1\rangle\,, \tag{4.141}$$

where $\langle j_2||T||j_1\rangle$ is called the *reduced matrix element* of the operator T, can be found by computing only one (e.g. the easiest one for a given operator T) of the $(2j_2 + 1)(2j + 1)(2j_1 + 1)$ matrix elements.

The Clebsch-Gordan coefficients appearing in the Wigner-Eckart formula (4.140) immediately determine the selection rules, that is, tell which of the possible $(2j_2 + 1)(2j + 1)(2j_1 + 1)$ matrix elements must vanish. In this way the Wigner-Eckart theorem determines e.g. possible electric quadrupole (and higher) transitions (induced and spontaneous alike) in atoms. Another its immediate consequence is that the system in a state characterized by the total angular momentum j cannot have electric or magnetic multipole moments of order 2^l with $l > 2j$ because the operators representing such moments are tensor operators of the type $T^{(l)}_m$ and

$$\langle j, m|T^{(l)}_{m'}\,|j, m\rangle = 0 \qquad \text{unless} \qquad l \leq 2j\,.$$

Therefore, spin $\frac{1}{2}$ fermions cannot (by the rotational invariance) have quadrupole ($l = 2$) moments, whereas spinless particles are forbidden to possess even dipole moments. (Spin $\frac{1}{2}$ particles generically do have magnetic dipole moments but electric dipole moment of a spin $\frac{1}{2}$ particles, allowed by the rotational invariance, violates the CP symmetry).

For vector operators, which are most frequently encountered in elementary applications the following simplified form of the Wigner-Eckart theorem proves very useful

$$\langle n, j, m|\mathbf{V}|n, j, m\rangle = \frac{\langle n, j, m|\mathbf{J}\cdot\mathbf{V}|n, j, m\rangle}{j(j+1)\hbar^2}\,\langle n, j, m|\mathbf{J}|n, j, m\rangle\,, \tag{4.142}$$

where n are some quantum numbers not related to the angular momentum. The proof of (4.142) goes as follows. From (4.140) and (4.133) we have

$$\langle n, j, j_z|V^{(1)}_m|n, j, j_z\rangle = C_{1j}(m, j_z|j, j_z)\,\mathcal{N}(j, 1, j, V, n)\,.$$

Consider now the matrix element $\langle n,j,m|\mathbf{J}|n,j,m\rangle$. Applying the Wigner-Eckart theorem to the vector $\mathbf{J}$ operator itself treated as $J^{(1)}_m$ we can write

$$j_z\hbar\,\delta_{m0} = \langle n,j,j_z|J^{(1)}_m|n,j,j_z\rangle = C_{1j}(m,j_z|j,j_z)\,\mathcal{N}(j,1,j,J,n)\,. \tag{4.143}$$

The first equality follows from the well known properties of the J^z and $J_\pm$ operators. In tables of the Clebsch-Gordan coefficients one can find that $C_{1j}(m,j_z|j,j_z) = j_z\delta_{m0}/\sqrt{j(j+1)}$. Hence,

$$\mathcal{N}(j,1,j,J,n) = \hbar\sqrt{j(j+1)}\,.$$

Inverting now the second equality in (4.143) we can therefore write

$$C_{1j}(m,j_z|j,j_z) = \frac{\langle n,j,j_z|J_m|n,j,j_z\rangle}{\hbar\sqrt{j(j+1)}}\ . \tag{4.144}$$

In order to find $\mathcal{N}(j,1,j,V,n)$ we consider[35]

$$\begin{aligned}
\langle n,j,j_z|\mathbf{V}\cdot\mathbf{J}|n,j,j_z\rangle &= \langle n,j,j_z|V^{(1)}_0J^z + \frac{1}{\sqrt{2}}\,V^{(1)}_{-1}J_+ - \frac{1}{\sqrt{2}}\,V^{(1)}_1J_-|n,j,j_z\rangle \\
&= j_z\hbar\,\langle j_z|V^{(1)}_0|j_z\rangle + \frac{\hbar}{\sqrt{2}}\,\sqrt{j(j+1)-j_z(j_z+1)}\,\langle j_z|V^{(1)}_{-1}|j_z+1\rangle \\
&\qquad -\frac{\hbar}{\sqrt{2}}\,\sqrt{j(j+1)-j_z(j_z-1)}\,\langle j_z|V^{(1)}_{+1}|j_z-1\rangle \\
&= \frac{\hbar}{\sqrt{2}}\,\Big[j_z\sqrt{2}\,C_{1j}(0,j_z|j,j_z) \\
&\qquad +\sqrt{j(j+1)-j_z(j_z+1)}\,C_{1j}(-1,j_z+1|j,j_z) \\
&\qquad -\sqrt{j(j+1)-j_z(j_z-1)}\,C_{1j}(1,j_z-1|j,j_z)\,\Big]\,\mathcal{N}(j,1,j,V,n)\,,
\end{aligned}$$

where at the intermediate stage we have dropped the unnecessary labels and applied the Wigner-Eckart theorem (4.140) to the matrix elements of $V^{(j)}_m$. Using again the properties of the Clebsch-Gordan coefficients one can show that the expression inside the square brackets equals $\sqrt{2j(j+1)}$, and we obtain

$$\mathcal{N}(j,1,j,V,n) = \frac{\langle n,j,m|\mathbf{J}\cdot\mathbf{V}|n,j,m\rangle}{\sqrt{2j(j+1)}\,\hbar}\,.$$

This, together with (4.144) completes the proof of the relation (4.142).

We illustrate the usefulness of the formula (4.142) by computing the splitting of the Hydrogen atom energy levels in a constant uniform magnetic field (the Zeeman effect)

[35]Notice that the standard J_+ and J_- operators treated as components of the tensor operator are not properly normalized.

taking into account the electron spin (i.e. its magnetic moment). To this end we have to consider the states with definite quantum numbers l, j and j_z. The magnetic field splits the states with different j_z. The Hamiltonian $V_{\rm int}$ of the electron spin interaction with an external magnetic field $\mathbf{B}$ reads

$$V_{\rm int} = \frac{e}{2mc}\,(\mathbf{L} + 2\mathbf{S})\cdot\mathbf{B}\,, \tag{4.145}$$

(we use $e > 0$). The factor 2 multiplying $\mathbf{S}$ is the anomalous magnetic moment of the electron: it is the well known relativistic effect that the ratio of the intrinsic magnetic moment of the electron to its spin is twice[36] as big as the ratio of the electron magnetic moment due to its orbital to its orbital angular momentum. Because of this factor of 2 the calculation of the energy splitting given by

$$\Delta E_{nljj_z} = \frac{e}{2mc}\,B^z \langle n,l,s,j,j_z|L^z + 2S^z|n,l,s,j,j_z\rangle\,, \tag{4.146}$$

is not straightforward and requires using (4.142). Since $L^z + 2S^z = J^z + S^z$ it is sufficient to consider the matrix element

$$\langle l,j,j_z|S^z|l,j,j_z\rangle = \frac{\langle l,j,j_z|\mathbf{J}\cdot\mathbf{S}|l,j,j_z\rangle}{j(j+1)\hbar^2}\,\langle l,j,j_z|J^z|l,j,j_z\rangle\,, \tag{4.147}$$

where we have used (4.142) and omitted inessential quantum numbers. We can now use the identity

$$\mathbf{J}\cdot\mathbf{S} = -\frac{1}{2}\,(\mathbf{J}-\mathbf{S})^2 + \frac{1}{2}\mathbf{J}^2 + \frac{1}{2}\mathbf{S}^2 = \frac{1}{2}\left(\mathbf{J}^2 + \mathbf{S}^2 - \mathbf{L}^2\right). \tag{4.148}$$

Since the states $|l,j,j_z\rangle$ are eigenstates of all these operators we get

$$\langle l,j,j_z|S^z|l,j,j_z\rangle = \frac{j(j+1) + \frac{3}{4} - l(l+1)}{2j(j+1)}\,\langle l,j,j_z|J^z|l,j,j_z\rangle\,. \tag{4.149}$$

Thus we finally obtain

$$\begin{aligned}\Delta E_{nljj_z} &= \frac{e}{2mc}B^z\left[1 + \frac{j(j+1)+\frac{3}{4}-l(l+1)}{2j(j+1)}\right]\,\langle l,j,j_z|J^z|l,j,j_z\rangle \\ &= \frac{e}{2mc}B^z\,g\,\langle l,j,j_z|J^z|l,j,j_z\rangle = \frac{e}{2mc}B^z\,g\,j_z\hbar\,,\end{aligned} \tag{4.150}$$

with

$$g = 1 + \frac{j(j+1)+\frac{3}{4}-l(l+1)}{2j(j+1)}\,, \tag{4.151}$$

the so-called Landé factor.

[36]The factor 2 comes out naturally from the Dirac equation. There are also tiny corrections to this result whose computation requires the use of the full Quantum Electrodynamics - see section 19.5.

4.7 Higher symmetries

In some special cases the spectrum of the Hamiltonian exhibits degeneracies higher than could be expected from the rotational invariance alone. Consider for example the two-dimensional isotropic harmonic oscillator with the Hamiltonian

$$H = \frac{1}{2M}\left(P_x^2 + P_y^2\right) + \frac{1}{2}M\omega^2\left(x^2 + y^2\right). \tag{4.152}$$

Its eigenvalues are given by $E_{n_x n_y} = \hbar\omega(n_x + n_y + 1)$ and depend only on $n_x + n_y$ and not on n_x and n_y separately. Hence, the N-th energy level has $(N+1)$-fold degeneracy. Of course, $L = xP_y - yP_x$ commutes with the Hamiltonian, but since the group of two-dimensional rotations it generates is Abelian, all the representations of its Lie algebra are one-dimensional. Thus, on the basis of the rotational symmetry one would not expect any degeneracy.

Similarly, the eigenvalues of the Hamiltonian of the three-dimensional isotropic harmonic oscillator are given by $E_{n_x n_y n_z} = \hbar\omega(n_x + n_y + n_z + \frac{3}{2})$ and the degeneracy of the N-th energy level is $\frac{1}{2}(N+1)(N+2)$-fold. Again, these multiplicities do not correspond to $(2l+1)$-fold degeneracies expected on the basis of the invariance with respect to three-dimensional rotations.

The degeneracy of the spectra of the two- and three- (and also higher) dimensional isotropic harmonic oscillators can be understood by noticing that in each case one can construct a number of Hermitian operators Q^a, which commute with the Hamiltonian and form a closed algebra

$$\left[Q^a,\ Q^b\right] = i\hbar f_c{}^{ab} Q^c\,, \qquad [Q^a,\ H] = 0\,, \tag{4.153}$$

with some structure constants $f_c{}^{ab}$. The operators $\mathbf{L}$ are part of the algebra of Q^a's. Since these algebras are closed, the operators Q^a generate some higher dimensional symmetry groups. In the case of two dimensions the algebra of Q^a's coincides with the one generated by $\mathbf{L}$ in three dimensions. Hence, the two-dimensional isotropic harmonic oscillator has the $SU(2)$ symmetry group which appears because of the special form of the potential. Similarly, the algebra of Q^a's in the case of the three-dimensional isotropic harmonic oscillator coincides with the algebra of the generators of the $SU(3)$ group.

These symmetries are easy to uncover if the Hamiltonian of the n-dimensional isotropic harmonic oscillator is written in terms of the creation and annihilation operators:

$$H = \hbar\omega \sum_{i=1}^{n} \left(a_i^\dagger a_i + \frac{1}{2}\right). \tag{4.154}$$

This form of H as well as the commutation relation $[a_i,\ a_j^\dagger] = \delta_{ij}$ are easily seen to be invariant under the transformations

$$a_i \to \left(e^{-i\theta^a T^a}\right)_{ij} a_j\ , \qquad a_i^\dagger \to a_j^\dagger \left(e^{i\theta^a T^a}\right)_{ji}\ , \tag{4.155}$$

where the n^2-1 Hermitian $n\times n$ matrices T^a form the so-called fundamental (i.e. the nontrivial one of the lowest dimension) representation of the $SU(n)$ group.[37] For $SU(2)$ the matrices T^a are the Pauli matrices divided by 2: $T^a=\frac{1}{2}\sigma^a$; for $SU(3)$ $T^a=\frac{1}{2}\lambda^a$, where λ^a are the eight 3×3 Gell-Mann matrices, etc.[38]

Invariance of the Hamiltonian under the transformations (4.155) immediately suggests that the hidden symmetry group is just $SU(n)$. Indeed, it is easy to see that if there exist unitary symmetry operators $U(\theta)\approx 1-\frac{i}{\hbar}\theta^a Q^a$ which commute with H and such that

$$U^\dagger(\theta)\,a_i\,U(\theta)=\left(e^{-i\theta^a T^a}\right)_{ij}a_j\,,\qquad U^\dagger(\theta)\,a_i^\dagger\,U(\theta)=a_j^\dagger\left(e^{i\theta^a T^a}\right)_{ji}\,, \tag{4.156}$$

then the Hamiltonian is automatically invariant

$$U^\dagger(\theta)\,H\,U(\theta)=H\,, \tag{4.157}$$

or, in other words, $[H,\ U(\theta)]=0$. For infinitesimal parameters θ^a we should therefore have

$$\frac{i}{\hbar}\,[Q^a,\ a_k]=-iT^a_{kj}a_j\ ,\qquad \frac{i}{\hbar}\left[Q^a,\ a_k^\dagger\right]=ia_j^\dagger T^a_{jk}\,, \tag{4.158}$$

and it is easy to see that these commutation rules are satisfied by the operators Q^a of the form

$$Q^a=\hbar\,a_k^\dagger\,T^a_{kj}\,a_j\,. \tag{4.159}$$

It is also straightforward to check that together with the Hamiltonian (4.154) the operators Q^a (4.159) satisfy the commutation rules (4.153) with the same structure constants of the $SU(n)$ group as do the finite dimensional c-number matrices T^a:

$$T^a_{ik}T^b_{kj}-T^b_{ik}T^a_{kj}=if_c{}^{ab}\,T^c_{ij}\,. \tag{4.160}$$

The symmetry group of the n-dimensional harmonic oscillator is therefore $SU(n)$ and the degeneracies of the successive energy levels correspond to the number of basis states of higher and higher dimensional representations of this group. For $n=2$ these representations are labeled by the values $k(k+1)$ with $k=0,\frac{1}{2},1,\ldots$ of the Casimir operator $\mathbf{Q}^2=\sum_{a=1}^3 Q^aQ^a$ and the multiplicity of the N-th energy level is easily seen to correspond to the representation with $k=N/2$. For the three-dimensional oscillator, $n=3$, the representations are in principle labeled by two Racah operators (one of them,

[37] In fact the Hamiltonian (4.154) is invariant under the larger, $U(n)$ symmetry group generated by the n^2-1 matrices T^a and one additional matrix T which is simply proportional to the unit $n\times n$ matrix (it generates transformations changing the phases of all the operators a_i in the same way). However, as can be checked, the Hilbert space operator generating these additional transformations coincides (up to a multiplicative constant factor) with the Hamiltonian itself. Hence, this additional symmetry is the time translation symmetry and is not reflected in the degeneracy of the energy levels.

[38] For the generators in the fundamental representation we adopt the normalization $\mathrm{tr}(T^aT^b)=\frac{1}{2}\delta^{ab}$.

the Casimir operator, is of the form $\mathbf{Q}^2 = \sum_{a=1}^{8} Q^a Q^a$ and the second one is built as some trilinear combination of Q^a's), but usually the representations of the $SU(3)$ Lie algebra are distinguished just by their dimension or by giving a pair of integers (u, v), where $u, v = 0, 1, 2, \ldots$, in which case the dimension of the representation is given by $\frac{1}{2}(u+1)(v+1)(u+v+2)$. Not all representations are realized in the spectrum of the three-dimensional oscillator: for example, the representations denoted in particle physics as **1**, **3**, **6** and **10** are realized at the 0-th, first, second and third energy levels, respectively, but the adjoint representation **8** does not appear. In fact, realized are only those representations which in the (u, v) classification are denoted as $(u, 0)$. It is left for the reader to investigate the reason for this.

Another celebrated example of a symmetry higher than expected explains the structure of the spectrum the nonrelativistic Hydrogen-like atom. Solving the Schrödinger equation with the potential $V(r) = -e^2/r$ (for simplicity we consider the Hydrogen atom with $Z = 1$) one finds that the $n = 1$ ground level is nondegenerate and consists of a single $1S$ state.[39] At the second $n = 2$ energy level there are four states: one $2S$ and three $2P$ states. For $n = 3$ there are: one $3S$ state, three $3P$ states and five $3D$ states, and so on. One immediately realizes that the multiplicity of states at the n-the energy level is n^2 instead of being equal $(2l + 1)$ for some integer $l = 0, 1, 2, \ldots$, as could be expected from the rotational invariance of the potential $V(r)$. Clearly, some higher symmetry must be responsible for this degeneracy. However, as will be seen, in contrast with the harmonic oscillator, this symmetry is only a dynamical one, that is, the Hilbert space symmetry generators forming a closed algebra can be defined only for subspaces corresponding to individual energy levels. As a result, the symmetry considerations will allow to explain not only the degeneracy of the energy levels but also to find purely algebraically the eigenvalues of the Hamiltonian.

As it is well known, from classical mechanics, the motion of a particle of mass m in the central potential $V(r) = -e^2/r$ is characterized not only by the four usual constants of motion (the energy E and the three components of the orbital angular momentum $\mathbf{L}$), but also by three other constant quantities - the three components of the so-called Lenz vector

$$\mathbf{M} = \dot{\mathbf{r}} \times \mathbf{L} - e^2 \frac{\mathbf{r}}{r}, \tag{4.161}$$

(the dot represents the time derivative). Indeed, differentiating $\mathbf{M}$ with respect to time and using the Newton's equation

$$\frac{d}{dt} m\dot{\mathbf{r}} = -e^2 \frac{\mathbf{r}}{r^3}, \tag{4.162}$$

one easily finds that $\mathbf{M}$ is constant. While the constancy of $\mathbf{L}$ expresses geometrically the fact that the motion occurs in a fixed plane, the constancy of $\mathbf{M}$ is related to the fact that the axes of the ellipses do not precess with time.

[39] In the considerations we ignore the doubling of each energy eigenstate due to the spin of the electron.

The analogy with classical mechanics suggests that in the quantum theory the three components of $\mathbf{M}$ will, together with the three components of $\mathbf{L}$, play the roles of the generators of some higher symmetry, which explains the degeneracy of the spectrum. There is however an ambiguity in defining $\mathbf{M}$ as the quantum mechanical operator because $\mathbf{L}$ and $\mathbf{P}$ do not commute with each other. It turns out that the correct definition is provided by the symmetric ordering

$$\begin{aligned}\mathbf{M} &= \frac{1}{2m}\left(\mathbf{P}\times\mathbf{L} - \mathbf{L}\times\mathbf{P}\right) - e^2\,\frac{\mathbf{r}}{r} \\ &= \frac{1}{m}\,\mathbf{P}\times\mathbf{L} - \frac{i\hbar}{m}\,\mathbf{P} - e^2\,\frac{\mathbf{r}}{r}\,,\end{aligned} \tag{4.163}$$

which also makes $\mathbf{M}$ Hermitian. With this definition it is straightforward (but in fact terribly tedious!) to check that the following commutation rules are satisfied:

$$\begin{aligned}&[H,\ \mathbf{L}] = 0\,, \qquad &&\left[L^i,\ L^j\right] = i\hbar\,\epsilon^{ijk}L^k\,, \\ &[H,\ \mathbf{M}] = 0\,, \qquad &&\left[L^i,\ M^j\right] = i\hbar\,\epsilon^{ijk}M^k\,.\end{aligned} \tag{4.164}$$

The last relation expresses simply the fact that $\mathbf{M}$ is a vector operator.

To have a closed algebra of generators - a property necessary to identify the results of the action of $Q^aQ^b - Q^bQ^a$ on states of the system with another transformation belonging to the group of symmetries (see Section 4.2) - it should be also possible to express the commutator of components of $\mathbf{M}$ as a linear combination of L^i and M^i. However, computing the commutator explicitly one finds (after a long calculation) instead:

$$\left[M^i,\ M^j\right] = -\frac{2}{m}\,i\hbar\,\epsilon^{ijk}\,HL^k\,, \tag{4.165}$$

(with the Hamiltonian H on the right hand side). In other words, one finds that the algebra of the operators $\mathbf{L}$ and $\mathbf{M}$ does not close.

The solution is provided by the observation, that if we restrict the consideration to a given discrete (with $E<0$) energy level, we can form the new operators

$$\mathbf{N} = \left(-\frac{m}{2E}\right)^{1/2}\mathbf{M}\,, \tag{4.166}$$

which are also vector operators commuting with H and satisfy the rule

$$\left[N^i,\ N^j\right] = i\hbar\,\epsilon^{ijk}L^k\,, \tag{4.167}$$

that is, on the subspace of states corresponding to fixed $E<0$ they form, together with the operators $\mathbf{L}$, a closed algebra of generators. Therefore, the six generators $\mathbf{L}$ and $\mathbf{N}$ can be promoted to the generators of the transformations forming the $SO(4)$ symmetry group. Of course, the operators $\mathbf{N}$ are defined only for a given energy level (different operators $\mathbf{N}$ form closed algebras at different energy levels), but apart from this, their implications for the degeneracies of the energy levels are the same as of "normal" symmetry generators.

Before finding the representations of the Lie algebra generated by $\mathbf{L}$ and $\mathbf{N}$ it is useful to note two relations. Firstly, computing (laboriously!) the square of the operator $\mathbf{M}$ one finds that

$$\mathbf{M}^2 = \frac{2}{m} H \left(\mathbf{L}^2 + \hbar^2\right) + e^4 \,. \tag{4.168}$$

On the subspace of states corresponding to a fixed value $E < 0$ of energy this is equivalent to

$$\mathbf{N}^2 + \mathbf{L}^2 = -\hbar^2 - \frac{me^4}{2E} \,. \tag{4.169}$$

Secondly, in the specific realization of the $SO(4)$ Lie algebra provided by the operators $\mathbf{L}$ and $\mathbf{N}$ one has[40] $\mathbf{M} \cdot \mathbf{L} = \mathbf{L} \cdot \mathbf{M} = 0$, or, equivalently,

$$\mathbf{N} \cdot \mathbf{L} = \mathbf{L} \cdot \mathbf{N} = 0 \,. \tag{4.170}$$

It is important to stress that this relation does not follow from the commutation rules of the $SO(4)$ Lie algebra; it is specific only for its realization by operators acting in the Hilbert space of the nonrelativistic Hydrogen atom.

It is now straightforward to find the representations of the Lie algebra generated by the operators $\mathbf{L}$ and $\mathbf{N}$. To this end, it is easier to define the new generators[41]

$$\mathbf{I} \equiv \frac{1}{2} \left(\mathbf{L} + \mathbf{N}\right) , \qquad \mathbf{K} \equiv \frac{1}{2} \left(\mathbf{L} - \mathbf{N}\right) , \tag{4.171}$$

which satisfy simpler commutation rules:

$$\begin{gathered} \left[I^i,\ I^j\right] = i\hbar\epsilon^{ijk} I^k \,, \qquad \left[K^i,\ K^j\right] = i\hbar\epsilon^{ijk} K^k \,, \\ \left[I^i,\ K^j\right] = 0 \,. \end{gathered} \tag{4.172}$$

Thus the Lie algebra of $\mathbf{L}$ and $\mathbf{N}$ is equivalent to the direct sum $su(2) \oplus su(2)$ of the two $su(2)$ Lie algebras generated by the $\mathbf{I}$ and $\mathbf{K}$ operators independently. The symmetry group is therefore

$$SU(2) \times SU(2) \sim SO(4) \,. \tag{4.173}$$

It is then easy to realize that the Lie algebra of the generators $\mathbf{L}$ and $\mathbf{N}$ is of rank two with I^z and K^z forming its Cartan subalgebra and $\mathbf{I}^2$ and $\mathbf{K}^2$ playing the roles of the two Racah operators. Irreducible representations of the $su(2) \oplus su(2)$ Lie algebra spanned by the Hilbert space vectors belonging to a given energy level are therefore labeled by pairs of $\mathbf{I}^2$ and $\mathbf{K}^2$ eigenvalues $\hbar^2 i(i+1)$ and $\hbar^2 k(k+1)$ - they are concisely denoted (i, k) -

[40] The equality $\mathbf{M} \cdot \mathbf{L} = 0$ is easy to check using the second form (4.163) of the operator $\mathbf{M}$, while $\mathbf{L} \cdot \mathbf{M} = 0$ using its third form with $\mathbf{L}$ standing to the left.

[41] A warning: the operator $\mathbf{K}$ defined here has nothing to do with the boost generator defined in (4.43)!

where $i, k = 0, \frac{1}{2}, 1, \frac{3}{2}, \ldots$, and have dimensions $(2i+1)(2k+1)$. State-vectors spanning a given representation are then labeled by eigenvalues $\hbar i_z$ and $\hbar k_z$ of the generators I^z and K^z and can be written as $|n, i_z, k_z\rangle$ (here n labels the energy level); the matrices of the first (second) $SU(2)$ group of the direct product $SU(2) \times SU(2)$ act only on the first (second) index i_z (k_z).

However, because of the operator relations (4.170), in the Hydrogen atom Hilbert space

$$\begin{aligned} \mathbf{I}^2 &= \frac{1}{4}\left(\mathbf{L}^2 + \mathbf{N}^2 + \mathbf{N}\cdot\mathbf{L} + \mathbf{L}\cdot\mathbf{N}\right) = \frac{1}{4}\left(\mathbf{L}^2 + \mathbf{N}^2\right), \\ \mathbf{K}^2 &= \frac{1}{4}\left(\mathbf{L}^2 + \mathbf{N}^2 - \mathbf{N}\cdot\mathbf{L} - \mathbf{L}\cdot\mathbf{N}\right) = \frac{1}{4}\left(\mathbf{L}^2 + \mathbf{N}^2\right), \end{aligned} \tag{4.174}$$

i.e. $\mathbf{I}^2 = \mathbf{K}^2$. Hence, in this particular case realized can only be those $su(2) \oplus su(2)$ algebra representations with $k = i$, and which, for this reason, are of dimensions $(2k+1)^2$ with $k = 0, \frac{1}{2}, 1, \frac{3}{2}, \ldots$. This explains why the multiplicity of states at each energy level is a square of an integer $n = 2k + 1$.

One can go further and notice that because

$$\frac{1}{2}\left(\mathbf{L}^2 + \mathbf{N}^2\right) = \mathbf{I}^2 + \mathbf{K}^2, \tag{4.175}$$

the operators appearing on the left-hand side of (4.169) can take only values $2{\cdot}2{\cdot}k(k{+}1)\hbar^2$. Hence,

$$-\hbar^2 - \frac{me^4}{2E} = 4k(k+1)\hbar^2, \tag{4.176}$$

which leads to the well known result

$$E = -\frac{me^4}{2\hbar^2(2k+1)^2}, \qquad \text{with} \qquad k = 0, \frac{1}{2}, 1, \frac{3}{2}, \ldots \tag{4.177}$$

This reproduces the spectrum of the nonrelativistic bound states of the Hydrogen atom and explains the rule that the multiplicity of the n-th energy level equals n^2.

4.8 Discrete symmetries: space and time reflection

The set of classical Galileo transformations (4.36) can be supplemented with two discrete symmetry transformations: P and T - the space and time reflection, respectively (often called simply parity and time reversal) - which act on coordinates in the following way

$$\begin{aligned} &\mathbf{r}' = -\mathbf{r}, \quad t' = t, \quad \text{(space reflection)} \\ &\mathbf{r}' = \mathbf{r}, \quad t' = -t, \quad \text{(time reversal).} \end{aligned} \tag{4.178}$$

From this it is easy to see that on coordinates $P^{-1} = P$, $T^{-1} = T$ and that

$$\begin{aligned} P \cdot (R,\, \mathbf{V},\, \mathbf{a},\, \tau) &= (R,\ -\mathbf{V},\ -\mathbf{a},\, \tau) \cdot P\,, \\ T \cdot (R,\, \mathbf{V},\, \mathbf{a},\, \tau) &= (R,\ -\mathbf{V},\, \mathbf{a},\ -\tau) \cdot T\,. \end{aligned} \tag{4.179}$$

In the Hilbert space these transformations are represented by the operators $U(P) = \mathcal{P}$ and $U(T) = \mathcal{T}$, which, according to the Wigner theorem, must be either unitary and linear or antiunitary and antilinear. The commutation rules of $\mathcal{P}$ and $\mathcal{T}$ with the generators of the Galileo group can be deduced by using the same procedure that led us to (4.48). Repeating the steps we find

$$\begin{aligned} &\mathcal{P}\, iJ^i\, \mathcal{P}^\dagger = iJ^i\,, && \mathcal{T}\, iJ^i\, \mathcal{T}^\dagger = iJ^i\,, \\ &\mathcal{P}\, iK^i\, \mathcal{P}^\dagger = -iK^i\,, && \mathcal{T}\, iK^i\, \mathcal{T}^\dagger = -iK^i\,, \\ &\mathcal{P}\, iP^i\, \mathcal{P}^\dagger = -iP^i\,, && \mathcal{T}\, iP^i\, \mathcal{T}^\dagger = iP^i\,, \\ &\mathcal{P}\, iH\, \mathcal{P}^\dagger = iH\,, && \mathcal{T}\, iH\, \mathcal{T}^\dagger = -iH\,. \end{aligned}$$

We have left the factors of i, for we still have to decide whether the operators $\mathcal{P}$ and $\mathcal{T}$ are linear or antilinear. This can be decided by looking at the last pair of relations: if the operations of space and time reflections are to be symmetries of the given physical system, they should transform it into (taking the active view) another realizable system with the same energy levels. In particular, the energy spectrum of the transformed system should not be unbounded from below (typically the spectrum of H is unbounded from above - there can be arbitrarily high excitations; recall also that $\mathcal{P}^\dagger H \mathcal{P}$ and $\mathcal{T}^\dagger H \mathcal{T}$ give on the states of the original system the same values as does H on the states of the parity transformed and time reversed systems, respectively). Hence we should require that

$$\mathcal{P}\, H\, \mathcal{P}^\dagger = H\,, \qquad \mathcal{T}\, H\, \mathcal{T}^\dagger = H\,, \tag{4.180}$$

from which it follows that $\mathcal{P}$ must be unitary and linear whereas $\mathcal{T}$ has to be antiunitary and antilinear (multiplying these relations from the right by $\mathcal{P}$ and $\mathcal{T}$ one gets the commutation relations in the standard form $[H,\ \mathcal{P}] = 0$, $[H,\ \mathcal{T}] = 0$). Thus,

$$\begin{aligned} &\mathcal{P}\, J^i\, \mathcal{P}^\dagger = J^i\,, && \mathcal{T}\, J^i\, \mathcal{T}^\dagger = -J^i\,, \\ &\mathcal{P}\, K^i\, \mathcal{P}^\dagger = -K^i\,, && \mathcal{T}\, K^i\, \mathcal{T}^\dagger = K^i\,, \\ &\mathcal{P}\, P^i\, \mathcal{P}^\dagger = -P^i\,, && \mathcal{T}\, P^i\, \mathcal{T}^\dagger = -P^i\,. \end{aligned} \tag{4.181}$$

We now come to specific realizations of $\mathcal{P}$ and $\mathcal{T}$ in Hilbert spaces.

We consider first the space reflection in the conventional nonrelativistic quantum mechanics of a single particle. As we will see studying the relativistic case, each particle[42]

[42] That is, each irreducible representation of the Poincaré group identified with some type of particles. Of course, parity is known to be broken in Nature by the weak interactions, so strictly speaking the parity operator $\mathcal{P}$ acting on full interacting state vectors of the Standard Theory cannot be constructed. However, considering the action of $\mathcal{P}$ on free particle states is still useful because in physics - as opposed to mathematics - we are not merely interested in the statement that the space reflection is not a symmetry, but rather in *how* it is broken by interactions.

can be characterized by a number η called its *intrinsic parity* which is the eigenvalue of the parity operator $\mathcal{P}$ on the vector state of this particle. Since classically P^2 is the identity, in the Hilbert space we can have $\mathcal{P}^2 = e^{i\varphi}$. Therefore η^2, and hence also η, is a complex number of modulus 1. We will see later, that for bosons (particles having integer spin) the possible eigenvalues of $\mathcal{P}$ are ± 1, whereas for fermions (particles having half-integer spin) η can assume values ± 1 and $\pm i$. (In nonrelativistic theory this is sometimes justified with the argument that since P^2 is like the rotation by 2π, for bosons one must have $\mathcal{P}^2 = +1$, while for fermions $\mathcal{P}^2$ can also equal -1; this argument is however not very convincing).

The intrinsic parity η is unique for a given particle and plays, hence, completely no role in quantum mechanic of a single particle. In principle the state vector $|\psi\rangle$ (the wave function $\psi(\mathbf{r})$ of the space reflected system should satisfy the relation

$$\psi'(\mathbf{r}) \equiv \langle \mathbf{r}|\psi'\rangle = \eta\psi(P^{-1}\mathbf{r}) = \eta\psi(-\mathbf{r}) = \eta\,\langle -\mathbf{r}|\psi\rangle\,, \tag{4.182}$$

and if the space reflection is a symmetry of the physical system then the operator $\mathcal{P}$ such that

$$|\psi'\rangle = \mathcal{P}|\psi\rangle\,, \tag{4.183}$$

commutes with the Hamiltonian.

In quantum mechanics of a single particle the action of $\mathcal{P}$ on the position operator $\hat{\mathbf{r}}$ can be deduced by noticing that since $\mathcal{P}\mathbf{J}\mathcal{P}^\dagger = \mathbf{J}$, where in general $\mathbf{J} = \hat{\mathbf{r}} \times \mathbf{P} + \mathbf{S}$, cf. (4.76), and $\mathcal{P}\,\mathbf{P}\,\mathcal{P}^\dagger = -\mathbf{P}$, one must have

$$\mathcal{P}\,\hat{\mathbf{r}}\,\mathcal{P}^\dagger = -\hat{\mathbf{r}}\,, \tag{4.184}$$

(and also $\mathcal{P}\mathbf{S}\mathcal{P}^\dagger = \mathbf{S}$). This is in line with the physically motivated expectation that if $\langle\psi|\hat{\mathbf{r}}|\psi\rangle = \mathbf{r}$, then $\langle\psi'|\hat{\mathbf{r}}|\psi'\rangle = \langle\psi|\mathcal{P}^\dagger\hat{\mathbf{r}}\mathcal{P}|\psi\rangle = -\mathbf{r}$.

If the Hamiltonian H of a system of *many* particles (not necessarily all identical) or, more frequently, its unperturbed part H_0, commutes with $\mathcal{P}$, the N-particle eigenstates of H or of H_0 denoted by $|\psi_N\rangle$, forming a basis of the system Hilbert space (see Section 5) can be chosen so that they satisfy

$$\mathcal{P}|\psi_N\rangle = \eta_\psi\eta_{\psi_1}\ldots\eta_{\psi_N}|\psi_N\rangle\,, \tag{4.185}$$

with $\eta_\psi = \pm 1$ the parity of the state $|\psi_N\rangle$ and η_{ψ_i} the intrinsic parities of the particles in this state. In such a case parity can be used to establish certain selection rules for matrix elements of those operators O which have definite reflection properties

$$\mathcal{P}^\dagger O\mathcal{P} = \eta_O O\,. \tag{4.186}$$

Indeed, in this case we have:

$$\begin{aligned}\eta_O\langle\chi_N|O|\psi_N\rangle &= \langle\chi_N|\mathcal{P}^\dagger O\mathcal{P}|\psi_N\rangle \\ &= \eta_\chi\eta_\psi\eta^*_{\chi_1}\ldots\eta^*_{\chi_N}\eta_{\psi_1}\ldots\eta_{\psi_N}\langle\chi_N|O|\psi_N\rangle\,,\end{aligned} \tag{4.187}$$

and the matrix element must vanish if

$$\eta_O^*\eta_\chi\eta_\psi\eta_{\chi_1}^*\dots\eta_{\chi_N}^*\eta_{\psi_1}\dots\eta_{\psi_N}\neq 1\,. \tag{4.188}$$

In particular, in quantum mechanics of a single particle ($N=1$) the operator $\hat{\mathbf{r}}$ has $\eta_{\mathbf{r}}=-1$ and the electric dipole transitions can occur only between states having opposite parities.

Consider now the time reversal. If $[H,\ \mathcal{T}]=0$, i.e. if the time reversal is the symmetry of the system, for an arbitrary state $|\psi(t)\rangle$ one can write

$$\mathcal{T}|\psi(t)\rangle=\mathcal{T}\,e^{-i\frac{H}{\hbar}t}|\psi(0)\rangle=e^{-i\frac{H}{\hbar}(-t)}\,|\psi'(0)\rangle=|\psi'(-t)\rangle\,, \tag{4.189}$$

where we have used the antilinearity of $\mathcal{T}$ and *defined*

$$|\psi'(0)\rangle\equiv\mathcal{T}|\psi(0)\rangle\,. \tag{4.190}$$

Thus, $\mathcal{T}|\psi(t)\rangle=|\psi'(-t)\rangle$. With this definition it is easy to see that if $|\psi(t)\rangle$ satisfies the Schrödinger equation, so does also $|\psi'(t)\rangle$:

$$\begin{aligned}i\hbar\frac{d}{dt}|\psi'(t)\rangle\equiv i\hbar\frac{d}{dt}\mathcal{T}|\psi(-t)\rangle&=\mathcal{T}i\hbar\frac{d}{d(-t)}|\psi(-t)\rangle\\&=\mathcal{T}H|\psi(-t)\rangle=\mathcal{T}H\mathcal{T}^\dagger\mathcal{T}|\psi(-t)\rangle=H|\psi'(t)\rangle\,,\end{aligned} \tag{4.191}$$

(we have used again the antilinearity of $\mathcal{T}$).

In concrete representations of quantum mechanics one represents the operator $\mathcal{T}$ as the product $\mathcal{T}=U\mathcal{K}$, in which U is a suitable unitary operator and $\mathcal{K}$ is the complex conjugation. The operator U is chosen so that the commutation rules (4.181) of $\mathcal{T}$ are satisfied.

For complex H (e.g. if the potential energy V is a complex function of the position, which is the case e.g. when inelastic scattering is modeled within the framework of quantum mechanics of a single particle) the time reversal symmetry would require

$$UH^*U^\dagger=H\ , \tag{4.192}$$

which usually is impossible - the time reversal is broken because the absorption effects (described by the imaginary part of V) single out (like friction or viscosity) one time direction.

In quantum mechanics of a single particle $\mathbf{J}=\hat{\mathbf{r}}\times\mathbf{P}+\mathbf{S}$ (c.f. (4.76)) and from (4.181) one deduces that

$$\mathcal{T}\,\hat{\mathbf{r}}\,\mathcal{T}^\dagger=\hat{\mathbf{r}}\,, \tag{4.193}$$

and $\mathcal{T}\mathbf{S}\mathcal{T}^\dagger=-\mathbf{S}$. The wave function of a spinless particle has only one component and it is easy to see that in usual the position representation the rules (4.181) are satisfied by

$U = 1$. Instead, in the momentum representation, in which $\hat{\mathbf{P}} = \mathbf{p}$ and $\hat{\mathbf{r}} = i\hbar\partial/\partial\mathbf{p}$, one must have $U\mathbf{p}U^\dagger = -\mathbf{p}$ in order to satisfy the relations (4.181) with $\hat{\mathbf{P}}$ and $\mathbf{J} = \mathbf{L}$.

For spinning particles the commutation rule (4.181) with $\mathbf{J} = \hat{\mathbf{r}} \times \mathbf{P} + \mathbf{S}$ imposes additional conditions on U. In the position representation assuming that the matrices S^i are such that S^x and S^z are real while S^y is purely imaginary (this can always be arranged for), we must have

$$US^{x,z}U^\dagger = -S^{x,z}\,, \qquad US^yU^\dagger = S^y\,. \tag{4.194}$$

It is easy to check that in this representation

$$\mathcal{T} = \exp\left(-\pi\frac{i}{\hbar}S^y\right)\mathcal{K}\,, \tag{4.195}$$

satisfies the requirements. In particular, for spin $\frac{1}{2}$ particles, for which $S^i = (\hbar/2)\sigma^i$, one has $\mathcal{T} = -i\sigma^y\mathcal{K}$.

Consider now a system of N identical particles. In the ordinary position representation, in which the state is represented by the wave function $\psi_{s_1,\ldots,s_N}(\mathbf{r}_1,\ldots,\mathbf{r}_N)$, where s_k is the spin label of the k-th particle, the time reversal operator takes the form

$$\mathcal{T} = e^{-\pi\frac{i}{\hbar}S_1^y}\cdot\ldots\cdot e^{-\pi\frac{i}{\hbar}S_N^y}\mathcal{K}\,, \tag{4.196}$$

where S_k^y acts on spin variables of the k-th particle only (so that $[S_k^i,\ S_l^j] = 0$ for $k \neq l$). If all the particles have integer spin, $\mathcal{T}^2 = 1$ independently of their number N. However,

$$\mathcal{T}^2 = (-1)^N = \begin{cases} +1 & \text{for} \quad N \quad \text{even} \\ -1 & \text{for} \quad N \quad \text{odd} \end{cases}, \tag{4.197}$$

if there are N half-integer spin particles. Consider now the energy eigenstates $|n\rangle$. If the time reversal is a symmetry, i.e. if $[H,\ \mathcal{T}] = 0$, the state $\mathcal{T}|n\rangle$ has the same energy as $|n\rangle$. Suppose now that $\mathcal{T}|n\rangle$ and $|n\rangle$ represent the same state, i.e. $\mathcal{T}|n\rangle = \lambda|n\rangle$ with λ a phase factor, that is, there is no degeneracy of the n-th energy level. Applying $\mathcal{T}$ twice we get

$$\mathcal{T}^2|n\rangle = \mathcal{T}\lambda|n\rangle = \lambda^*\mathcal{T}|n\rangle = |\lambda|^2\,|n\rangle = |n\rangle\,, \tag{4.198}$$

(antilinearity!) which is only possible if $\mathcal{T}^2 = 1$. Hence, for an odd number N of fermions, the states $|n\rangle$ and $\mathcal{T}|n\rangle$ must be distinct and, therefore, there must be at least a two-fold degeneracy - called *the Kramers degeneracy* - of the energy levels of the Hamiltonian. The states $|n\rangle$ and $\mathcal{T}|n\rangle$ are then orthogonal to each other: for arbitrary two states Ψ and Φ (we again resort to the mathematical notation) we can write (cf. 4.11)

$$(\Phi|\Psi) = (\Phi|\mathcal{T}^\dagger\mathcal{T}\Psi) = (\mathcal{T}\Psi|\mathcal{T}\Phi)\,. \tag{4.199}$$

Setting now $\Psi = \mathcal{T}|n\rangle \equiv \mathcal{T}\Psi_n$ and $\Phi = |n\rangle \equiv \Psi_n$ we get

$$(\Psi_n|\mathcal{T}\Psi_n) = (\mathcal{T}^2\Psi_n|\mathcal{T}\Psi_n) = \pm(\Psi_n|\mathcal{T}\Psi_n)\,, \tag{4.200}$$

so that for the minus sign ($\mathcal{T}^2 = -1$) we must have $(\Psi_n|\mathcal{T}\Psi_n) = 0$. Usually the state $\mathcal{T}|n\rangle$ together with $|n\rangle$ belong to a larger multiplet of some continuous symmetry,[43] so that the Kramers degeneracy does not introduce any additional doubling of states with a given energy. The two-fold degeneracy exclusively due to the time reversal can be observed in some special situations, though. Consider for example a crystal which has a low symmetry. Each atom of the crystal lattice can be then viewed as feeling the electrostatic field of the neighbouring atoms. This field is *not* rotationally invariant and, superficially, one would not expect any degeneracy of the atomic energy levels. However, the electrostatic field felt by the electron at the position $\mathbf{r}$ of a given atom described by the Hamiltonian term $\sum_i \phi(\mathbf{r} - \mathbf{r}_i)$ ($\mathbf{r}_i$ are the positions of the other atoms) does not break the time reversal symmetry (recall that $\mathcal{T}\mathbf{r}\,\mathcal{T}^\dagger = \mathbf{r}$ so that $\mathcal{T}\phi(\mathbf{r} - \mathbf{r}_i)\mathcal{T}^\dagger = \phi(\mathbf{r} - \mathbf{r}_i)$). Therefore, if the number of atom's electrons is odd, there must still be a two-fold degeneracy of each atomic energy level. It is lifted only if the crystal is placed in an external magnetic field, because the term $H' \propto \mathbf{B} \cdot (\mathbf{L} + 2\mathbf{S})$ does break the time reversal: $\mathcal{T}\mathbf{B} \cdot (\mathbf{L} + 2\mathbf{S})\mathcal{T}^\dagger = \mathbf{B} \cdot \mathcal{T}(\mathbf{L} + 2\mathbf{S})\mathcal{T}^\dagger = -\mathbf{B} \cdot (\mathbf{L} + 2\mathbf{S})$ and the full Hamiltonian $H_0 + V_{\rm int}$ does not commute with $\mathcal{T}$.

Another important conclusion is that fermions cannot have electric dipole moments without violating the time reversal invariance. Consider a free spin s (half-integer) fermion at rest,[44] so that only its spin degrees of freedom matter. It has $(2s + 1)$ degenerate spin states. If the particle possesses an electric dipole moment $\mathbf{d}$, an external electric field $\mathbf{E}$ lifts this degeneracy completely.[45] If the time reversal were a good symmetry, a two-fold degeneracy should remain. Since it is not the case, symmetry with respect to the time-reversal must be broken. In the context of relativistic quantum field theory this means that also the CP (the combination of parity and the charge conjugation - the operation of replacing particles by their antiparticles) must be broken, because the CPT operation is always a good symmetry of relativistically invariant quantum field theory models (with Hermitian Hamiltonians).

[43] For example, in the Hydrogen atom the Kramers doubling of energy states is related to the doubling introduced by the spin degree of freedom: indeed, since $\mathcal{T}^\dagger \mathbf{J} \mathcal{T} = -\mathbf{J}$ one has $\mathcal{T}|n, l, m, s^z\rangle = |n, l, -m, -s^z\rangle$, but the fact that $E_{n,l,m,s^z} = E_{n,l,-m,-s^z}$ follows also from the rotational invariance. (If the spin degree of freedom is neglected, electrons are treated as bosons and the fact that the ground state is nondegenerate is not in conflict with the time reversal invariance.)

[44] Clearly, this reasoning applies to massive fermions only.

[45] The Wigner-Eckart theorem (4.142) can be used to calculate shifts of the energy levels due to the interaction $V_{\rm int} = \mathbf{E} \cdot \mathbf{d}$. In particular, application of this theorem makes it clear that the degeneracy is lifted completely.