Appendix A Angular Momentum

A.1 Orbital Momentum

In spherical coordinates the Laplace operator is a sum of the radial and angular parts,

$$\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r} - \frac{1}{r^2}\mathbf{l}^2, \tag{A.1}$$

$$\mathbf{l}^2 = -\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2} - \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta}. \tag{A.2}$$

A simple transformation of variables shows that the operator in the angular part (A.1) is nothing but the square of the vector $\mathbf{l}$ of orbital momentum (in units of $\hbar$),

$$\mathbf{l} = \frac{[\mathbf{r}\times\mathbf{p}]}{\hbar} = -i[\mathbf{r}\times\nabla]. \tag{A.3}$$

The orbital momentum components in spherical polar coordinates are

$$l_\pm \equiv l_x \pm il_y = e^{\pm i\varphi}\left[\pm\frac{\partial}{\partial\theta} + i\cot\theta\frac{\partial}{\partial\varphi}\right], \tag{A.4}$$

$$l_z = -i\frac{\partial}{\partial\varphi}. \tag{A.5}$$

Obviously, the decomposition (A.1) physically means that kinetic energy can be presented as a sum of the radial and rotational part. Being rotationally invariant, it does not imply the specification of a quantization axis.

A.2 Spherical Functions

Explicitly acting on a function of angles by the operator (A.1), we obtain

$$\mathbf{l}^2 F_l(\theta,\varphi) = l(l+1) F_l(\theta,\varphi). \quad \text{(A.6)}$$

This means that the functions $F_l(\theta,\phi)$ are the *eigenfunctions* of the orbital momentum squared with the eigenvalue $l(l+1)$, where, by construction, $l = 0, 1, 2, \ldots$. One can construct $(2l+1)$ various angular functions F that are called *spherical harmonics* of rank l,

$$Y_{lm}(\theta,\varphi) = \Theta_{lm}(\theta)\frac{1}{\sqrt{2\pi}}e^{im\varphi}, \quad \text{(A.7)}$$

with $m = -l, -l+1, \ldots, -1, 0, 1, \ldots, l-1, l$. Of course, the function (A.7) is an eigenfunction of the operator (A.5) with the eigenvalue $l_z = m$,

$$l_z Y_{lm} = m Y_{lm}. \quad \text{(A.8)}$$

By construction, all values of l and m are integer.

According to general properties of Hermitian operators, the spherical functions with different quantum numbers (l, m) are automatically orthogonal, and the total normalization will always be taken as

$$\int do Y^*_{l'm'}(\mathbf{n}) Y_{lm}(\mathbf{n}) \equiv \int_0^{2\pi} d\varphi \int_0^{\pi} \sin\theta d\theta \, Y^*_{l'm'}(\theta,\varphi) Y_{lm}(\theta,\varphi) = \delta_{l'l}\delta_{m'm}. \quad \text{(A.9)}$$

There can still be a phase factor in the definition of Y_{lm} that can be fixed arbitrarily. A conventional choice is given by the condition

$$Y_{l-m}(\theta,\varphi) = (-)^m Y^*_{lm}(\theta,\varphi). \quad \text{(A.10)}$$

A.3 Generation of Rotations

Consider a rotation through an infinitesimal angle $\delta\alpha$ around the axis characterized by the unit vector $\mathbf{n}$. Under this rotation, a wavefunction ψ changes by an amount proportional to $\delta\alpha$. This transformation, $R_{\mathbf{n}}(\delta\alpha)$, is generated via the action of the operator $(\mathbf{J}\cdot\mathbf{n})$, the projection of the angular momentum onto the rotation axis,

$$\psi \to \psi' = \left[1 - i(\mathbf{J}\cdot\mathbf{n})\delta\alpha\right]\psi; \quad \text{(A.11)}$$

here and always we measure all angular momentum operators in units of $\hbar$. Equation (A.11) is nothing more than a *definition* of the angular momentum operator for a given system; we should find the transformed function explicitly and compare with (A.11) in order to determine the operator $\mathbf{J}$.

A *finite rotation* by an angle α can be achieved as a limit of a large number, $N \to \infty$, of sequential small rotations by $\delta\alpha = \alpha/N$. The operator of a finite rotation is

$$R_{\mathbf{n}}(\alpha) = \lim_{N\to\infty}\left[1 - i(\mathbf{J}\cdot\mathbf{n})\alpha/N\right]^N = \exp\left[-i(\mathbf{J}\cdot\mathbf{n})\alpha\right]. \quad \text{(A.12)}$$

Here we used the fact that the rotations through different angles around the same axis commute. Rotations preserve relations between the state vectors in Hilbert space: amplitudes are the same before and after any rotation R of the entire space,

$$\langle\psi_2'|\psi_1'\rangle \equiv \langle R\psi_2|R\psi_1\rangle \equiv \langle\psi_2|R^\dagger R\psi_1\rangle = \langle\psi_2|\psi_1\rangle. \tag{A.13}$$

Therefore the transformation operator (A.12) has to be *unitary*,

$$R^\dagger R = 1 \Rightarrow R^\dagger = R^{-1}. \tag{A.14}$$

Any unitary operator U can be expressed as

$$U = e^{iG} \equiv \sum_{n=0}^{\infty} \frac{(iG)^n}{n!}, \tag{A.15}$$

where the exponent is a symbolic representation of the infinite series and the generator G of the unitary transformation, $\mathbf{J}$ in our case, is Hermitian.

A.4 Orbital Rotations

Let us see how (A.12) goes into the definition (A.3) in the particular case of the *orbital momentum* of a particle, $\mathbf{J} \Rightarrow \mathbf{l}$. In this case it is convenient to deal with the direct coordinate representation $\psi(\mathbf{r})$ of the particle wavefunction. The result of the rotational transformation of $\psi(\mathbf{r})$ is known: after the rotation one sees at the point $\mathbf{r}$ the value of the function that before the rotation was at the point $R^{-1}\mathbf{r}$, with R^{-1} denoting the inverse rotation,

$$\psi'(\mathbf{r}) = R\psi(\mathbf{r}) = \psi(R^{-1}\mathbf{r}). \tag{A.16}$$

For example, take the rotation around the z-axis through an angle α. A vector

$$\mathbf{r} = (x, y, z) = (r\sin\theta\cos\varphi, r\sin\theta\sin\varphi, r\cos\theta) \tag{A.17}$$

goes into

$$\mathbf{r}' = (r\sin\theta\cos(\varphi+\alpha), r\sin\theta\sin(\varphi+\alpha), r\cos\theta), \tag{A.18}$$

or, in the limit of the infinitesimal $\delta\alpha$,

$$R_z(\delta\alpha)(x, y, z) = (x - \delta\alpha\, y, y + \delta\alpha\, x, z). \tag{A.19}$$

The arguments of the transformed function in (A.16) correspond to the *opposite* rotation, so that, using the linear momentum operator in the coordinate representation, $\mathbf{p} = -i\hbar\nabla$, we get

$$\begin{aligned} R_z(\delta\alpha)\psi(x, y, z) &= \psi(x + \delta\alpha\, y, y - \delta\alpha\, x, z) = \psi(x, y, z) + \delta\alpha\left[y\frac{\partial\psi}{\partial x} - x\frac{\partial\psi}{\partial y}\right] \\ &= \{1 - (i/\hbar)\delta\alpha(xp_y - yp_x)\}\psi = \{1 - i\delta\alpha l_z\}\psi. \end{aligned} \tag{A.20}$$

It means that the generator of rotations (A.11) is here the orbital angular momentum $\mathbf{l}$, (A.3).

Our definition (A.16) of the rotation implies that we rotate a physical object ("active" picture). Rotation of a coordinate frame is equivalent, from a viewpoint of transformations, to an opposite rotation of the system ("passive" picture). The corresponding rotation operators would be conjugate to ours (A.16).

We can compare this procedure with a simpler case of the linear momentum $\mathbf{p}$ that is the generator of *translations* $D(\mathbf{a})$, when the coordinate $\mathbf{r}$ of the object is shifted by a constant vector $\mathbf{a}$, and the new function after the shift comes to the point $\mathbf{r}$ from the point $\mathbf{r}-\mathbf{a}$,

$$D(\mathbf{a})\psi(\mathbf{r}) = \psi'(\mathbf{r}) = \psi(\mathbf{r}-\mathbf{a}). \tag{A.21}$$

For an infinitesimal translation, $\mathbf{a} \to \delta\mathbf{a}$,

$$\psi'(\mathbf{r}) \approx \psi(\mathbf{r}) - (\delta\mathbf{a}\cdot\nabla)\psi(\mathbf{r}) = \left\{1 - \frac{i}{\hbar}(\delta\mathbf{a}\cdot\mathbf{p})\right\}\psi(\mathbf{r}). \tag{A.22}$$

Comparison with the rotational case (A.11) shows that the linear momentum (in units of $\hbar$) is the generator of translations. A finite translation $D(\mathbf{a})$, analogous to (A.12), is a product of an infinite number of infinitesimal translations,

$$D(\mathbf{a}) = e^{-(i/\hbar)(\mathbf{a}\cdot\mathbf{p})}. \tag{A.23}$$

Since the translations along different axes commute, here it is not necessary to take all small shifts $\delta\mathbf{a}$ along the same direction.

A.5 Spin

The result of a rotation in general cannot be reduced to the explicit coordinate transformation (A.20). The wavefunction may consist of several components that undergo a linear transformation between themselves, in addition to the transformation (A.20) of their coordinate dependence. Such components describe different possible *intrinsic* states of an object and usually are referred to as *spin* degrees of freedom. If $\mathbf{S}$ is the vector generator (A.11) of this transformation, the whole effect of the rotation onto the wavefunction of a system is described by the *total* angular momentum,

$$\mathbf{J} = \mathbf{L} + \mathbf{S}, \tag{A.24}$$

where $\mathbf{L}$ generalizes the single-particle orbital momentum $\mathbf{l}$ of (A.3) for an arbitrary system. For a many-body system, the global rotation acts on all particles in the same way so that the total momenta are additive combinations of the single-particle ones,

$$\mathbf{J} = \sum_a \mathbf{j}_a, \quad \mathbf{L} = \sum_a \mathbf{l}_a, \quad \mathbf{S} = \sum_a \mathbf{s}_a, \quad \mathbf{j}_a = \mathbf{l}_a + \mathbf{s}_a. \tag{A.25}$$

As a natural example we consider a *vector function* $\mathbf{V}(\mathbf{r})$. At each point $\mathbf{r}$ we have three functions $V_i(\mathbf{r})$, but they are components of the same vector object. Under rotations not only should each of these functions be transformed as we have seen earlier but, apart from that, the components V_i are transformed among themselves, as would occur even for a constant vector $\mathbf{V}$ with no coordinate dependence.

For an arbitrary rotation R we have

$$RV_x(x, y, z) = V'_x(R^{-1}x, R^{-1}y, R^{-1}z), \tag{A.26}$$

where the notation V' means that the components of the vector also undergo a transformation. As we have seen in (A.19), for an infinitesimal rotation $R = R_z(\delta\alpha)$ by an angle $\delta\alpha$ around the z-axis,

$$R^{-1}x = x + \delta\alpha\, y, \quad R^{-1}y = y - \delta\alpha\, x, \quad R^{-1}z = z. \tag{A.27}$$

This shows what argument is to be taken for the vector as a function of the coordinates in the right-hand side of (A.26). On the other hand, in addition to this parallel transport, the vector $\mathbf{V}$ itself rotates around the z-axis by an angle $\delta\alpha$, so its azimuthal angle ϕ_0 changes to $\phi_0 + \delta\alpha$ (the angles with subscript 0 are those of the direction of $\mathbf{V}$ rather than of the coordinate point $\mathbf{r}$). Then

$$V'_x = |\mathbf{V}| \sin\theta_0\, \cos(\phi_0 + \delta\alpha) \approx V_x - \delta\alpha\, V_y, \tag{A.28}$$

and, analogously,

$$V'_y \approx V_y + \delta\alpha\, V_x, \quad V'_z = V_z. \tag{A.29}$$

The result of the transformation of the components (note that it again has a sign corresponding to an active rotation opposite to that for the arguments of the wave function) can be expressed as an action of a 3×3 matrix S_z on a column of the components V_i,

$$R_z(\delta\alpha)\mathbf{V} = (1 - i\delta\alpha S_z)\mathbf{V}, \quad S_z = \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}. \tag{A.30}$$

The total infinitesimal transformation of our vector function is given by

$$\begin{aligned} R_z(\delta\alpha)\, V_x(\mathbf{r}) &= V'_x(x + y\delta\alpha, y - x\delta\alpha, z) \\ &= V_x(x + y\delta\alpha, y - x\delta\alpha, z) - \delta\alpha\, V_y(x + y\delta\alpha, y - x\delta\alpha, z), \end{aligned} \tag{A.31}$$

or, collecting all terms of the first order with respect to $\delta\alpha$,

$$R_z(\delta\alpha)\, V_x(\mathbf{r}) = V_x(x, y, z) - \delta\alpha\, V_y(x, y, z) - \delta\alpha \left(x\frac{\partial V_x}{\partial y} - \frac{\partial V_x}{\partial x} \right). \tag{A.32}$$

In operator form this means that for the vector field

$$R_z(\delta\alpha) = 1 - i\delta\alpha(S_z + L_z) = 1 - i\delta\alpha J_z, \tag{A.33}$$

where the orbital momentum **L** is, as usual, $-i[\mathbf{r} \times \nabla]$. Finite rotations require the exponentiation of the total angular momentum operator, as in (A.12). We need to stress that the operators **S** and **L** act on different variables and therefore always commute.

A.6 Ladder Operators

We now consider the one-dimensional case of a particle described by a coordinate x and conjugate momentum p, operators with the standard commutation relation

$$[x, p] = i\hbar. \tag{A.34}$$

The operators x and p are Hermitian. Instead we can introduce their non-Hermitian linear combinations

$$a = \sqrt{\frac{1}{2\nu\hbar}}(\nu x + ip), \quad a^\dagger = \sqrt{\frac{1}{2\nu\hbar}}(\nu x - ip), \tag{A.35}$$

which are Hermitian conjugate to each other. In (A.35) we introduced an arbitrary positive constant ν of dimension (mass/time), which makes the new variables a and $a^\dagger$ dimensionless.

The *Heisenberg-Weyl algebra* (A.34) is translated to the new variables (A.35) as

$$[a, a^\dagger] = 1. \tag{A.36}$$

The operator product of these operators,

$$N = a^\dagger a, \tag{A.37}$$

is Hermitian and in terms of the original variables equals

$$N = \frac{\hbar}{2\nu}(\nu x - ip)(\nu x + ip) = \frac{\nu x^2}{2\hbar} + \frac{p^2}{2\nu\hbar} - \frac{1}{2}, \tag{A.38}$$

where the commutator (A.34) was taken into account. With a specific choice of

$$\nu = m\omega, \tag{A.39}$$

we come to the Hamiltonian of a harmonic oscillator with mass m and frequency ω presented in the form

$$H = \frac{m\omega^2 x^2}{2} + \frac{p^2}{2m} = \hbar\omega\left(N + \frac{1}{2}\right), \tag{A.40}$$

although the entire construction is meaningful independently of any oscillator system.

The ladder of the eigenvalues of N can be built if one notices that

$$[a, N] = a, \quad [a^\dagger, N] = -a^\dagger. \tag{A.41}$$

Thus, N has a spectrum $\{\dots, n-1, n, n+1, \dots\}$, where n is an eigenvalue at the point where we have started building the ladder. The specific features of the ladder in this case are determined by the fact that the operator N is positively defined. Indeed, for any state $|\psi\rangle$ we can construct the state $|\psi_a\rangle \equiv a|\psi\rangle$ and see that the expectation value of N for the state $|\psi\rangle$ reduces to the norm of the state $|\psi_a\rangle$ and therefore it is not negative:

$$\langle\psi|N|\psi\rangle = \langle\psi|a^\dagger a|\psi\rangle = \langle\psi_a|\psi_a\rangle \geq 0. \tag{A.42}$$

Together with (A.38), this shows that for any state of a particle and any value of the positive parameter ν,

$$\left\langle \nu x^2 + \frac{p^2}{\nu} \right\rangle \geq \hbar, \tag{A.43}$$

an alternative form of the *uncertainty relation*. The minimum of this relation is achieved at the ground state of the harmonic oscillator, (A.39) and (A.40).

Equation (A.42) implies that all eigenvalues n of the operator N are non-negative, $n \geq 0$. The expectation value (A.42) can vanish if and only if the norm of $|\psi_a\rangle$ vanishes, that is, this state is the zero vector. Let us call the state $|\psi\rangle$ annihilated by the lowering operator the *vacuum* state and denote this state as $|\text{vac}\rangle$,

$$|\psi\rangle = |\text{vac}\rangle \Rightarrow |\psi_a\rangle = a|\text{vac}\rangle = 0. \tag{A.44}$$

For the vacuum state

$$\langle\text{vac}|N|\text{vac}\rangle = 0. \tag{A.45}$$

On the other hand, any state can be represented with the help of the complete set of the eigenstates of a Hermitian operator. Taking the family of the eigenstates $|n\rangle$ of the operator N with the eigenvalues n as a basis, we can write down for the vacuum state

$$|\text{vac}\rangle = \sum_n C_n^{\text{vac}} |n\rangle. \tag{A.46}$$

Then (A.45) shows that

$$\sum_{n=0}^{\infty} |C_n^{\text{vac}}|^2 n = 0. \tag{A.47}$$

Since all $n \geq 0$, this is possible only if for the vacuum state

$$C_n^{\text{vac}} = \delta_{n0} \to |\text{vac}\rangle = |n=0\rangle \equiv |0\rangle, \tag{A.48}$$

the vacuum state is an *eigenstate* of N with eigenvalue $n = 0$. Because of (A.44), the ladder cannot continue down from the vacuum state: this would bring us to impossible negative eigenvalues of N. But applying the raising operator $a^\dagger$ we can go upstairs in steps by $\Delta n = 1$ with no restriction. Thus, the ladder is limited from below but any *integer* $n \geq 0$ is an allowed eigenvalue of the operator N.

In order to complete our algebraic consideration we have to build explicitly the set of eigenstates $|n\rangle$ that satisfy the following equations (now we can label the states by the eigenvalues of N):

$$N|n\rangle = n|n\rangle, \quad a|n\rangle = \mu_n|n-1\rangle, \quad a^\dagger|n\rangle = \tilde{\mu}_n|n+1\rangle. \tag{A.49}$$

Here we assume that the states are normalized,

$$\langle n'|n\rangle = \delta_{nn'}, \tag{A.50}$$

so that the factors μ_n and $\tilde{\mu}_n$ are unknown matrix elements interrelated by the Hermitian conjugation,

$$\mu_n = \langle n-1|a|n\rangle, \quad \tilde{\mu}_n = \langle n+1|a^\dagger|n\rangle = \langle n|a|n+1\rangle^* = \mu^*_{n+1}. \tag{A.51}$$

For a consistent determination of the matrix elements we need a *nonlinear* relation. For example, we can take the commutator (A.36) or the definition (A.37) of N,

$$\langle n|N|n\rangle = n = \langle n|a^\dagger|n+1\rangle\langle n+1|a|n\rangle = |\mu_n|^2. \tag{A.52}$$

The *phase* of the matrix elements remains arbitrary. Indeed, the commutator (A.36), which determines the Heisenberg-Weyl algebra, does not change under a phase transformation

$$a \to a' = ae^{i\alpha}, \quad a^\dagger \to a^{\dagger'} = a^\dagger e^{-i\alpha} \tag{A.53}$$

with any real value of α. The transformations preserving the operator algebra can be called *canonical* in analogy with classical mechanics. Therefore the matrix elements can be determined up to an arbitrary phase. The simplest choice is to make them *real*,

$$\mu_n = \sqrt{n}, \quad \tilde{\mu}_n = \sqrt{n+1}. \tag{A.54}$$

Now we can recurrently construct the entire ladder starting from the vacuum state $|0\rangle$ and raising n:

$$a^\dagger|0\rangle = |1\rangle, \tag{A.55}$$

$$a^\dagger|1\rangle = \sqrt{2}|2\rangle \to |2\rangle = \frac{a^\dagger}{\sqrt{2}}\bigg|1\bigg\rangle = \frac{(a^\dagger)^2}{\sqrt{2}}\bigg|0\bigg\rangle, \tag{A.56}$$

and so on. The general recipe is evident,

$$|n\rangle = \frac{(a^\dagger)^n}{\sqrt{n!}}\bigg|0\bigg\rangle. \tag{A.57}$$

Parenthetically we can mention that the structure of the spectrum we obtained is that of noniteracting but *indistinguishable* quanta, and the quantum number n can be interpreted as a number of quanta in the quantum state $|n\rangle$. This approach is used in the general procedure of *secondary quantization* applicable to the general case of identical particles treated as quanta of a *quantum field*. The quantal picture attributes an important physical meaning to formal relations (A.49) and (A.54). Now we can rename raising and lowering operators into those of *creation* and *annihilation* of quanta, respectively. The annihilation operator a may describe the *absorption* of quanta. The probability of this process is proportional to the square of the matrix element $|\mu_n|^2 = n$, that is, to the number of available quanta (they are indistinguishable). The probability of the inverse process of *radiation* of a quantum is proportional to $|\tilde{\mu}_n|^2 = n + 1$ and contains, along with the *spontaneous* radiation independent of the number of quanta in the system also the effect of the *induced*, or *stimulated*, emission that is proportional to n. This effect is at the heart of laser physics.

A.7 Angular Momentum Multiplets

As clear from elementary geometric arguments, the result of two consecutive rotations around *different* axes depend on their order—the corresponding rotation operators do not commute. Using the explicit expression of the orbital momentum components as in (A.4) and (A.5) we obtain

$$[l_j, l_k] = i\epsilon_{jkn} l_n, \tag{A.58}$$

Since the commutation relations reflect a geometrical connection of rotations, they should be the same for any angular momentum operator $\mathbf{J}$, spin or orbital, single-particle or many-body,

$$[J_j, J_k] = i\epsilon_{jkn} J_n. \tag{A.59}$$

It is worthwhile to notice that the linear momentum components p_j commute since these operators generate the shifts of Cartesian coordinates (A.22), and the results of two consecutive translations performed in different order coincide (the *abelian* group of translations in contrast to the *non-abelian* rotation group). As follows from the algebra (A.59), different components of $\mathbf{J}$ cannot simultaneously have certain values.

The most important new element that appears in this algebra compared to the simple case of the previous section is the possibility to construct an operator C, the so-called *Casimir operator*, that commutes with all generators J_k. Of course, any function of C also satisfies this condition but a more complicated algebra can have several *independent* Casimir operators. It is easy to see that the absolute value squared of the angular momentum plays the role of the Casimir operator,

$$\left[J_k, \mathbf{J}^2\right] = \left[J_k, J_x^2 + J_y^2 + J_z^2\right] = 0. \tag{A.60}$$

One of the projections, let us say J_z, and $\mathbf{J}^2$ can have certain values simultaneously. As we have seen for the orbital momentum, this characterization is associated with the choice of the quantization axis and therefore with the apparent violation of rotational symmetry. The symmetry is restored by the potential possibility of rotation to another frame.

Analogously to (A.35), instead of two Hermitian components of the angular momentum in the plane transverse to the quantization axis, J_x and J_y, we introduce two new operators. Hermitian conjugate to each other,

$$J_{\pm} = J_x \pm iJ_y, \quad J_{+} = (J_{-})^{\dagger}. \tag{A.61}$$

According to (A.59), these operators satisfy

$$[J_{\mp}, J_z] = \pm J_{\mp}, \tag{A.62}$$

$$[J_{-}, J_{+}] = -2J_z. \tag{A.63}$$

The first relation (A.62) is of the ladder type, (A.41). Starting with a state with a certain value M of the projection J_z, the operator J_{-} lowers this eigenvalue, $M \to M-1$, whereas J_{+} raises M, $M \to M+1$. Let the initial state, apart from M, have also a certain value of $\mathbf{J}^2$. The Casimir operator commutes with $J_{\pm}$; therefore all states encountered along the ladder of various values of M still belong to the same value of $\mathbf{J}^2$. Geometrically it means that $J_{\pm}$ generate small rotations around the perpendicular axis that change the orientation (projection $J_z = M$) of the angular momentum vector relative to the quantization axis but do not change the absolute value that is invariant under rotations and characterizes the ladder as a whole.

Consider the ladder family of the states with a given value of $\mathbf{J}^2$ and various values of M. Since for any state

$$C = \langle \mathbf{J}^2 \rangle = \langle J_x^2 + J_y^2 + J_z^2 \rangle \geq \langle J_z^2 \rangle = M^2, \tag{A.64}$$

the ladder cannot be infinite, it ends (in both directions) at some limiting values $M_{\max}$ and $M_{\min}$. These values are determined by the value C of the Casimir operator for the family under consideration. At the upper (lower) end of the multiplet the action of the raising (lowering) operator should give zero, similarly to eq. (A.44) for the Heisenberg-Weyl algebra. Using the equivalent expressions for the Casimir operator that follow from (A.60) and (A.63),

$$\begin{aligned} \mathbf{J}^2 &= J_z^2 + \frac{1}{2}(J_{+}J_{-} + J_{-}J_{+}) \\ &= J_{+}J_{-} + J_z^2 - J_z = J_{-}J_{+} + J_z^2 + J_z, \end{aligned} \tag{A.65}$$

having in mind that the expectation value of C is the same all over the ladder, and applying two last forms of (A.65) to the states with $M_{\min}$ and $M_{\max}$, respectively, we obtain

$$C = M_{\min}^2 - M_{\min} = M_{\max}^2 + M_{\max}. \tag{A.66}$$

The appropriate solution for $M_{\min}$ is $M_{\min} = -M_{\max}$. The maximum possible projection $M_{\max}$ will be denoted as J. Usually this number is simply called "angular momentum" and

$$C = J(J+1). \tag{A.67}$$

We see that the value of the Casimir operator $\mathbf{J}^2$ in the multiplet $|JM\rangle$ is *larger* than the squared maximum projection $M^2_{\max} = J^2$. This can be interpreted as a consequence of the uncertainty relation. In the state with the certain values of $\mathbf{J}^2$ and J_z, the noncommuting with J_z transverse components $J_{x,y}$ of the angular momentum cannot have definite values which would be the case if one could align the vector $\mathbf{J}$ along the z-axis, $\mathbf{J}^2 = J_z^2 = M^2_{\max}$. The difference is due to the quantum fluctuations of $J_x^2 + J_y^2$. In other words, it is impossible to construct a state with a certain value of the angular momentum and a certain orientation in space, for example, along the quantization axis. The uncertainty relation $(\Delta J_x)(\Delta J_y) \geq |\langle J_z\rangle|/2$ is similar to the relation between a coordinate x and conjugate linear momentum p_x. From classical mechanics we remember that the angular momentum components are conjugate to angular coordinates.

Starting from the lowest state $M_{\min} = -M_{\max} = -J$ and applying the raising operator J_+, one can construct the entire ladder. The number of steps k from $M = -J$ to $M = +J$ is always integer and equals $2J$. Therefore only *integer* and *half-integer* values of J are possible. Correspondingly, the values of the projection M along the ladder are all integer or all half-integer. They can be labeled $|JM\rangle$ by the common value J (the family name) and the individual tag M (the first name of the family member), where $-J \leq M \leq +J$. The total number of states in the family (*multiplet*) $|JM\rangle$ is $k + 1 = 2J + 1$.

Now we can find the matrix elements of the generators inside the multiplet $|JM\rangle$. Being the eigenstates of the Hermitian operators $\mathbf{J}^2$ and J_z, the states $|JM\rangle$ are orthogonal and assumed to be normalized,

$$\langle J'M'|JM\rangle = \delta_{J'J}\delta_{M'M}. \tag{A.68}$$

The operators $J_\pm$ connect the adjacent states in the multiplet,

$$J_\pm|JM\rangle = \mu_\pm(JM)|JM \pm 1\rangle, \tag{A.69}$$

where, as a result of Hermitian conjugation,

$$\mu_-(JM) = \mu_+^*(JM - 1). \tag{A.70}$$

Taking the expectation value of the Casimir operator (A.65) in an arbitrary state $|JM\rangle$, we find the absolute values of the matrix elements $\mu_\pm(JM)$. Their phases remain arbitrary, and as we did earlier in (A.54), we take them real:

$$\mu_\pm(JM) = \sqrt{(J \mp M)(J \pm M + 1)}. \tag{A.71}$$

Thus, the Cartesian components of the angular momentum have simple selection rules with respect to quantum numbers of the states in the multiplet:

$$\langle J'M'|J_x|JM\rangle = \frac{1}{2}\left(\mu_+(JM)\delta_{M',M+1} + \mu_-(JM)\delta_{M',M-1}\right)\delta_{J'J}, \tag{A.72}$$

$$\langle J'M'|J_y|JM\rangle = \frac{1}{2i}\left(\mu_+(JM)\delta_{M',M+1} - \mu_-(JM)\delta_{M',M-1}\right)\delta_{J'J}, \tag{A.73}$$

$$\langle J'M'|J_z|JM\rangle = M\delta_{M'M}\delta_{J'J}. \tag{A.74}$$

The physical image corresponding to the state $|JM\rangle$ is that of *precession* of the angular momentum vector around the quantization axis z, then $\mathbf{J}^2$ and J_z are fixed, the expectation values $\langle J_x \rangle$ and $\langle J_y \rangle$ are averaged out and vanish, and the expectation values of J_x^2 and J_y^2 are positive.

A.8 Multiplets as Irreducible Representations

Any rotation can be represented as a function (A.12) of the generators. None of them can change the magnitude J: starting from a state $|JM\rangle$ and applying various finite rotations we are always confined to the family of states with different M and the same J. Thus, any state $|JM\rangle$ transforms under rotation R into a superposition of the states belonging to the same multiplet $|JM\rangle$. This fact can be written explicitly as

$$R|JM\rangle = \sum_{M'} D^J_{M'M}(R)|JM'\rangle, \tag{A.75}$$

where

$$D^J_{M'M}(R) = \langle JM'|R|JM\rangle \tag{A.76}$$

are matrix elements of the *finite rotation* R in a given *representation*; here we take into account that the states $|JM\rangle$ with different values of M are orthogonal and assume that they are normalized (A.68). The unitarity of rotations implies the unitarity of matrices (A.75),

$$D^J(D^J)^\dagger = (D^J)^\dagger D^J = 1, \tag{A.77}$$

or, explicitly in matrix elements,

$$\sum_M D^J_{KM}(R)D^{J*}_{K'M}(R) = \delta_{KK'}, \quad \sum_K D^{J*}_{KM'}(R)D^J_{KM}(R) = \delta_{M'M}. \tag{A.78}$$

In algebraic terms, matrices (A.76) give a *unitary representation* of the rotation group of the dimension $2J+1$. It means that for a rotation performed in two steps, $R = R_2R_1$, the corresponding matrix (A.76), $D^J(R)$, is the matrix product of the matrices representing individual rotations performed in the same order,

$$D^J(R) = D^J(R_2)D^J(R_1). \tag{A.79}$$

All geometric properties of rotations are adequately reflected in relations between the corresponding matrices. Thus, the unit matrix corresponds to the rotation by zero angle and for the inverse rotation $D^J(R^{-1}) = (D^J(R))^{-1}$. The representation D^J is *irreducible*: the multiplet $|JM\rangle$ of dimension $2J+1$ does not contain any smaller subset of states that transform only within this subset under all rotations.

A.9 SU (2) Group and Spin $\frac{1}{2}$

The orbital momentum **l** generates multiplets with an *integer* $J = l$. The spin angular momentum s can take both integer and half-integer values. We can understand the physical reason for this difference. Under rotation (A.12) around the z-axis, the wavefunction of the state $|JM\rangle$ acquires a phase,

$$R_z(\alpha)|JM\rangle = e^{-iJ_z\alpha}|JM\rangle = e^{-iM\alpha}|JM\rangle. \tag{A.80}$$

This determines a particular matrix element

$$D^J_{M'M}(R_z(\alpha)) = e^{-iM\alpha}\delta_{M'M}. \tag{A.81}$$

Consider rotation through an angle $\alpha = 2\pi$. The states with integer J do not change, $\exp(-i2\pi M) = 1$, but the states with half-integer J gain a factor -1. As we have seen, the orbital momentum transforms the explicit coordinate dependence of the wavefunctions. Since the directions marked by the angles 0 and 2π physically coincide, a single-valued wavefunction has to be periodic as a function of angles with the period 2π, that is, it should have *integer* angular momentum. Spin wavefunctions are not explicit functions of coordinates, so the requirement of periodicity is absent. Since the physical predictions are given in terms of the amplitudes, which are bilinear in wavefunctions, the *double-valued* representations of the rotation corresponding to a half-integer spin are allowed.

Spin $\frac{1}{2}$ plays an exceptional role because the objects with $J = s = \frac{1}{2}$ are the most fundamental objects in nature. The main building blocks of matter, electrons and quarks, have spin $\frac{1}{2}$. Combining constituents of spin $\frac{1}{2}$ one can construct an arbitrary high angular momentum J. The spin-$\frac{1}{2}$ objects realize the lowest nontrivial representation of the SU(2) group with dimension $2s + 1 = 2$. In a general SU(n) group the *fundamental* representation of dimension n describes similar basic constituents (the simplest nontrivial set of objects which is irreducible under all group transformations).

Our canonical basis $\chi_M = |J = 1/2, M\rangle$ consists of two basis vectors, $M = \pm\frac{1}{2}$. Sometimes it is convenient to call them "spin up," $\chi_{1/2} \equiv \chi_+ \equiv\uparrow$, and "spin down," $\chi_{-1/2} \equiv \chi_- \equiv\downarrow$. All operators in this space are 2×2 matrices. The algebra (A.59) is satisfied with $\mathbf{s} = \frac{1}{2}\boldsymbol{\sigma}$, where the components of $\boldsymbol{\sigma}$ are *Pauli matrices*

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{A.82}$$

It is easy to check the commutation relations (A.59) and the matrix elements (A.72)–(A.74); the matrices are traceless.

Together with the unit matrix, the matrices (A.82) form a complete set of four independent matrices in 2×2 space. In particular, their products are again matrices of the same set. This allows one to accumulate the entire spin algebra in the identity

$$\sigma_k\sigma_l = \delta_{kl} + i\epsilon_{kln}\sigma_n. \tag{A.83}$$

It follows that any operator function of Pauli matrices σ_k can be reduced to a linear expression. The first term of (A.83) is Hermitian and *symmetric* in vector subscripts k, l; the second one is anti-Hermitian and *antisymmetric*. Frequently one has to deal with scalar products $\mathbf{a} \cdot \vec{\sigma}$ of Pauli matrices with (nonmatrix) vectors. Then (A.83) gives

$$(\mathbf{a} \cdot \boldsymbol{\sigma})(\mathbf{b} \cdot \boldsymbol{\sigma}) = (\mathbf{a} \cdot \mathbf{b}) + i[\mathbf{a} \times \mathbf{b}] \cdot \boldsymbol{\sigma}. \tag{A.84}$$

According to (A.84),

$$(\mathbf{n} \cdot \boldsymbol{\sigma})^2 = \mathbf{n}^2 = 1 \tag{A.85}$$

for any unit vector $\mathbf{n}$.

In the representation (A.82) the matrix $\sigma_z = 2s_z$ is diagonal, and taking the basis states $\chi_\pm$ as the eigenstates of σ_z with the eigenvalues ± 1, we obtain our canonical angular momentum basis with z as the quantization axis. In the representation corresponding to the matrices (A.82), the basis states $|1/2\, m\rangle$ are two-component columns

$$\chi_+ = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \chi_- = \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \tag{A.86}$$

Such objects implementing the fundamental representation of the SU(2) algebra are called *spinors*. Any state of spin $\frac{1}{2}$ can be represented as a superposition $a_+\chi_+ + a_-\chi_-$ of basic spinors (A.86) with the upper (lower) component $a_+(a_-)$ giving an amplitude of finding the value of s_z equal to $\frac{1}{2}$ $(\frac{1}{2})$. Starting from the state χ_+ (spin *polarized* along the z-axis) and applying various rotations $\exp -(i/2)(\boldsymbol{\sigma} \cdot \mathbf{n})\alpha$, one can get states with any spin orientation.

A.10 Properties of Spherical Harmonics

A.10.1 *Explicit derivation*

The spherical harmonics $Y_{lm}(\mathbf{n}) \equiv Y_{lm}(\theta, \varphi)$ are the eigenfunctions of the orbital momentum operators $\mathbf{l}^2$ and l_z and therefore they transform among themselves under rotations generated by the orbital momentum $\mathbf{l}$, (A.11), (A.16), and (A.75), according to an integer irreducible representation, $J = l$ (integer), $J_z = m = -l, \dots, +l$.

Given the coordinate frame with the quantization axis z, we define the polar, θ, and azimuthal, φ, angles for any direction $\mathbf{n}$. Using the general recipe (A.16) and the result (A.80) for rotation around the z-axis, we obtain

$$R_z(\alpha) Y_{lm}(\theta, \varphi) = Y_{lm}(\theta, \varphi - \alpha) = e^{-im\alpha} Y_{lm}(\theta, \varphi). \tag{A.87}$$

The second equation (A.87) determines the universal periodic dependence of spherical functions on the azimuthal angle, (A.7). As it should be, the raising and lowering operators (A.4) change the φ-dependence of the functions (A.87) in an appropriate, way adding the factor $\exp(\pm i\varphi)$. The Casimir operator $\mathbf{l}^2$ is, in this representation, the angular part (A.2 of the Laplace operator.

Since the upper state with $m = l$ is annihilated by the raising operator, we should have $l_+ Y_{ll} = 0$. It gives the simple equation of the first order for $\Theta_{ll}(\theta)$ defined by (A.7),

$$\frac{d\Theta_{ll}}{d\theta} = l \cot\theta\, \Theta_{ll}. \tag{A.88}$$

The solution of (A.88) normalized in accordance with (A.9) is

$$\Theta_{ll}(\theta) = \sqrt{\frac{(2l+1)!}{2}}\,\frac{1}{2^l l!}\sin^l\theta. \tag{A.89}$$

The larger l is, the more this function becomes concentrated near the equator, $\theta = \pi/2$, which characterizes the semiclassical orbit in the plane perpendicular to the direction of the angular momentum.

Now we can act by the lowering operator l_-, (A.4), and go down to all members of the multiplet. Using the matrix elements (A.71), we obtain

$$Y_{ll-1} = \frac{1}{\sqrt{2l}} l_- Y_{ll}, \ldots, \quad Y_{lm} = \left[\frac{(l+m)!}{(l-m)!(2l)!}\right]^{1/2} (l_-)^{l-m} Y_{ll}. \tag{A.90}$$

After simple algebra, the result can be expressed in terms of the *associated Legendre polynomials* $P_{lm}(x)$,

$$\Theta_{lm}(\theta) = (-)^m \left[\frac{2l+1}{2}\frac{(l-m)!}{(l+m)!}\right]^{1/2} P_{lm}(\cos\theta), \tag{A.91}$$

$$P_{lm}(\cos\theta) = (-)^{l-m}\frac{(l+m)!}{(l-m)!}\frac{1}{2^l l!}\frac{1}{\sin^m\theta}\frac{d^{l-m}}{(d\cos\theta)^{l-m}}\sin^{2l}\theta, \tag{A.92}$$

where the so-called normalization according to *Condon and Shortley* [CS51] was used which implies the symmetry properties (A.10). Note that the definitions by various authors can differ in phase conventions.

A.10.2 *Legendre polynomials*

For the forward angles, $\theta \to 0$, a regular function of angles, as Y_{lm}, cannot depend on φ since the azimuthal angle is not defined for $\theta = 0$. Therefore all Y_{lm} vanish at $\theta = 0$ except for Y_{l0}, which does not carry any φ-dependence. At $m = 0$ the associated Legendre polynomials (A.92) reduce to the ordinary Legendre polynomials,

$$P_l(x) \equiv P_{l0}(x), \tag{A.93}$$

so that

$$Y_{l0}(\mathbf{n}) = \sqrt{\frac{2l+1}{4\pi}} P_l(\cos\theta). \tag{A.94}$$

It is easy to see from (A.92) that all Legendre polynomials are equal in the forward direction,

$$P_l(1) = 1. \tag{A.95}$$

Hence, for the direction along the quantization axis,

$$Y_{lm}(\theta = 0) = \delta_{m0}\sqrt{\frac{2l+1}{4\pi}}. \tag{A.96}$$

The Legendre polynomials are orthonormalized on the segment from -1 to $+1$,

$$\int_{-1}^{1} dx P_{l'}(x) P_l(x) = \frac{2}{2l+1}\delta_{l'l}. \tag{A.97}$$

The first four polynomials are

$$P_0(x) = 1, \quad P_1(x) = x, \quad P_2(x) = \frac{1}{2}(3x^2 - 1), \quad P_3(x) = \frac{1}{2}(5x^3 - 3x). \tag{A.98}$$

A.10.3 Completeness

The set of spherical functions $Y_{lm}(\theta, \varphi)$ for all l and m is complete, so any regular function of angles can be expanded over Y_{lm}. The coefficients of the expansion can be readily found with the aid of the orthonormality conditions (A.9). Azimuth-independent functions of $\cos\theta$ can be expanded into a series of Legendre polynomials with the help of (A.97). For an arbitrary function of angles $F(\mathbf{n})$, the expansion is

$$F(\mathbf{n}) = \sum_{lm} F_{lm} Y_{lm}(\mathbf{n}). \tag{A.99}$$

According to (A.9),

$$F_{lm} = \int do Y^*_{lm}(\mathbf{n}) F(\mathbf{n}). \tag{A.100}$$

Inserting (A.100) back into the expansion (A.99), one obtains the identity

$$F(\mathbf{n}) = \int do' F(\mathbf{n}') \sum_{lm} Y^*_{lm}(\mathbf{n}') Y_{lm}(\mathbf{n}). \tag{A.101}$$

Therefore the completeness of the set of spherical harmonics can be written as

$$\sum_{lm} Y^*_{lm}(\mathbf{n}') Y_{lm}(\mathbf{n}) = \delta(\mathbf{n} - \mathbf{n}'). \tag{A.102}$$

Taking $\mathbf{n}' = \mathbf{e}_z$, the unit vector along the z-axis, and applying (A.94) and (A.96), we get another useful relation,

$$\sum_{l} (2l+1) P_l(x) = 4\pi\,\delta(x - 1), \tag{A.103}$$

showing that the Legendre polynomials cancel each other in all directions except for the forward one.

A.10.4 Spherical functions as matrix elements of finite rotations

The spherical harmonics $Y_{lm}(\mathbf{n})$ are the wavefunctions in the coordinate representation of the states $|lm\rangle$ (described in the frame with the fixed quantization axis),

$$Y_{lm}(\mathbf{n}) \equiv \langle \mathbf{n}|lm\rangle. \tag{A.104}$$

Let R be a rotation that brings the directional vector $\mathbf{e}_z$ of the quantization axis to a new direction $\mathbf{n}$,

$$R\mathbf{e}_z = \mathbf{n}(\theta, \varphi). \tag{A.105}$$

The rotation R^{-1}, inverse to that in (A.105), acting on the state $|lm\rangle$, transforms it into a superposition of the multiplet states according to the general rule (A.75):

$$R^{-1}|lm\rangle = \sum_{m'} D^{l}_{m'm}(R^{-1})|lm'\rangle. \tag{A.106}$$

The coordinate representation of this equality is obtained by the projecting on the localized state vector $\mathbf{n}_0$,

$$\langle \mathbf{n}_0|R^{-1}|lm\rangle = \sum_{m'} D^{l}_{m'm}(R^{-1})\langle \mathbf{n}_0|lm'\rangle = \sum_{m'} D^{l}_{m'm}(R^{-1})Y_{lm'}(\mathbf{n}_0). \tag{A.107}$$

Due to unitarity of rotations, the left hand side here is

$$\langle \mathbf{n}_0|R^{-1}|lm\rangle = \langle R\mathbf{n}_0|lm\rangle = Y_{lm}(R\mathbf{n}_0). \tag{A.108}$$

The direction $\mathbf{n}_0$ is arbitrary. Taking this function in the direction of the polar axis, $\mathbf{n}_0 \to \mathbf{e}_z$, we come to $Y_{lm}(R\mathbf{e}_z)$. that is, the spherical function of the original angles θ, φ, (A.105). In the right-hand side of (A.107) we can use the result (A.96) for $Y_{lm'}(\mathbf{e}_z)$. This leads to the connection sought for,

$$Y_{lm}(\mathbf{n}) = \sqrt{\frac{2l+1}{4\pi}}\, D^{l}_{0m}(R^{-1}) = \sqrt{\frac{2l+1}{4\pi}}\, D^{l*}_{m0}(R), \tag{A.109}$$

where the $D(R^{-1})$ is the matrix element for the rotation that, inversely to (A.105), brings the vector $\mathbf{n}$ to the direction of the polar axis, and the second equality uses the relation between $D(R)$ and $D(R^{-1}) = D^{\dagger}(R)$. The Legendre polynomials, (A.94), are

$$P_l(\cos\theta) = D^{l}_{00}(R^{-1}) = D^{l}_{00}(R). \tag{A.110}$$

A.10.5 Addition theorem

Frequently one needs a scalar function of an angle γ between two directions, $\mathbf{n}(\theta, \varphi)$ and $\mathbf{n}'(\theta', \varphi')$. Being a scalar, such a function is in fact a function of the scalar product $(\mathbf{n}\cdot\mathbf{n}')$

and can be expanded with the use of the Legendre polynomials $P_l(\cos\gamma)$, where

$$\cos\gamma = (\mathbf{n}\cdot\mathbf{n}') = \sin\theta\sin\theta'\cos(\varphi-\varphi') + \cos\theta\cos\theta'. \tag{A.111}$$

Using the rotation transformation properties of the spherical harmonics one can prove the addition theorem for spherical harmonics,

$$P_l(\mathbf{n}\cdot\mathbf{n}') = \frac{4\pi}{2l+1}\sum_m Y_{lm}(\mathbf{n})Y^*_{lm}(\mathbf{n}'). \tag{A.112}$$

As a particular case, for coinciding $\mathbf{n}$ and $\mathbf{n}'$,

$$\sum_m |Y_{lm}(\mathbf{n})|^2 = \frac{2l+1}{4\pi}. \tag{A.113}$$